State-of-the-Art Digital Twin Applications for Shipping Sector Decarbonization

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Shipping decarbonisation is a challenge that can only be tackled by a holistic approach that combines advancements in technology, optimisation of the ship design, taking into account also the decarbonisation solutions, operational strategies, whilst considering economic incentives and policies. Although several technological innovations in different ship areas (hull, propulsion, fuel, and others) are contributing towards decarbonisation, and operational strategies such as slow steaming, have been proposed, in practice, selecting the most effective ones for a specific ship and timeframe represents a multifaceted problem which slows down progress. This chapter's main focus is on how digital twining (DT) can support the selection of decarbonisation technologies and operational strategies in designing decarbonisation solutions in a rolling time-horizon to meet regulations with the goal of achieving green shipping (zero-emission shipping) by 2050. For this a DT-centric design methodology is described offering shipping companies continuous decision support to manage the decarbonisation transition, utilising a multi-objective optimisation approach that balances the conflicting goals of minimising investment, maximising profitability, and reducing emissions in line with regulations. Both solutions for retrofitting existing ships and new buildings are considered. Furthermore, the chapter illustrates the application of DTs to specific use cases, namely energy production, distribution, and recovery onboard process management with the help of a simulator, and hull performance prediction utilising simulation.

This chapter explores the data management challenges inherent in a digital twin framework and elucidates the pivotal role of knowledge graphs in meeting these demands. The author introduces a functional metamodel designed to semantically convert scenarios related to the green transition into a standardized format. This metamodel emerges as a vital instrument for both business and technical stakeholders, streamlining the intricate interplay among operational requisites, environmental factors, optimization strategies, and decarbonization technologies. It adeptly encapsulates the ship's environmental and economic performance indicators. In synergy with the metamodel, a knowledge graph (KG) encodes industry-specific parameters, laying a robust groundwork that depicts the vessel's functionalities, variables, and operational processes, and serves as a repository for model metadata. This facilitates the automation of shortest path computations, effectively bridging the divide between overarching platform operations and the complex nuances of maritime assets and activities. The utility of the metamodel and knowledge graph in translating real-world issues into a digital twin-compatible format is exemplified through a case study focusing on the application of variable frequency drives for enhancing the efficiency of the high-temperature cooling system. The chapter concludes by summarizing the data management hurdles encountered in maritime digital twins and offering a perspective on future developments.

Edge computing is a solution that prioritizes data processing for low-latency and specialised applications, particularly those involving complex and mission-critical processes. An ideal example of an edge device is a ship, which heavily relies on its onboard computing capabilities to autonomously perform various navigation tasks. The transportation sector, including shipping, has witnessed the emergence of software-defined vehicles where sensor data, analytics, and algorithms play a pivotal role in optimising operations such as propulsion, cargo handling, energy management, communication, and human-machine interactions. This chapter delves into the significance of edge computing in the shipping industry, outlining its ability to enhance operational efficiencies. It explores the specific user requirements for an effective edge computing solution and highlights the role of AI in enabling scalable and continuous computation. Additionally, the chapter provides a comprehensive overview of edge infrastructure, platform requirements, and considerations pertaining to data and AI at the edge. The discussion incorporates the Mayflower autonomous ship as a case study, illustrating the criticality of edge computing for the future of shipping.

The chapter is concerned with the potential of alternative fuels, i.e., any other fuel than conventional fossil fuels, for powering ships. The alternative fuels surveyed in this chapter include liquefied natural gas (LNG), methanol, hydrogen, ammonia, as well as synthetic fuels (e-fuels). The chapter explains how digital twin's simulation capabilities, can be used to model complex energy systems and alternative fuels and compute emissions, power consumption/output, etc., virtually. The chapter provides a comparison of alternative marine fuels, in terms of storage requirements and energy converters (e.g., combustion engines, fuel cells) suitability. Finally, the chapter discusses the role of digital twins in supporting further research and development towards the evolution of alternative fuels.

The chapter explains techniques and approaches to optimize a ship's voyage in terms of environmental and business parameters, utilizing the digital twin (DT) concept. It demonstrates how voyage planning and navigation management, in general, is enhanced by taking into account vessel state in real time as reflected and analyzed by the digital twin ecosystem. The theoretical backbone of voyage planning entails a multitude of state-of-the-art processes from trajectory mining and path finding algorithms to multi constraining optimization by including a variety of parameters to the initial problem, such as

design method is proposed which is then evaluated through a case study on an LNG-powered handysize bulk carrier. Four design scenarios are presented to show the ability of the design approach to simulate vessel behaviour, providing a feasible design space, and supporting early design decision-making. Second, an optimization-based DT design approach is proposed also covering the early concept design phase. Combined, the two complimentary DT design approaches help address the gap in enabling DTs in the design of green transport vessels.

Shipping is responsible for over 90% of global trade. Although it is generally considered a safe and clean mode of transportation, it still has a significant impact on the environment. Thus, state-of-the-art models that may contribute to the sustainable management of the life cycle of shipping operations without compromising safety standards are urgently needed. This chapter discusses the potential of artificial intelligence (AI) based digital twin models to monitor ship safety and efficiency. A paradigm shift is introduced in the form of a model that can predict ship motions and fuel consumption under real operational conditions using deep learning models. A bi-directional long short-term memory (LSTM) network with attention mechanisms is used to predict ship fuel consumption and a transformer neural network is employed to capture ship motions in realistic hydrometeorological conditions. By comparing the predicted results with available full scale measurement data, it is suggested that following further testing and validation, these models could perform satisfactorily in real conditions. Accordingly, they could be integrated into a framework for safe and sustainable ship operations.

This chapter presents three applications of digital twin in shipping, namely the predictive maintenance of ship machinery, cargo load area cleaning, and hull biofouling treatment. The chapter discusses the business importance of each of these applications and surveys the current state of the art practices. The chapter then illustrates novel approaches that utilise digital twins and bring improvements in terms of costs, safety, and environmental impact.

Pollutant emissions constitute a critical aspect of vessel operation, impacting both environmental compliance and sustainability goals. However, direct measurement of pollutants is often a complex endeavor. The contemporary maritime landscape further complicates matters with the introduction of diverse fuel variants, rendering emissions prediction an intricate challenge. In this chapter, the author employs a sophisticated multizone combustion model as a powerful tool to estimate engine performance and NOx emissions. This model serves a dual purpose: it enables real-time assessment of emissions based on basic engine operational parameters and functions as a decision support system for forecasting emissions across various fuel types and engine operational schemes. By integrating this implementation into the digital twin framework, the author augments it with invaluable insights. These insights, in turn, facilitate the reduction of carbon emissions while ensuring compliance with stringent NOx regulations.

Foreword

The title of this book connects two seemingly distant and independent industries. How can digital twin technology help decarbonization of a well-established, global, and complex industry such as the shipping industry? How can computational tools and Artificial intelligence contribute to diverse engineering problems concerning efficiency and safety of maritime operations, including choice of fuel and emission reduction, ship design and routing optimization as well as onshore activities related to shipping?

The thesis of this book is that digital tools are not only essential but indispensable when we orchestrate the green transition of the maritime industry. The analysis is based on the results of a project funded by Horizon Europe, namely Digital Twins for Green Shipping. This consortium assembles a diverse group of European stakeholders, whose researchers are the authors of the book chapters. More generally, at Athena Research Center we regularly witness a variety of instances, besides transportation and logistics, where digital transformation acts as a cornerstone in our society's quest for sustainable development and environment-friendly development.

The book offers a rich and multifaceted discussion of the above issues by shedding light on cutting edge methods in all types of digital processes and models for the maritime industry. At the same time, it pays attention to motivating these technical advances by real needs of the industry. The chapter authors constitute a relevant mix of computer scientists, maritime engineers, and professionals of shipping companies. Let me point out that, although the term "digital twins" has been coined and used during the past couple of decades, automatization and digitization on ships has a long history, which can also be traced in the pages that follow.

Decarbonization is meant to address the planet's top priority today, and the European Union has set ambitious goals, some of which have imminent deadlines. The maritime industry is a major part of this plan and one of the oldest industries that needs to adopt a radical gamechanger in order to lead the way in terms of the green transition and sustainable development. This is already happening today, and the change relies on a long array of sophisticated technologies including big data analytics, sensor networks, Internet of things, edge computing, optimization, geometric modeling, computer-aided design, Virtual reality, scientific computing, machine learning, and Artificial Intelligence for decision making.

In conclusion, this is an exciting and often surprising book, articulated around a sequence of quite independent chapters. Readers of different backgrounds will be introduced to the advanced technologies mentioned above, which makes for quite exciting and fun reading. It will also be very useful to engineers and executives alike in order to decide and deploy the next steps of the green transition in the maritime industry.

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Preface

Shipping accounts for 80% of global trade. Roughly 50,000 ships carry 90% of the world's traded cargo every year, and most of these ships run on heavily polluting oil known as bunker fuel. According to the International Maritime Organisation (IMO), the share of shipping emissions in global anthropogenic emissions has increased from 2.76% in 2012 to 2.89% in 2018. IMO has mandated therefore, that all ships built in the future must reduce pollution from today's averages.

The World Commission on Environment and Development (WCED), defines *sustainability* as development that meets the needs of the present generation without compromising the ability of future generations to meet their own needs. Technology whose use is intended to mitigate or reverse the effects of human activity on the environment is known as *green technology*. Consequently, technological developments that reduce environmental effects due to waterborne transportation is known as *green ship technology*. There has been recently a new impetus for green technology application in shipping, towards halving current emission levels by 2050.

An information technology with a great potential to support the acceleration of green shipping technologies is *digital twins*. A digital twin is a representation of a physical entity in a digital format. A ship digital twin is a digital replica of the real (physical) ship in terms of its structure (e.g. hull type, component layout, hull parameters), its equipment (e.g. engines, propeller, rudder) and its behaviour and functions (e.g. propulsion, navigation, loading), as well as its integration in a fleet management system or multimodal supply chains. It provides a unique, intelligent ship model merging technical specifications, component models, and parameters with management information on the components and processes of the ship, ultimately enabling computerised simulation and optimisation of all its functions along a matrix of performance metrics that can emphasise environmental goals.

Digital twins (contrary to similar concepts such as 'digital shadows') use bi-directional communication links with the ICT infrastructure on the physical ship. The communication link from the ship to the digital twin is used to monitor the physical ship constantly through several data collection techniques and devices, and communication channels to transfer this information. This allows the (virtual) digital twin to constantly learn from its physical counterpart and evolve mirroring its lifecycle. A digital twin can therefore be used in place of its physical counterpart to carry out simulations, analyse data and make predictions in order to prevent unnecessary outcomes, reduce downtime, redesign and improve equipment or processes. Recently, digital twins have been receiving attention in the context of green shipping. This has been largely accelerated by the emergence of the *smart ship*, i.e. ships where a large number of sensors are installed to collect all possible information about the state of the vessel, various indicators, etc.

At the same time, the maturity of digital twin technologies has been advancing rapidly, with the growth of digital twin underpinning technologies such as Internet of Things (IoT), Big Data Machine

Learning, Cloud and Edge computing. This has made possible the use of digital twins in areas such as new ship design. Digital twin technology has started to penetrate through the whole ship lifecycle to include activities such as the design of more energy efficient ships, the installation and retrofitting of energy efficiency subsystems, greener fuels, the optimisation of the ship's voyage, operation, and finally the decommissioning or retire stages.

While digital twining advances have been mainly concentrating to manufacturing (i.e. in the emergent Industry 4.0), research in the application of digital twins to the shipping sector lags behind, with the maritime industry registering lower levels of digital twin research and development than aerospace or automotive engineering. To reduce this gap, several national and international initiatives have been introduced, notably the European Commission's research and development in waterborne transport (https://research-and-innovation.ec.europa.eu/research-area/transport/waterborne_en), aiming to balance optimal energy use with environmental impact. Within this context, the theme of this book, i.e. the application of digital twin technologies to green shipping is both novel and timely.

The shipping and maritime ecosystem is a complex one. Decarbonisation of shipping with the use of digital twins is a paradigm that spans technical and business disciplines. The book therefore Is both authored by a truly interdisciplinary team and addresses a broad audience of readers, including:

- Ship owners /operators.
- Ship Designers & Builders (academia, consultancies, shipbuilders).
- Ship building service providers (engineering services, retrofitters, maintainers).
- Shipping Decarbonisation solution providers, including engine manufacturers, green fuel producers, alternative energy manufacturers.
- Shipping ICT services and application providers
- Classification societies.
- EU and national government policy makers
- Maritime Authorities such as port authorities.
- Researchers in a broad range of disciplines including naval architecture and engineering and computer science.

To understand the context and scope of this book, the diagram shown in the figure needs to be consulted. According to that diagram, green shipping can be classified along a number of parallel streams of innovations, products and technologies that address different perspectives. Underlying all these alternative green shipping approaches is however, Information Technology and more specifically, digital twins. The book therefore covers all different spheres of green shipping activity under the prism of a unified paradigm of digital twins. In the following section we illustrate how the different chapters of the book address the above green shipping areas and collectively construct an integrated view of green shipping through the prism of the digital twin paradigm.

Chapter 1 ("Shipping Digital Twin Landscape"), provides a historical overview, as well as the current state-of-the-art solutions, recent advancements, and emerging approaches in the maritime industry.

Furthermore, the chapter delves into the regulatory aspects associated with the adoption of digital twins in the shipping sector.

Chapter 2 ("A Digital Twin Approach for Selection and Deployment of Decarbonisation Solutions"), main focus is on how Digital Twining can support the selection of decarbonisation technologies and

Figure 1. A classification of green shipping technologies

operational strategies in designing decarbonisation solutions in a rolling time-horizon to meet regulations with the goal of achieving green shipping (zero-emission shipping) by 2050. Furthermore, the chapter illustrates the application of DTs to energy production, distribution, recovery onboard process management, and hull performance prediction utilising simulations.

Chapter 3 ("Shipping Digital Twin Data Management With The Use Of Knowledge Graphs"), presents a model for shipping operations management expressed as a Knowledge Graph that provides data management functionality, and links ship data to operational models and automates model pipeline executions. The Knowledge Graph serves as a host for the digital twin of the vessel and functions as a semantic layer that integrates structural and operational ship models and facilitates model pipeline execution as well as interlinking of digital twins.

Chapter 4 ("Towards Intelligent Ship Edge Computing Enabling Automated Configuration Of Ship Models And Adaptive Self-Learning"), delves into the significance of edge computing in the shipping industry, outlining its ability to enhance operational efficiencies. It explores the specific user requirements for an effective edge computing solution and highlights the role of AI in enabling scalable and continuous computation. Additionally, the chapter provides a comprehensive overview of edge infrastructure, platform requirements, and considerations pertaining to data and AI at the edge.

Chapter 5 (“Shipping Green Fuels Strategies And Benchmarking Supported By Digital Twins”), explains how digital twin’s simulation capabilities, can be used to model complex energy systems and alternative fuels and compute emissions, power consumption/output, etc., virtually. The Chapter provides a comparison of alternative marine fuels, in terms of storage requirements and suitability of energy converters such as combustion engines and fuel cells.

Chapter 6 (“Enhanced and Holistic Voyage Planning Using Digital Twins”), presents techniques and approaches to optimize a ship’s voyage using digital twins in terms of environmental and business parameters controlling ship speed, trim, route, as well as estimated time of arrivals. It demonstrates how voyage planning is enhanced taking into account actual current vessel status reflected by the digital twin. The theoretical backbone of Voyage Planning entails a multitude of state-of-the-art processes from trajectory mining and shortest path algorithms to multi constraining optimization by including a variety of parameters to the initial problem, such as bunkering, JIT and hull condition.

Chapter 7 (“Digital Twins For Synchronised Port Centric Optimisation Enabling Shipping Emissions Reduction”), discusses the context for emission regulations, port operations and hinterland capabilities, and frames a general methodology for port authorities, terminal operators, shipping companies and logistics operators to implement collaborative, emission reducing practices such as slow steaming and synchro-modality.

Chapter 8 (“Application Of Digital Twins In The Design Of New Green Transport Vessels”), discusses the role of optimization in the early design phases. Two complimentary design approaches are proposed aimed at the concept design phases of green ships, and an optimization based DT design approach covering the early concept design phase, are presented.

Chapter 9 (“A Ship Digital Twin For Safe And Sustainable Ship Operations”), discusses the potential of AI based digital twin models to monitor ship safety and efficiency. A paradigm shift is introduced in the form of a model that can predict ship motions and fuel consumption under real operational conditions using deep learning models. A bi-directional Long Short-Term Memory (LSTM) network with attention mechanisms is used to predict ship fuel consumption and a transformer neural network is employed to capture ship motions in realistic hydrometeorological conditions.

Chapter 10 (“Shipping Applications of Digital Twins”), presents three applications of digital twin in shipping, namely the predictive maintenance of ship machinery, cargo load area cleaning and hull biofouling treatment. The Chapter discusses the business importance of each of these applications and surveys the current state of the art practices. The Chapter then illustrates novel approaches that utilise digital twins and bring improvements in terms of costs, safety and environmental impact.

Lastly, Chapter 11 (“Enhancing A Digital Twin With A Multizone Combustion Model For Pollutant Emissions Estimation And Engine Operational Optimization”), presents a sophisticated multizone combustion model used to estimate engine performance and NOx emissions. This model enables real-time assessment of emissions based on basic engine operational parameters and functions as a decision support system for forecasting emissions across various fuel types and engine operational schemes.

This book aims to inform researchers and practitioners alike about the State of the Art in digital twin applications for shipping sector decarbonisation, as well as all important emerging developments in the area. It contains expert views from a broad array of disciplines such as naval architecture, naval engineering, shipping operations management, ship modelling and simulation, and Computer Science, on how to apply digital twinning for maximum waterborne industry decarbonisation. The book addresses a timely and important issue at the intersection of a societal and business imperative (maritime industry decarbonisation) with a promising emerging technology of digital twins.

Review of current developments of digital twins in the maritime industry, indicates that mostly conceptual papers are available and even fewer industry applications and case studies.

This indicates an imbalance between the levels of research and development of digital twins for maritime compared to other areas such as aerospace and manufacturing. The book aims to address such imbalance with a comprehensive review of the current state of digital twins in waterborne transportation, in a green shipping context, together with a set of key industrial applications of digital twins, both existing as well as emerging ones.

Hopefully, in the chapters of this book the readers will find useful insights and valuable knowledge about the true potential of digital twins for ship decarbonisation, and subsequently use it to further research and practice.

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Chapter 1
Shipping Digital Twin Landscape

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ABSTRACT

The evolution of ship computerization towards digital twinning (DT) has been gradual, having its roots in the 1970s, when the first automated navigation and control systems were developed. Over the course of the past decades, the increased automation of ship functions, coupled in ICT advances, paved for the development and analysis of highly realistic ship models. These models are now enhanced and supported by sensor technologies that provide real-time data from ships. This chapter explores the transformative potential of digital twin technology to create virtual replicas of ships, their systems and broader shipping processes. These digital twins empower decision-makers in various stages, including ship design and operational management, both onboard and ashore, regarding ship and fleet management as well as optimised integration in multimodal transport networks. Additionally, they facilitate optimized integration within multimodal transport networks. The chapter provides insights into current state-of-the-art (SOTA) solutions, recent advancements, and emerging approaches in the maritime industry. Furthermore, the chapter delves into the regulatory aspects associated with the adoption of digital twins in the shipping sector, shedding light on potential risks and limitations. To assist in understanding and implementing digital twins effectively, the chapter introduces a comprehensive shipping digital twining architecture and a capabilities model. These frameworks can accommodate diverse technologies, enabling different levels of ambition and customization in the realm of shipping digital twins.

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DIGITAL TWINS

In the most general term, a digital twin (DT) represents a digital counterpart of a physical entity, encompassing its entire lifecycle, continually updated with real-time data, and serving as a decision support tool (IBM-A, nd). The digital twin concept has been around since the 1960s; however, it has started to gain traction only relatively recently, due to technological advances that we discuss later in the chapter. Digital Twin models are gaining more and more interest for their potentials and strong impact in application fields, such as manufacturing (Lu et al., 2020), aerospace (Li et al., 2022), healthcare (Copley, 2018), and medicine (Hempel et al., 2019).

The potential advantages that organizations can gain through the implementation of digital twins are substantial. In the medium to long term, having a digital twin is anticipated to become a prerequisite for competitiveness, particularly in manufacturing, transport logistics, and shipping. Indeed, digital twin technology earned recognition as one of the top ten strategic technologies by IT market research firm Gartner (Gartner, 2017). Digital twins now stand as a business imperative that covers the entire lifecycle of assets and processes, forming the foundation for connected products and services. SAP underscores that companies failing to embrace the digital twin mandate risk falling behind (Forbes, 2017). This growing imperative is driven by the increasing significance of data and digital technologies in contemporary business operations.

Furthermore, digital twins empower companies to bridge physical assets with digital data, enabling the development of new products and services that are more responsive to customer needs. The maritime industry has already witnessed the applications of digital transformation in automated procedures, operational measurement and control, and the creation of digital products and product information models (Erikstad, 2018; 2019).

The primary drivers for the adoption of digital twins in shipping encompass:

1. *Technology*: The development of new technologies, such as the Internet of Things (IoT), Edge Computing and advanced data analytics, has made it possible to create and use digital twins for maritime applications. This has led to a growing number of companies offering digital twin solutions for ships, which can provide valuable insights into ship performance and operations.
2. *Business drivers*: Ship owners and operators are increasingly recognizing the benefits of digital twin technology for improving efficiency and reducing operational costs. The use of digital twins can help to identify areas for improvement, reduce maintenance costs, and minimize the risk of operational downtime. These benefits are driving the adoption of digital twin technology in the maritime industry.
3. *Environmental Regulation*: The maritime industry is highly regulated, and there is a growing focus on improving safety and reducing the environmental impact of shipping. The use of digital twins can help to support these regulatory efforts by providing real-time monitoring and analysis of ship operations, allowing operators to identify and address potential safety or environmental issues before they become problematic.
4. *Shipping value chains and ecosystem*: The shipping/maritime industry is a complex ecosystem made up of a diverse range of stakeholders, including ship owners and operators, shipbuilders, classification societies, and port authorities. The use of digital twin technology is being embraced by these stakeholders as a way to improve efficiency, reduce costs, and enhance safety and environmental performance.

In summary, digital twinning creates substantial business value in shipping by effectively managing the complexities arising from the interdependencies between technical, operational, chartering, safety, and regulatory perspectives, all of which impact ship operators' performance metrics. Projected benefits, as indicated by RINA (nd), include the potential for a significant reduction in ship operating expenditures (up to 40%) and a decrease in port time (up to 30%). Equally important, DT-enhanced shipping companies are expected to handle increased volumes, resulting in higher revenue and profitability, while shipbuilding costs may decrease by 15-20%.

This chapter is dedicated to exploring the current state and future potential of digital twins in the shipping and waterborne sector. Subsequent sections will delve into::

The historical background to digital twin for shipping (Section 2).
General concepts and principles related to shipping digital twins (Section 3).
Approaches for the development of digital twins (Section 4).
Digital Twin development drivers in shipping industry (Section 5).
The application landscape for digital twins in a shipping context (Section 6).
An architecture and capabilities model for shipping DTs (Section 7).

Current trends, conclusions and directions and future outlook of digital twins in shipping/maritime (Section 8).

HISTORICAL BACKGROUND OF SHIPPING DTS AND OF THEIR PRECURSORS

While shipping digital twinning is currently at its infancy, ship digitisation has been widely researched and is increasingly used today (DNV, 2021). The use of computer technology on ships has its roots in the 1960s, when the first automated navigation and control systems were developed. These early systems had limited capabilities, but they started the integration of computer technology in the maritime industry. In the 1970s and 1980s, more advanced computer systems were developed for use on ships, including automatic radar plotting aids (ARPA), shipboard management information systems (SMIS), Advanced Alarm Handling (AAH), and ship condition monitoring and planned maintenance systems. These systems were designed to improve the efficiency and safety of shipping operations by automating various tasks and processes.

In the 1990s and early 2000s, Integrated Bridge Systems (IBS), combined multiple ship systems and functions into a single ship management platform. This allowed for greater automation and increased situational awareness for the officers and crew, improving safety and efficiency. Notably, *e-Maritime* introduced by the European Commission working closely with industry stakeholders, member states, is a concept that predates digital twins in shipping, and it aims to harness the potential of digital technologies by ameliorating complexities that hinder networking of different stakeholders, helping to increase automation of operational processes particularly compliance management and facilitating the management of information from disparate sources to assist decision making.

Closely associated with the Ship DT concepts are also developments in *e-navigation*, initiated in the late 90's and becoming part of the International Maritime Organisation's (IMO) strategy. E-navigation is defined as "the harmonized collection, integration, exchange, presentation and analysis of marine information on board and ashore by electronic means to enhance berth to berth navigation and related services for safety and security at sea and protection of the marine environment." (IMO, nd). E-navigation is "intended to meet present and future user needs through harmonization of marine navigation systems and supporting shore services. The development and implementation of the concept is coordinated by the International Maritime Organization in accordance with the "E-Navigation Strategy Implementation Plan – Update 1" adopted in 2018 by the Maritime Safety Committee (MSC). Potential synergies are self-evident particularly on ship information standardisation.

More recent developments include the creation of 'smart' ship' or cyber-enabled ships, referring to ships equipped to monitor the state of the vessel through onboard sensors enabling increasing ship automated operation. A smart ship is equipped with automation that provides multiple systems control and data driven decisions (Reilly and Jorgensen, 2016). In smart or cyber-enabled ships (Lloyds Register, 2018), onboard sensors monitor the state of the vessel through and are essentially utilising the maturing developments for autonomous ships (IBM-B. nd).

Digital technology relies on the ship-to-shore connectivity using hardware equipment on board vessels and sharing data and information to support decision-making either on board or at shore. Integration of data from navigation, propulsion, cargo management and energy systems, provides the means to manage effectively ship and fleet performance and operations. A typical ship monitoring system is depicted in Figure 1.

A layered model of shipping processes produced by the eMAR EU project (cordis.europa.eu/project/id/265851) is shown in Figure 2, providing an overview of the diversity of processes and technologies interacting in a ship operational management context.

Figure 1. Significant ICT developments facilitating shipping digitalisation

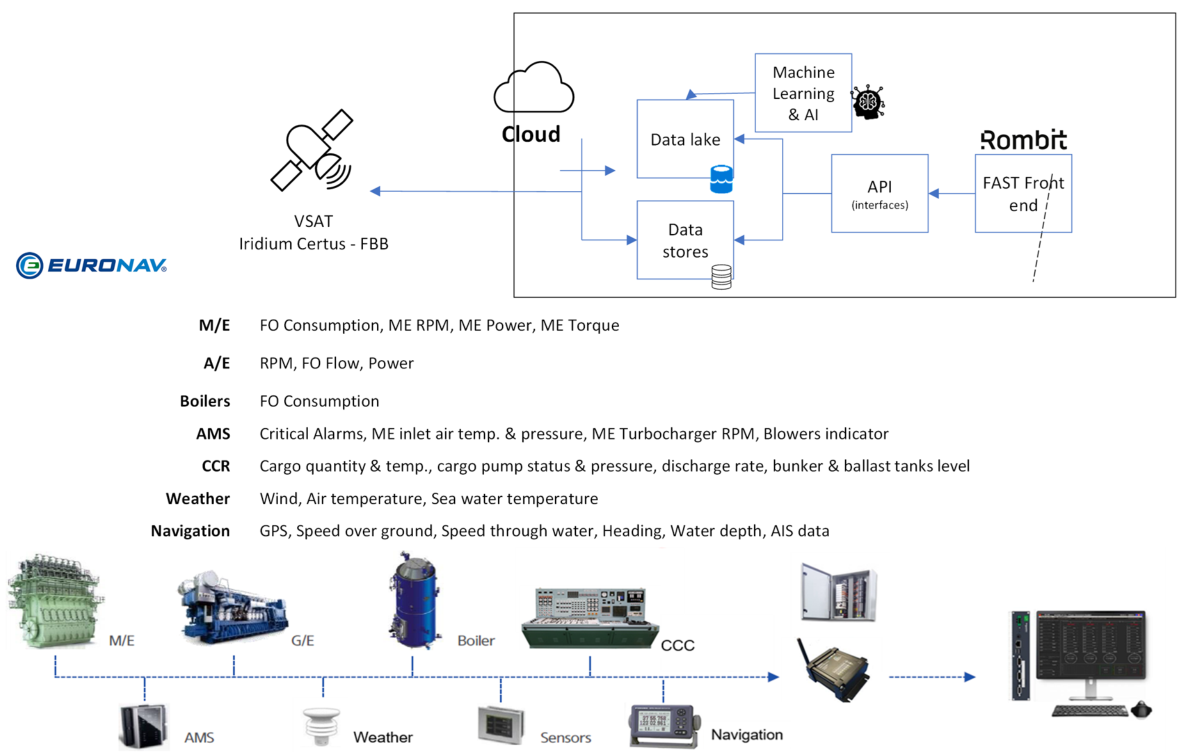


Figure 2. eMAR layered model of shipping processes

DIGITAL TWINS AND THE SHIPPING INDUSTRY

What is a Ship Digital Twin

A digital twin is a digital replica of a physical entity, but what sets it apart from a static digital image is its dynamic nature and the ability to evolve alongside its physical counterpart ('physical twin'). In the context of shipping, the digital twin of a ship is therefore a digital model of the physical ship including its structure, behaviour, and characteristics. Unlike a static digital image or model, a digital twin is dynamic. It is designed to evolve and change over time in response to changes in the ship systems and operating profile. This means that as the ship object undergoes changes, such as health conditions, modifications, or upgrades, the digital twin is updated to reflect those changes in real-time. One of the distinguishing features of a digital twin is its ability to simulate and represent the behaviour of the ship. It is not just a static 3D ship model; it also includes algorithms and models that mimic how the ship operates and responds to different sailing, port call, charter conditions, etc.

A central part of Digital Twins is the use of bi-directional communication links with the ICT infrastructure on a physical ship (Tao et al., 2007). The communication link from the ship to the Digital Twin is used to monitor the physical ship constantly through sensor and data collection instrumentation, and through communication channels to transfer this information to local (Edge) or central (Cloud) processing modules. Overall, the ship responds to the changes according to the optimized scheme received from the DT (Jones et al., 2020). The sensors continuously send real-time data describing novel statuses, and are used to update the state of the DT. When the bi-directional features of DT applications are not fully used, and emphasis is given in one direction flow of data from the ship to the DT, the digital twin is termed *digital shadow*.

This bidirectional communication allows the virtual Digital Twin to constantly learn from its physical counterpart and evolve using mirrored data. As a result, a Digital Twin can be used to get insights into the current state of the physical ship as well as to predict future states of the ship through simulation or predictive algorithms. The Digital Twin can, therefore, provide remote monitoring and control functions.

Information Technologies Underpinning DTs

The digital twin serves as a repository of ship information that can include ship specifications, historical operational data, maintenance records, and real-time sensor data. This wealth of information allows for in-depth analysis and decision-making. Using real-time data from IoT sensors and other sources enables real-time monitoring and analysis of the ship's performance. Three information technologies underpin digital twins in shipping: Big Data, Machine Learning (ML)/Pattern Recognition (PR) and the Internet of Things (IoT) combined with Edge Computing (Baricelli et al., 2019).

Over the past twenty years, the advent of the Internet of Things (Ashton, 2009) is changing the way data are exchanged among different sources. Improvements in technologies such as (embedded) sensors and actuators connected through the Internet, allows a continuous exchange of Big Data between the ship and its DT. Recent years has seen the evolution and maturation of IoT technology from primarily a data collection and transmission approach to devices with significant compute capabilities and the ability to deploy workloads to the data.

Big Data is measured in terms of Volume (storage of large amounts of data), Variety (data with heterogeneous nature, belonging to different sources), Velocity (referring to the speed of production and acquisition), and Value (the importance of the information carried by data) (Gandomi and Haider, 2015).

Big Data technologies are required to process the vast amounts of ship data generated by the onboard sensors and collected by the DT. Data pipelines implement data preprocessing (e.g. cleaning to remove noise, errors, missing values etc). Clean data are then enriched with metadata, indexed and stored in suitable Big Data storage technologies (such as data lakes) where they are made available for online processing, or they are consumed in real time by message and event driven systems residing on the back office or onboard the ship (Edge computing).

Scientific advances in data fusion techniques, high dimensional data processing, Big Data analytics and cloud computing allow to store and analyse Big Data to obtain important knowledge and improve the performance of physical systems. Machine learning and pattern recognition can detect hidden patterns and information encoded by the data.

Descriptive, predictive and prescriptive analytics applications act upon the data in order to provide insights into the ship and its environment, predict future behaviour and support the making of correct decisions regarding the ship operations.

The synergy between AI models, Big Data Analytics, and IoT data is therefore, a fundamental aspect of digital twins' usefulness and potential. It enables these virtual representations of physical objects or systems to not only mirror reality, but also to enhance it by offering predictive insights, optimization opportunities, and advanced monitoring and control capabilities.

Types of Shipping Digital Twins

According to (IBM-B, nd), the types of digital twins include: Component/Part Twin, Asset Twin, System Twin and Process Twin.

In the context of shipping, two types of shipping DTs can be distinguished:

ship operational digital twin managed by the ship operator
collaborative ship life cycle management digital twin managed by a ship service provider.

A 'ship operational digital twin', is defined as a digital replica of a ship in terms of its structure (e.g., hull characteristics, structural and component layout), its equipment (e.g., engines, propeller, rudder) and its functions (e.g., propulsion, navigation, loading), as well as its integration in a fleet management system and ports and multimodal transportation network system.

A 'collaborative ship life cycle management digital twin' supports integrated ship design, manufacturing, operational management and decommissioning. This involves all the actors of the shipping ecosystem including charterers, ship owners and operators, ship designer, shipyards, equipment and service providers, regulators and class societies. A 'collaborative ship life cycle management digital twin' is closely associated with Product Lifecycle Management (PLM) (Grieves et al, 2015) that offer a holistic approach to shipbuilding and a single source of service knowledge that increases accuracy and coordination across the global service network, enabling fleet upgrades, improvements, and modifications that are crucial to overall fleet performance, ship safety and regulatory management.

Both types of ship DT should provide a unique, intelligent ship data and simulation platform merging technical specifications, component models, and parameters with management information on the components and processes of the ship, ultimately enabling computerised simulation and optimisation of all its functions along a matrix of performance metrics linked to economic, environmental and social criteria or goals. The central advantage of DTs Is that allows the use of heterogeneous data sources to be integrated and interpreted in a meaningful way by DT models. Further, the combination of data, AI, and simulation allows stakeholders to rapidly generate multiple scenarios exploring different aspects of ship management and operations and identify optimal configuration.

Current Status of Shipping DT Research

Digital Twins have started to be explored by the shipping industry, throughout the ship life cycle.

'Shipbuilding & Lifecycle Technology 4.0' focuses on enhancing the development of smart technologies, solutions, and processes to support simultaneously effective design and build processes, efficient operational procedures, and sustainable end-end lifespans. Product lifecycle management (PLM) solutions offer a holistic approach to shipbuilding and a single source of service knowledge that increases accuracy and coordination across the global service network, enabling fleet upgrades, improvements, and modifications that are crucial to overall fleet performance. Installed Shipbuilding & Lifecycle Technology 4.0 is essentially DT based approach for delivering enhanced productivity and high design quality incentivising adoption by shipyards. Crucial future developments are standardisation and components enabling integration of equipment DTs and their sensors.

Multiple research paths for the digitisation in life cycle of ships are active. According to the literature review on the maritime industry and its relation with general manufacturing application of digital twin concepts, the following areas have been identified as main streams for future research on DT applications in the maritime sector:

- Construction of multi-physics model libraries, either modular or specific per ship type.
- Application of Digital Twins in the operation phase onboard ships as an aid for operators, including full scale testing and validation exercises.
- Design methodologies based on DT.

The former point is likely to be pursued first, as the DT research in the maritime sector has been principally active in the last years in the developing of models for future DT applications. Especially concerning the power generation on board (power systems and engine) the status of the research is continuously progressing, forced by the upcoming green transition for ships. Besides, prediction of voyage characteristics is also considerably developed, as such topic are strictly related to the real-time evaluation of fuel consumption and, consequently, to the optimisation of the actual route of the sailing ship.

Potential Applications of the Digital Twin in Shipping

DT applications in shipping cover all aspects of ship design, ship production, ship operation and ship decommissioning as well as fleet management and integration in multimodal transport systems. innovations will largely result from the way aforementioned capabilities will be used in the various applications. For this purpose, core DT capabilities include:

Realistic Simulation: highly detailed and realistic simulation models of ship systems' performance. These models can take into account a vast array of variables and parameters, allowing for accurate representations of how the ship or specific subsystems behave under different conditions. When combined with IoT data, these simulations can be continuously updated and refined, ensuring that the digital twin remains an accurate representation of the ship and of its environment.

Optimization: optimization algorithms can be used within DTs to find the best balance between competing objectives and optimised operational setpoints taking into account the overall multimodal transport system when necessary.

Remote Monitoring and Control: Digital twins can enable remote monitoring and control of a variety of ship functions particularly ships are moving towards increased automation for navigation and machinery control and maintenance.

Applications of DTs in Ship design

This includes the following areas:

- Integration and interoperability of different simulation models and tools into a holistic ship design process and extended use of Model-Based System Engineering (Douglass, 2016).
- Internal connectivity of equipment of different vendors and their sensors (IoT) supported by standardisation – extended use of ship data connectors.

- Improved "design for operation", based on operational data, collected from existing vessels. And solutions for automated integration of real data into the design decision-making process
- Vessel Digital Twin, supporting the vessel throughout its full lifecycle, from design to decommissioning.
- Data sharing among different stakeholders and operators to enable everyone to improve its own contribution to new designs, towards better cost-efficiency (CAPEX, OPEX, Return of Investment) and environmental protection.
- Design and verification of digital equipment and ship automation towards higher safety and security.
- Design for retrofitting / technology upgrade.
- Design and classification of Unmanned & Autonomous vessels.

Ship Production

Shipbuilding DTs are expected to support the Collaborative Ship Life-cycle Management DTs domain and allow designers to test and optimize a ship design before it is built. Digital twins allow for virtual prototyping, which is the simulation of a ship's behaviour under different conditions that impact cost and safety considerations in order to test and optimize the ship's design. Important DT feature is provision of APIs for key ship design tools and equipment manufacturers. Special attention areas include:

- More efficient, cost-effective and environmentally friendly processes for building / maintaining / converting / recycling ships and their equipment.
- Reduce waste of materials, in a circular economy perspective.
- Full digitalisation of the production process.

Safe and Efficient Operation of a Single Vessel

Applications are aimed at supporting efficient operations of an individual vessel and all equipment, in normal operation and in emergency, and also to Improve a ship's operational profile. The main subdomains are:

- Propulsion Performance modelling for main engine, shafting, hull, propeller, rudder, and propulsion performance enhancement devices. Ship propulsion performance is a measure of the energy (fuel) consumption at a certain state/speed. During the lifetime of the ship the performance will decrease (fuel consumption will increase or speed decrease) because of fouling of the hull and propeller. In this case useful will be monitoring of the fuel consumption and fouling. Propulsion performance is strongly related to "ship health")
- Voyage Optimisation (VO) against economic, operational and environmental criteria (route, speed, trim, draft, JIT arrivals, weather) using real-time predictive wind and wave energy spectra analysis, just-in-time port arrival scenarios and interaction with Fleet Management, Charter Party, Bunkering, CII Analysis. The VO models will be able to utilise a variety of inputs such as location, destination, wave and current direction and intensity, fuel cost, local weather information, and other ship and voyage-specific parameters to determine the optimal route for the ship, and optimal engine, trim and rudder settings at regular intervals.

- Power Management models for integrated ship energy production, distribution and optimisation incorporating optimisation models to configure the Heat Recovery (HR) system, and simulation models to determine the effects of implementing additional HR Units.
- Ship health monitoring and prediction models, utilising sensors /IoT system, supporting accurate estimation of ship condition and updating of maintenance plans.
- Managing ship inventory and monitoring spare parts using a Digital Twin (DT) can bring significant benefits, particularly in the context of supply chain environmental optimization and the efficiency of maintenance activities.. Through predictive analytics, the DT can anticipate when spare parts will be needed based on historical data, usage patterns, and the condition of onboard equipment. This predictive capability helps in reducing excess inventory, minimizing carrying costs, and avoiding shortages.
- Cargo Management modelling focusing on loading and unloading processes to optimise energy consumption for running pumps and/or cargo equipment.
- Decarbonisation solutions modelling energy systems and related components (constant efficiency, lifetime, carbon content, mass & volume footprint, etc…) enabling the estimation of CO2 from blending fuels including green fuels (synthetic fuels) given engine and heat recovery particulars. Regarding carbon capture the focus is on coupling fuel cells with batteries, modularization and optimized control and operating strategies, which makes the development of performance models for hybrid solutions for different ship types, essential.

Fleet Management Applications

DTs can support a range of strategies and practices:

Chartering Strategies: Effective chartering strategies to maximize the utilization of each ship in the fleet scheduling cargo shipments in a way that minimizes idle time and optimizes revenue. Also support for negotiating favourable chartering contracts. Chartering strategies and freight rate estimation play a crucial role in the maritime industry, enabling shipowners and operators to adapt vessel utilization and availability effectively. For example, using historical data and predictive analytics, a DT can estimate future freight rates. By considering factors like vessel type, route, cargo, and market conditions, ship operators can optimize their chartering decisions.:

Fleet Benchmarking: against key performance indicators (KPIs) such as fuel consumption per nautical mile, on-time arrival rates, and cargo loading/unloading times. Advanced data analytics tools can be used to compare the performance of similar vessels within the flee toinform decisions on maintenance, upgrades, and operational improvements.

Port Call Optimisation

The efficiency of a port is defined by the equilibrium maintained between the demand and supply chains, which happens when the entire integration of the transport system is flexible. Ports are now occupied by various cargoes and passengers from all over the world, necessitating strategic planning to control such continuous output and input of assets in the port. A DT incorporating all available data, can support port decision-makers regarding port design, terminal capacity, and construction investments.

Addressing problems like berth allocation models, improving punctuality, or optimising the use of cargo space, can be achieved with digital twin models. A real-time data-fed DT can help coordinate port operations with synchronized operational planning (coordinated arrivals, slow steaming etc.).

Owners of cargo, good dealers, and customers waiting for the deliveries constantly need to track their shipments with transparency over their movement across ports. To meet such requirements DTs, allow simulation and analysis of operations, allowing real time adjustments to plans.

Connected DTs, can report to key stakeholders on infrastructure investments and serve as an investigation tool across ports linked like the web. This enriches the awareness of each situation in the long-term run and creates a portal for collaborative decision-making over goals such as emission control measures.

The dynamically updated DT makes it easier to understand operational parameters of remote assets such as ships, oil rigs etc. This makes possible the estimation of risk levels, structural reliability, conduct tests to make it more productive by just analysing data. DT can help optimize inspection regimes, making the cost of expenditure transparent and providing visibility and traceability.

DT ARCHITECTURES AND DEVELOPMENT APPROACHES

DT Data Management

Building on the previously discussed technologies, a digital twin platform requires the underpinning of technologies such as Industrial Internet of Things (IIoT) as well as ship blueprint models, both for the ship as a whole, as well as for its individual subsystems.

The vast amounts of data generated by ships and their systems must be collected, processed, and stored in a centralized database to allow for real-time monitoring and analysis. This requires the implementation of robust data management systems, including data security protocols, to ensure the integrity and confidentiality of the data,

Increasingly, ship data used to build the digital twin will be collected automatically, from sensors. *Internet of Things (IoT)* is a digital technology that allows the control of machinery remotely by using machine to machine communication using digital signals. When IoT is used on ships, it allows remote and unmanned operations of machines thereby making the operation safer and efficient, reducing maintenance, downtime, and fuel consumption. This effectively allows the reduction of carbon emissions as a result of efficient operations (Plaza-Hernández, et al., 2021).

As the volume and heterogeneity of data continues to grow, data gravity is an increasing challenge facing organisations. To eliminate connectivity limitations and ensure continued operations across 100s of ships each containing 1000s of sensors and devices, edge computing is developing as part of a multicloud paradigm that ensures that ship stakeholders can leverage digital twin capabilities in any locations, with safety mechanisms around software security and data sovereignty.

An important area for development is specifying a ‘standard’ data acquisition system identifying the key sensors to be used for each ship subsystem. To keep track of metadata and to structure the storage and processing of sensor data, there is a need for a unique identification of sensors as well as the components and systems subject to monitoring by sensors. In that direction, a standardised sensor naming scheme, developed by DNV (Geneva, 2017) provides a reference in this area.

Data used to build the digital twin will need to be based on some reference schema(s). Standardisation is expected to speed up the adoption of digital twinning. Standard industry wide schemas will therefore need to be introduced, while for data types that are shared within different domains (e.g., geospatial data) existing models can be utilised. Ship data models are used by classification societies and provide an important baseline in this area. A notable example is the DNV Functionally Oriented Vessel Data Model (DNV, nd) utilising the principles outlined in ISO 15926A. Ship functions include structural integrity, anchoring, propulsion, navigation, fire prevention, etc.

Remote monitoring with the use of IoT devices and other technologies, enables monitoring of a ship's performance and operations from a remote location enabling optimization of ship operations and reduce costs. Edge computing (subsection 6.4??), supports decision making on the ship and provides autonomy in case of connectivity limitations or outages.

Approaches for Developing Digital Twins

Various types of modelling techniques can be employed for the construction of digital twins. 'White Box' approaches rely on creating analytical models of the ship where relationships between the model variables are represented by mathematical models (e.g., differential equations) that are derived theoretically and are validated from experimental data, e.g., from towing tank or sea trials, or from actual operational data collection (e.g. 'noon reports'). Computational Fluid Dynamics (CFD) are used to model the flow of fluids, such as air or water, around a ship. to predict the performance of a ship's propulsion system, including its speed and fuel consumption, as well as its manoeuvrability and stability (Wang and Dan, 2020).

In contrast to white box methods, 'Black Box' or data-driven models utilise mainly statistical techniques to derive the relationships between the digital twin data, without reliance on a prior model of each component or process that generates them. Black box approaches establish relations (functions) between variables that can be used for the prediction of future states. For instance, consumed energy or fuel can be modelled as a function of the speed and other ship related input variables (e.g., trim, displacement, hull condition), along with the environment related input variables (wind, current, wave…). The function need not be known from the start, but can be derived, e.g., using regression, based on data collected from the vessel in question. Amongst the black box model prediction techniques. We can distinguish three types of data-driven depending on intended usage:

Descriptive models provide a snapshot of the current state or behavior such as ship health condition, navigation status, port status, cargo status etc., based on real-time monitoring of the ships, subsystems and voyage information (sensor data integration, data aggregation, and visualization techniques)

Predictive models that use historical data to forecast future behaviors or conditions of the system. They enable proactive decision-making by anticipating issues before they occur using Time-series forecasting, machine learning models, and statistical algorithms

Prescriptive models that not only predict future outcomes but also recommend actions to achieve desired outcomes using prescriptive analytics and optimization algorithms,

Machine learning algorithms, such as reinforcement learning, can be applied to digital twins to enable autonomous learning from new data

Federated learning provides a privacy-preserving technique that allows multiple ship digital twins to collaboratively train a shared model while keeping their data decentralized

Machine Learning (ML) based algorithms have found significant impact in many fields of engineering including naval engineering, to estimate the ship's power and fuel consumption. Accurate voyage fuel consumption prediction under variable sea environment has been reported using Artificial Neural Networks (ANNs) and Multi-Regression (MR) techniques (Panda, 2023).

The use of black box approaches in machine learning and artificial intelligence come with several disadvantages, with the need for comprehensive quality datasets being one of them. Also, predictions are made without clear explanations and many black box models, especially deep learning models, require significant computational resources and time for both training and inference.

Finally, hybrid (or 'grey box') models, combine the benefits of the white box and black box approaches discussed above, meaning that the physical laws governing the relationships between the ship variables (white box) can be used where feasible, together with statistical approaches (black box), in order to decrease the error margin and give better prediction accuracy with reasonable computational times (Leifsson et al., 2008). In practice, when the grey model relies more on the physical ship model than the volume of the historical data, it requires deep initial information about the ship's physical characteristics to obtain good results. On the other hand, when the model employs fewer physical assumptions, and relies more on historical data and/or empirical rules, it requires a broader set of data describing as many as possible of the operational conditions. Real-time simulation models of a ship's behaviour allow for the continuous monitoring of key parameters, such as speed, fuel consumption, and propulsion performance, and the prediction of how these parameters will change over time (Erikstad, 2017).

System Dynamics: simulation method that focuses on the behaviour of complex systems over time. It is used to model the interconnections between the various components of a ship, including the propulsion system, cargo handling, and power generation, to predict how the system will behave under different conditions. This allows designers to identify potential safety issues and make changes to the design to improve the ship's stability, manoeuvrability, and other safety-critical parameters.

DT DRIVERS

The shift from traditional Information Technology (IT) to digital transformation is a major trend in the maritime industry, driven by advances in AI, IoT, network connectivity, and edge computing. A digital culture can help to drive innovation and improve the efficiency of maritime operations by providing real-time insights, optimizing operations, and improving safety and sustainability.

The World Economic Forum estimates that the digital transformation in logistics will be valued at \$4 trillion: \$1.5 trillion for logistics stakeholders and \$2.4 trillion worth of societal benefits. The data-driven information services will bring \$810 billion to the industry as these services are used to optimise routes, reduce costs and improve utilisation (World Economic Forum, nd)

Essentially, Digital twining can create business value by managing complexity when dealing with the interdependencies between technical, operations, chartering, safety, regulations, and other aspects that affect all performance metrics for ship operators. This can generate 40% reductions in ship operating expenditure, and 30% reductions in port time (RINA, nd). Equally important, the enhanced shipping company capabilities are expected to increase cargo volumes, revenue and profitability, while shipbuilding costs are expected to decrease by 15-20% (RINA, nd).

The trend towards the adoption of digital twin technology in the maritime industry is being driven by the need for increased efficiency, safety, environmental performance and competitiveness. The environment and competitiveness are two key battlefields that shipping companies try to navigate. The industry has identified several economic advantages in driving the energy transition – by implementing more energy efficient technologies. These drivers include increased demand for eco-efficient vessels from shippers and charterers, as well as hesitancy and concern from insurers and investors regarding stranded carbon assets (International Transport Forum, 2018). In this section we identify key stakeholders, considerations, opportunities and pitfalls of DT introduction in the shipping sector.

Digital Transformation of Waterborne Assets

Digital Transformation of waterborne assets is driven by production needs, access and use of data, continuous evolution of digital technology and the development of new business-driven applications answering a variety of goals (environmental, societal, economical).

Digital Transformation can support the optimisation of assets and operations, but the commercial return on investment may be a long-term, multi-stakeholder and complex journey, sometimes requiring the introduction of new business models.

Therefore, Digital Twins need to be considered as part of an integrated and evolving process, i.e., iterative, interactive and cyclical, in which the developments in design and operation are interacting and converting to reach the expected business expectations. Digital twins and associated data are ship and application specific, and this increases their complexity. The general risk is the proliferation of isolated, one-off developments leading to a lack of coherence or even incompatible solutions.

A proper digital governance would enable coordinated development and integration of specific digital applications and technologies, with due regards to industry goals and strategies and business requirements.

Legislative Imperatives Such as Decarbonisation Related Regulation

Digital twining can play a pivotal role in supporting the transition to zero emissions shipping, which is addressed in Chapter 2 of this book.

New vessels are gaining in complexity particularly as they introduce novel decarbonisation technologies. Optimal performance is only achieved when all subsystems are working optimally; together as one system. The assessment of the functioning of all subsystems and overall system behaviour is getting increasingly difficult to MANAGE requiring new simulation models to ensure success and paving the way for the use of DT solutions (Giering and Dyck, 2021.)

Green shipping corridors are attracting attention as a way to accelerate decarbonisation and adoption of green ships, because these can help mitigate the risks associated with the introduction of zero-emission ships/fuels, as the risks are shared by all the stakeholders operating in the green corridor (Joerss et al, 2021).

Digital Governance: A Regulatory Perspective

A modern, future-oriented, harmonised regulatory framework is needed to provide continuous, seamless and transparent governance and regulatory support to stakeholders, towards faster and easier implementation of digital models and applications.

Digitalisation governance in shipping should ideally involve not only authorities and regulators (IMO, EC, flag state administrations, port authorities…) but also, all key stakeholders: ship owners, ship operators, shipyards, ship designers, ship system suppliers, cargo owners, port operators, classification societies. It is noted that, so far, THE International Association of Classification Societies (IACS) has not approved the establishment of a dedicated working group on Digital Twins and related issues.

The digital transformation of the waterborne sector should follow a transversal process, based upon harmonised and standardised regulations to enable a consistent and future proof development, validation and implementation of tools, models, systems and technologies. The involvement of regulatory bodies is essential to streamline these applications on a level playing field, enabling continuous compliance but also allowing a continuous evolution to match the technology progress (e.g., Digital Twin models and software simulations).

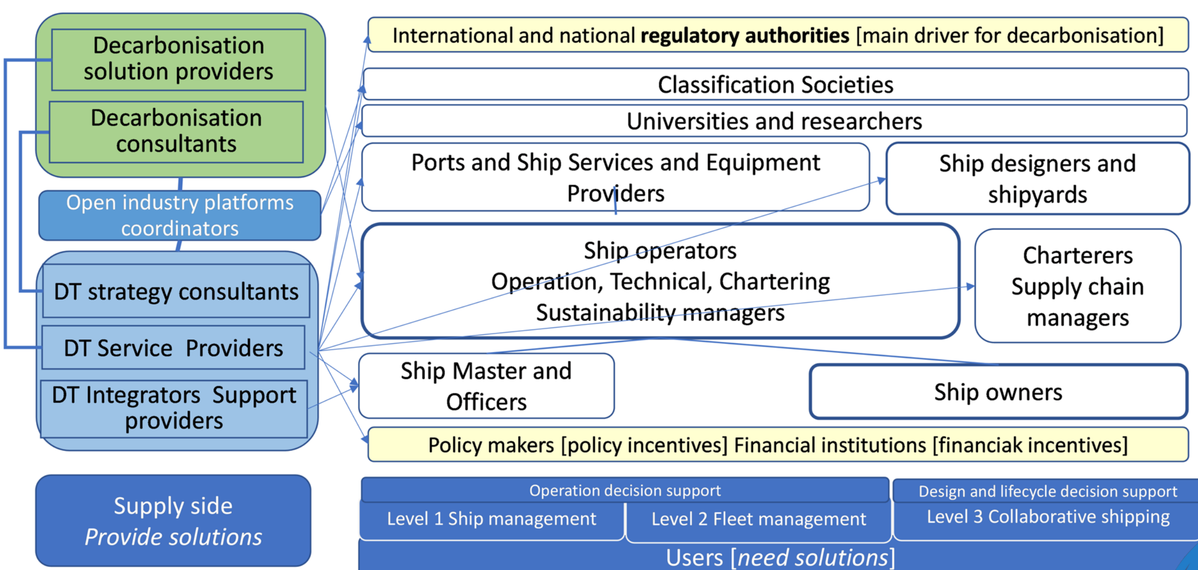
Classification Societies: A Potential Catalyst for Adoption of Ship DTs

Classification societies are responsible for developing and enforcing Class Rules and provide guidelines, Interpretations, and Additional Class notations supplementing the safety and environmental regulations issued by the International Maritime Organization (IMO), the European Commission or the flag Administrations. Classification societies may also act on behalf of the national flag Administrations as Recognized Organization for the implementation of the statutory requirements. It should be noted that industry standards are usually developed and issued by international standard organizations (ISO, IEC...) and that Unified interpretations and Recommendations are harmonized at IACS (International Association of Class Societies) level on some key IMO regulations. In this context Classification societies may promote the standardisation of ship models such as the Functionally Oriented Vessel Data Model based on the principles outlined in ISO 15926A.

Stakeholders for Shipping Digital Twins

The shipping DT stakeholder user groups can be described as shown in Figure 3 below.

Figure 3. Digital twin shipping stakeholders



- **Ship Owners/operators:** They benefit from the more complete knowledge and insights about their ships, that digital twins bring about in order to improve their decision making related to ship financial and operational aspects and for planning and implementing decarbonisation and competitiveness strategies. The HQ departments, e.g., operations, technical, chartering and sustainability, will be DT users, often utilising collaborative decision-making support. The ship master and officers are also potential users, even though their interaction with the system is likely to differ from company to company and will evolve with time.
- **Shipping Customers** They benefit from associating themselves with greener ships and thus elevating their public profile. Potentially, thy can link up with ship DTs to be better informed and create better decision support for using more environmentally friendly and seaworthy/safe ships, they improve the performance of their logistics and supply chains.
- **Ship Designers & Builders:** They develop and use ship design digital twins, but arguably they also learn from deployed digital twins and use such knowledge to optimise and improve the parameters of the actual ship design or improve the simulation models for development of future ships.
- **Ship Services and equipment providers** (equipment providers, engineering services, retrofitters, maintainers): This category of organisations benefits from the detailed and accurate knowledge contained in a digital twin that improves all engineering (e.g., maintaining, retrofitting, decommissioning) and other ship related activities.
- **Decarbonisation solution providers** including green fuels, emerging carbon capture solutions and fuel/ hydrogen cells. Expected to use DTs for the design and deployment/operation of their solutions. It will be important to provide standard ‘connectors’ enabling integration of their products in new ships or retrofits and to enable robust assessment of the performance of a product for specific types of ships.
- **Ports** are developing their own DTs to support their own operation and decarbonisation operations. Integration of port and ships DT is an essential route to increased ship voyage efficiency and improved integration of ships in supply chains. Further ports are directly involved with green fuels supply.
- **Classification societies**: main role is to assess DT applications on safety and regulatory implication and develop/provide e-compliance services and support services including guidelines and standardisation as outlined earlier. Also, likely to be users of DT technologies, to support their own approval and survey/ inspection services.
- **EU and national government policy makers** could use DTs to monitor decarbonisation progress and assess potential policy instruments; data-based evidence of the efficiency of different technologies and policies with respect to specific objectives such as decarbonisation.
- **Authorities including Safet and Emergency support:** These include organisations such as authorities directly interacting with the ship’s operations such as port authorities or legislation setting organisations (national or supranational). The former, such as IMO, provide the regulations that constitute the main driver for decarbonisation. As users, they could link-up with ship DTs to benefit from a more complete (and hopefully accurate and representative) understanding of the ship with a compliance view. Safety and emergency support services including traffic management can be efficiently integrated in DTs.

Related Standards for DTs in Shipping

Relevant initiatives that may be considered as parts of the ship digitalisation strategy are listed below.

GAIA-X (https://gaia-x.eu/) GAIA-X is an EU-supported initiative proposing an open Forum. It developed a Digital Transformation framework of control and governance and implements a common set of policies and rules that can be applied to any existing cloud/edge technology stack to obtain transparency, controllability, portability and interoperability across data and services. The framework is meant to be deployed on top of any existing cloud platform that decides to adhere to the GAIA-X standard. Synergy with requirements for a shipping Digitalisation governance framework outlined in the previous section worth exploring.

IMO Compendium (https://imo.org/en/OurWork/Facilitation/Pages/IMOCompendium.aspx)**:** the International Maritime Organisation has developed a reference data model that is used to harmonise information exchanges between the authorities sector (World Customs Organisation), the trade sector (UNECE), and the ship operation sector (ISO).

Common Maritime Data Structure (CMDS) (http://s100.iho.int/home/s100-introduction)**:** International Hydrographic Office (IHO) maintains the S-100 framework that is also used by other organisations such as IALA and IEC to develop information models and protocols in the maritime sector. S-100 is generally acknowledged as the realisation of the CMDS from IMO's e-navigation definitions.

Maritime Information Technology Standards (MITS) http://www.mits-forum.org/architecture.html: Provides background information on ship architectures.

OXC Consortium (https://3docx.org/) **-** The Open Class 3D Exchange Format. Shipyards and classification societies must modify the traditional design documentation and review process and enable a direct 3D digital classification process to improve the exchange of information between the different stakeholders and ultimately accelerate the classification process. The Open Class 3D Exchange (OCX) standard represents a step-change in this context. The OCX is a vessel-specific standard addressing the information needs by the classification society and is a key enabler to replace traditional 2D class drawings with a 3D model.

Uniquely, OCX addresses the needs of the classification society and shipbuilders for fully digital information exchange. Effectively, OCX acts as a conduit between the design tools and class confirmation tools, highlighting the structural information the class society requires and idealizing and formatting it in an efficient way that can be easily processed.

Major Challenges Inhibitors and Constraints to DT Developments

These can be summarised as:

- Lack of trust among stakeholders on holistic DT solutions applied to the shipbuilding industry (Giering and Dyck, 2021).
- Because vessels have long lifespans with an average of 20 to 25 years of operating life (Joerss, et al 2021), transition towards zero-emission ship designs can be slow. It is necessary to act quickly to prevent locked-in emissions for a long time (Istrate, et al., 2022)
- The lack of standardised quality assurance and validation models for DT systems may limit adoption of digital twins particularly for shipbuilding (Giering & Dyck, 2021)
- Increased risk of cyber-attacks (Markets & Markets, 2022).

Close collaboration between stakeholders will be key to minimise the risks of deploying new zero-emission vessels: collaboration between cargo owners, vessel operators and fuel producers will be crucial to achieve zero-emission shipping (M. Joerss, et al., 2021). This means that federation between different DTs is needed which may take longer to achieve.

Under the same theme, typical information silos can limit the extent of uptake of DTs in the shipping industry. Most of the data obtained during shipbuilding is lost before the vessel is transferred to the shipowner, who would need to develop their own DT. Additionally, classification societies use their own system, creating further redundancies and complexities (Giering and Dyck, 2021).

Cost of establishing DTs must be proportionate to ensuing benefits with rapid return on investment. In Europe, most shipyards (≈98%) are small or medium-sized (Markets & Markets, 2022.) limiting their investment capacity in new technologies/solutions. The same applies to the large number of small ship operators. Cost must include any additional training.

DT APPLICATIONS

Business Decision Support With DT Analytics

As explained so far, shipping digital twins are dynamic, data driven, multi-dimensional digital replicas of a physical entity such as a ship, a subsystem such as ship propulsion, or digital representations of complex processes such as the ship voyage management or fleet management, potentially covering the continuum of ship design, construction and lifecycle management. DTs can support predictive or reactive decision-making at different operational, tactical and strategic levels in order to achieve the performance goal of a company or broader community or industry goals.

A ship DT can support reactive and predictive decision-making tasks at different levels in order to achieve multiple performance goals, including enhanced economic and safety KPIs and minimisation of environmental impact. Shipping companies can use federations of DTs for fleet optimization on the grounds of its cargo-carrying capacity. DTs can support market intelligence and sensitivity analysis of market transactions in terms of past, present, and future scenarios.

DTs can be used to detect trade patterns and enhance both operational and strategic decision-making. Analytics applications for anomaly detection can detect atypical situations such as weather reports and coordinate with ship control systems.

At the operational level, predictive decision-making involves using real-time data from sensors and systems to anticipate and prevent undesirable incidents. For example, a predictive maintenance system can use data from sensors and historical trends to predict more accurately the remaining useful life of a component allowing proactively maintenance and preventing system failure. Reactive decision-making at the operational level involves responding to unexpected equipment failures.

At the tactical level, predictive decision-making involves using historical and real-time data to optimize ship operations, taking into account weather patterns and trend of fuel prices to determine optimal energy management strategies. Reactive decision-making at the tactical level involves responding to unexpected changes in the environment or operational conditions, such as a sudden change in weather conditions.

At the strategic level, predictive decision-making involves using historical and market data to make long-term planning decisions, to optimize fleet deployment and fuel procurement strategies and plan for new facilities. Reactive decision-making at the strategic level involves responding to unexpected changes in the market or regulatory environment, such as changes in fuel emissions regulations or geopolitical changes that affect supply chains.

Supply Chain Visibility

With the establishing development in standards for IoT connectivity, smart containers can be realised. Digital twins containing smart container data can be used to optimize the fleet, create awareness in different situations and address various port and terminal operations.

Throughout the supply chain, the containers transit through various shipping hubs, while flowing data stream generated by connecting containers globally can provide important data that can be utilized by digital twins. Digital twins can therefore further optimise the supply chain by providing opportunities for the stakeholders to select their ideal route for serving customers and coordinating transport buyers. In turn, this could facilitate the establishment of strategic relationships between the transport producers and the hubs for trans-shipment. Digital twins can also monitor the efficient movement of the empty containers, further reducing their environmental footprint.

Cyber-Security

As cyber-physical systems and connections expand, digital twins can assist tackle the growing worry concerning cybersecurity issues. Outside networks are increasingly compromising corporate information technology and operational technology systems as more assets are remotely overseen, managed, and preserved through the Industrial IoT. Digital twins can supervise the security of digital assets and aid the security upgrades and control of remotely accessible system data. Additionally, digital twins not only manage the exterior cyber-possessed security threats such as cyber-attacks done intentionally with some third-party interest, but also the cyber safety threats which develop due to internal complexities and properties, emerging and residing within the integrated systems (NIST, 2023). The priority is to restrict hazards at their early stage when their risks are minimal, which stops the operations from being manipulated. So, a digital twin which has capabilities such as testing based on simulation and verification yields the best solution possible.

Advanced Future DT Enabled Applications

Trends in networking, edge computing and AI offer many opportunities for enhanced DT capabilities for shipping to enhance sustainability, efficiencies, safety, and customer satisfaction.

The development of 5G capabilities and future evolution of 6G, 7G, and beyond enable high fidelity interaction between ships and HQ to disseminate highly realistic simulations or digital twins of every aspect of the ship operation. Remote operations and augmented reality guided maintenance can streamline complex processes on the ship and greatly enhance the productivity of key engineers and personnel.

Mobile computing has revolutionised our world since the first iPhone was released in 2007. Together with the proliferation of IoT devices, and the growth of highly elastic cloud computing, it enabled computing and disparate software applications to penetrate people's daily lives. Today, edge computing is bringing computing to the enterprise edge and allows organisations to process data, deploy AI models, and augment decision support tools to every portion of their operations.

AI has been described as having its "Netscape moment" in 2023 (NY Times: https://www.nytimes.com/interactive/2023/05/19/business/what-is-a-netscape-moment-artificial-intelligence.html#:~:text=There%20are%20parallels%20between%20today%E2%80%99s%20fervor%20for%20A.I.-powered,around%20an%20existing%20technology%2C%20leading%20to%20new%20innovation.) with the release of highly powerful chat assistants such as OpenAI ChatGPT or Google Bard. Foundation models, also known as pre-trained language models, are core to this and have demonstrated impressive performance across tasks. While they have gained recognition for their performance in language-related tasks, they can also be customized for various domains beyond NLP, including computer vision, IT operations, and industry applications. The advantage of foundation models is that since they are pre-trained on vast volumes of data, they can be fine-tuned to downstream applications at a fraction of the cost. Foundation models can be trained to ship-specific data to create generalisable representation of ship processes and their interfaces with other factors such as environment, land-borne transport, and customers. As these models become more energy efficient, and more explainable, they can be deployed on the edge of even the smallest vessel and have sufficient robustness to be trusted by the largest of organisations.

A SHIPPING DIGITAL TWINING ARCHITECTURE AND CAPABILITIES MODEL

Overall, Shipping Digital Twinning systems consist of several key components that work together to create a virtual replica of a ship and its operations. Creating a shipping Digital Twin (DT) involves a sophisticated infrastructure and various services to ensure efficient data management, orchestration, scheduling, version control, and continuous integration/continuous deployment. Figure 4, provides a Shipping Digital Twining architecture which highlights four areas:

- (Open) Shipping Digital Twining Infrastructure Support Tools

Figure 4. Shipping digital twining architecture
(SOURCE: EU project DT4GS https://dt4gs.eu)

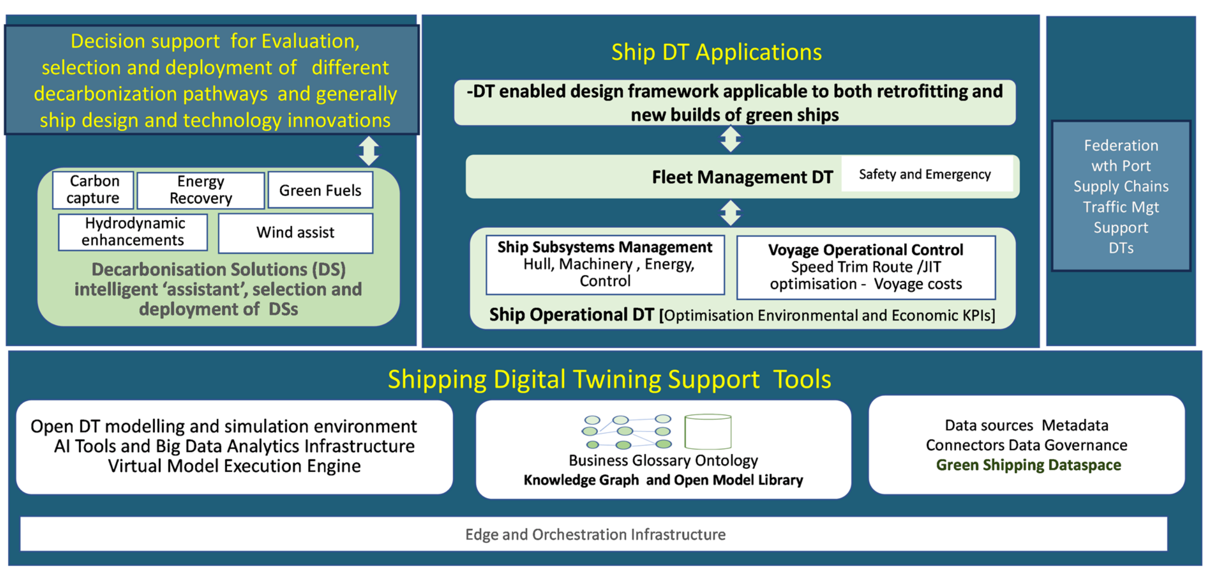


Table 1. Digital twin configurations

Autonomy Level	Level name	Description	Comments				
5	Autonomous (in 1 or more of federated DTs)	Bi-directional communication and control (navigation, mooring, prolusion) Autonomous operations by live synchronization to respond to changing conditions and orchestration without any human intervention (edge) Critical system parameters such as confidentiality, integrity, and availability considered by the DT autonomic manager / remediation process	These capabilities represent the cutting edge of digital twin technology. The ability to seamlessly integrate real-time data, orchestrate complex tasks, and ensure cybersecurity is crucial for the safe and efficient functioning of autonomous systems. compliance with regulations and standards is essential	**Supported by**	**Data Services**	**Integration**	**Intelligence Learning**
4	Federated DTs	Federated, synchronized, and interactive operations among Digital Twins, enabling coordinated decision-making or sharing of insights and recommendations data sharing through a federation interface among participants defines the protocols and standards for data exchange	IDS DTLF Instrumental in achieving efficiency, resilience, and agility in ship operation and in interconnected transportation system				
3	Modelling and simulation capabilities	Ship behaviours and dynamics modelled enabling Simulation based performance assessment and optimisation, What-if simulations for predictive decision support and deviations cause analysis including reproductive simulation recreating the conditions and events leading to a deviation Data threading throughout a process and analytics work flow	Core capabilities supported by CAE, HILS, CPS, Digital Factory, Digital mock-up. Standardisation and interoperability are main challenges which can be supported by evolving modelling and simulation tools. Open libraries of actual reference models particularly for new technologies essential				
2	Monitoring (state measurements)	Persistent, static, and initial data connection interoperable equipment communication system Real time display, historical data, action instructions, alarms and KPIs	Supported by SCADA, DCS, CAM- provides the first phase of DT deployment enabling calibration, tuning and familiarisation objectives.				
1	Mirroring	Reality capture (2D or 3D for a physical object, i.e ship, fleet, port	CAD, HS, GIS, etc.				

- Shipping Digital Twin Applications (Digital Twins managed by different stakeholders)
- Decision support for evaluation, selection and deployment of different decarbonization pathways and generally, ship design and technology innovations.
- Federation with Port, Supply Chains, Traffic Management, and shipping Support DTs

Holistic performance optimisation of the ship, incorporating incremental improvements in environmental performance, requires the consideration of the different optimisation trade-offs between variables of different subdomains and is a complex multifaceted problem, particularly in view of the environment of a ship's operation which changes constantly, as well as the changing landscape of decarbonisation solutions. DT implementations so far have been focused on distinct areas such as machinery, hull, energy or port call optimisation which represents the normal and 'safe' way of testing and creating confidence. Next, increased integration between ship subdomain applications and federation between DTs across industry players will result in increased benefits for the whole industry. Table 1 below presents a DT capabilities model that can be served by different technologies, providing different levels of ambition in shipping DTs. Levels of ambition range from digital blueprints (2D or 3D models of ships, fleets, ports) to real time monitoring, inferencing and real-time predictive decision support, through Visualisation Data Services, Integration technologies, and AI techniques.

CONCLUSION AND FUTURE OUTLOOK

Overview

This chapter has provided a broad view of shipping digital twinning, from technology, business, environment, regulation, and industry stakeholder perspectives. The Chapter has also outlined a capabilities model for current and future shipping DT applications, that can be served by different technologies, and supports different levels of ambition in shipping DTs. By taking a holistic view of digital twinning, the shipping industry can realize the full potential of this technology and promote more sustainable and efficient operations.

Sharing DT Knowledge

Flexibility and adaptability are necessary to ensure the progressive integration of new digital technologies to match business requirements. This means fast adaptability of new solutions, automation systems, digital simulations of multiple scenarios and technologies or operational options. In this context, flexibility is motivated by the goal of achieving "continuous innovation": to manage complexity and uncertainty. Reliable digital twins of the ship in operation, including data verification, validation, and accreditation (VV&A) (architecture, modelling, hybridisation). Reliability of (distributed) architectures and infrastructures.

Digital Twin technologies represent a transversal field of application of digital technologies across different fields, enabling a closed loop connection between different phases, such as design, manufacturing, testing and operations. It may be applied to any waterborne asset under operations, such as ships, offshore platforms, vessels trading in inland waters or ports. For this reason, Digital Twin models may appear with different specificities and scopes.

A key principle underlying successful, advanced digital twinning is that there needs be one unique digital twin for a given ship (possibly consisting of smaller, interconnected DTs). However, knowledge gained from a single DT may be transferrable to the DTs of other ships. Indeed, sharing data and knowledge is a key aspect of creating a strategic industry capability to provide more accurate and reliable ship models and to support shipping industry strategic goals by making DT technology easily accessible to shipping stakeholders. Potentially, digital twin data need to be shared across different communities and therefore be easily exported in different formats and granularities.

Evolution of Information Technologies Underpinning DTs

The integration of DTs into a wide range of ship applications is expected to continue to grow, leading to the development of new data-driven smart ship applications for predictive maintenance, fuel efficiency optimization, and real-time monitoring of ship performance. Regulations for the use of DTs in the maritime industry will likely focus on data privacy and security and the quality and accuracy of DT data. As the concept of DTs gains in popularity, there is an increased need to implement digital frameworks and standards for DTs. For this to happen, the following preconditions are essential:

Provide reference standards, and architectures to the developers, for the sectoral implementation and application development.

Define the verification process and verification criteria of digital twins (models / simulations)

Define quality and accuracy criteria of digital twin data.

Define data trustworthiness, traceability and protection against tampering and corruption and operational data protection.

Establish DT sovereignty guidelines providing privacy consideration as well as access and usage rights.

Establish cybersecurity and Intellectual Property Rights governance to ensure transparency, trustworthiness and secure portability of information (set of requirements for a Trusted Framework).

Furthermore, the future DT enabled Digital Ship may be characterised by dedicated (non-mandatory) Additional Class Notations, issued by Classification societies and assigned to ships which are:

Fitted with navigation & machinery automatic data collection system and transmission to shore.

Continuously monitored according to a set of key parameters

Linked to data collection system surveyed yearly via a remote connection to class platforms.

Industrial benefits are expected from accurate data management (e.g., measuring the level of hull and machinery degradation…), primarily for safety and for environmental compliance.

The technology is becoming more sophisticated and accessible, and the benefits it can provide are being recognized by an increasing number of stakeholders in the industry. Many sensors can be used to provide and generate different types of data, but leveraging data to deliver value requires not only the information generated by systems, but also the recognition of their value potential and use for the business. The identification of business priorities and objectives would then guide the innovation process and development of digital applications. As a result, it is likely that the use of digital twin technology will become more widespread in the coming years. However, the development of shipping DTs is an ongoing process, and will depend on advances in technology are expected to continue to improve the accuracy and reliability of DTs, as well as their integration into a wide range of ship applications. The development of new data-driven smart ship applications, shipping data spaces, and advanced machine learning and AI technologies will play a critical role in this process.

Digital Twin is also the key to approach the classification of Unmanned and Autonomous Vessels. Autonomous ships (IBM-B, nd) are another future fertile area for DT applications. Enabling technologies for autonomous ships have been investigated by EU Horizon H2020 projects, particularly for inland waterway barges, and have created knowledge around accurate positioning, 5G connectivity to support high-bandwidth camera feeds and real-time sensor data coming from vessels to a command centre that remotely controls vessels. Future smart waterways, smart ports, smart ships, and maritime intelligence compose the smart shipping system, likely to be implemented by federated DTs.

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Chapter 2
A Digital Twin Approach for Selection and Deployment of Decarbonization Solutions for the Maritime Sector

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ABSTRACT

Shipping decarbonisation is a challenge that can only be tackled by a holistic approach that combines advancements in technology, optimisation of the ship design, taking into account also the decarbonisation solutions, operational strategies, whilst considering economic incentives and policies. Although several technological innovations in different ship areas (hull, propulsion, fuel, and others) are contributing towards decarbonisation, and operational strategies such as slow steaming, have been proposed, in practice, selecting the most effective ones for a specific ship and timeframe represents a multifaceted problem which slows down progress. This chapter's main focus is on how digital twining (DT) can support the selection of decarbonisation technologies and operational strategies in designing decarbonisation solutions in a rolling time-horizon to meet regulations with the goal of achieving green shipping (zero-emission shipping) by 2050. For this a DT-centric design methodology is described offering shipping companies continuous decision support to manage the decarbonisation transition, utilising a multi-objective optimisation approach that balances the conflicting goals of minimising investment, maximising profitability, and reducing emissions in line with regulations. Both solutions for retrofitting existing

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ships and new buildings are considered. Furthermore, the chapter illustrates the application of DTs to specific use cases, namely energy production, distribution, and recovery onboard process management with the help of a simulator, and hull performance prediction utilising simulation.

INTRODUCTION

International shipping provides 80–90% of global trade, but strict environmental regulations around NOX, SOX and greenhouse gas (GHG) emissions create new imperatives for short-, medium- and long-term emission reduction targets. As shown in an EU survey (EU, n.d.), in 2018 the global shipping emissions represented 1076 million tonnes of CO_2, which represents the 2.9% of global emissions caused by human activities. In that review it was also projected that, if no actions will be taken, the emissions from shipping can be increased by up to 130% of the 2008 baseline by 2050, which are far from the EU targets.

The shipping industry emissions generation continues to rise due to increased global trade and the growing demand for maritime transport. The greatest source of GHG emissions are the container ships, bulk carriers, and oil tankers, however due to their larger engines, their emissions intensity (emissions per unit of cargo transported) is often more favourable compared to smaller vessels (Olmer et al, 2017).

The pathway to achieving the international target of 50% GHG reduction by 2050, which has been recently upped to 100%, is not certain, but numerous promising options exist. Efficiency measures, for GHG reductions can be classified along three axes:

- Operational efficiency, e.g., slow-steaming.
- New, more efficient ship designs and,
- Utilisation of renewable resources, such as wind, and carbon free or low carbon emitting fuels.

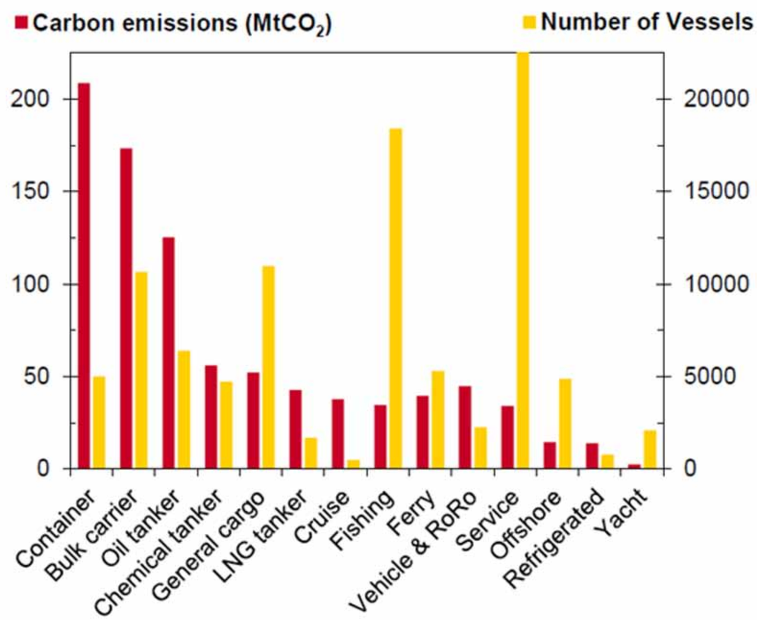
There is clearly no single route, and a multifaceted response is required for managing decarbonisation pathways for each ship. The scale of this challenge is explored by estimating the combined decarbonisation potential of multiple options. A recent study by Transport and Environment on Decarbonisation pathways for EU-related shipping concludes that a mix of different technologies is required to achieve the International Maritime Organization's (IMO) and EU targets leading to 2050 zero emission shipping. For instance, 50% decarbonisation with LNG or electric propulsion would likely require four or more complementary efficiency measures to be applied simultaneously. Broadly, as GHG reductions need to be achieved at increasing rates over the next 30 years we can differentiate between short- and long-term approaches. Short-term approaches can include operational changes and fuel switching, while long-term efforts involve developing and adopting new technologies and infrastructure.

The complexity of the challenge in achieving the IMO required emission reduction rates leading to full decarbonization underscores the need for a holistic and multifaceted approach. It also highlights the importance of ongoing research and development, investment in clean technologies, and global cooperation to transition the maritime industry toward zero-emission shipping by 2050 and beyond.

The Chapter is organised as follows:

The next section discusses the most important energy efficiency measures set by organisations such as IMO which current and future ships must adhere to. These provide the yardsticks against which decarbonisation technologies will be evaluated.

Figure 1. Number of ships and their carbon emissions by category in 2017
(Source: Balcombe et al. (2019)



Section 3 outlines a methodology that employs digital twins to select and evaluate decarbonization measures for the physical ship. Then it describes methods to assess the effectiveness of specific decarbonization technologies and how these results can have added value employing a knowledge hub within a dataspace. Two applications of DTs for the selection and deployment of decarbonisation solutions are described in sections 4 and 5, pertinent to waste heat recovery and hull performance, respectively. The final section of the chapter reviews the potential of the presented methodology for the optimal selection of current and future decarbonisation technologies and resources.

ENERGY EFFICIENCY ASSESSMENT AND COMPLIANCE

Global shipping decarbonisation measures driven by the IMO aim to improve the energy efficiency of ships. Since 2015, all newly delivered ships must meet the Energy Efficiency Design Index (EEDI), a minimum design energy efficiency standard, which becomes more stringent every five years. The EEDI is an index formulated for new ships at the design stage to cut down the amount of emissions from these ships. In that direction, DNV (2018) has developed a tool to compute the EEDI for the whole fleet. The EEDI is expressed in grams of CO2 per tonne-mile, or in other words, the ratio of environmental cost to the benefit for society. Each ship has to obey to different limits accordingly to the type of ship. However, the values of these limits will be reduced by 30% by 2025 compared to the zero phases in 2013 (Puisa, 2015); therefore, different technologies are required for ships to comply to significantly reduced EEDI limits (El-Gohary, 2013; Palomares, 2011; Papanikolaou et al., 2011).

Moreover, for existing ships, since the 1st of January 2023, the Energy Efficiency Existing Ship index (EEXI) has entered into force and applies to all vessels above 400 gross tonnage (GT) falling under MARPOL Annex VI. The decision to adopt this short-term measure has been taken at the IMO MEPC 76 and proposed in the MEPC 75 (IMO, 2020). The EEXI is a one-time certification targeting design parameters. The calculation guidelines refer to the corresponding EEDI guideline for new buildings. Most of the guidelines have been finalized at MEPC 76, while some are still not, according to (DNV, 2019).

Also, since 2015, the IMO has introduced voluntary guidance on the Ship Energy Efficiency Management Plan (SEEMP) that applies to both new and existing ships and aims to improve energy efficiency via operational measures such as optimising routes and speeds. The Ship Energy Efficiency Management Plan (SEEMP) establishes a cost-effective mechanism to improve the ship's energy efficiency (IMO, 2016).

SEEMP is based on four steps: planning, implementation, monitoring, and evaluation and improvement. Firs, it is important to define the current status of energy consumption and how it can be reduced. Secondly, implementing the SEEMP is the responsibility of the involved stakeholders, and then monitoring the effectiveness of the implemented SEEMP. Finally, it is necessary to evaluate the previous stage's results to check the effectiveness of the applied SEEMP to improve the plan. This procedure is applied to new and existing ships to manage ship and fleet efficiency performance over time, based on the Energy Efficiency Operational Indicator (EEOI) as a monitoring tool. This operational measure can optimize and improve voyage planning, introduce the timing of ship hull cleaning, and suggest installing new types of equipment onboard (Tikka, 2011). The EEOI is considered a monitoring tool to support the decisions in SEEMP (IMO, 2009). It is used to monitor and identify the operation and personnel performance as well as the quality control procedures. It aims to provide a transparent and recognized approach to assessing the level of GHG emissions from the ships in their real operating condition along the route.

Tran (2017) developed an open tool to support the computation of the EEOI for different types of ships based on the fuel type, the amount of cargo carried, the distance of the voyage and the sailing speed. For an accurate estimate of EEOI, real data is important to be provided by the fleet to take the right action (Perera et al., 2015). Such data relate to factors such as biofouling, which can reduce the propeller performance by 30% (Owen et al., 2018).

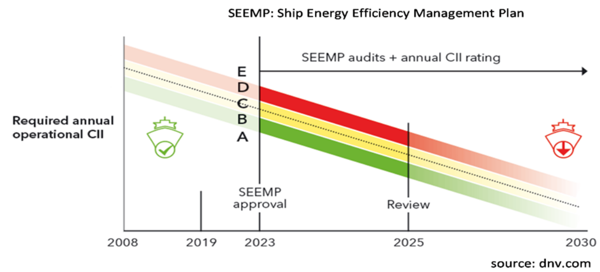
Another metric that has been introduced is the Environmental Ship Index, ESI, developed by the World Ports Climate Initiative (WPCI), complements existing indicators, like EEXI (WPSP, 2019). This index aims to identify seagoing ships with better performance by monitoring real-time emissions data from ships participating in port-based initiatives.

Since 1st January 2023 it has been mandatory for all ships not only to calculate their attained Energy Efficiency Existing Ship Index (EEXI), in order to measure their energy efficiency, but also to collect data for reporting their annual operational Carbon Intensity Indicator (CII) and their CII rating (fig. 2) (Czermański et al., 2022). CII index will be used to rate ships on a scale from A to E,. This is shaped to drive improvements in vessel operations, e.g., by technology upgrades. The decision to adopt this short-term measure has been taken at the IMO MEPC 76 (IMO, 2021) and proposed in MEPC 75.

The CII requirements have taken effect for all cargo, RoPax and cruise vessels above 5,000 GT and trading internationally. The metric addresses the actual emissions in operation by measuring how efficiently a ship transports goods or passengers and is given in grams of CO2 emitted per cargo-carrying capacity and nautical mile [$\frac{g_{CO_2}}{t \cdot nm}$]. Then, the ship is given an annual rating ranging from A to E, whereby the rating thresholds will become increasingly stringent towards 2030. If the ship fails to com-

Figure 2. CII calculation

$$CII = \frac{Annual\ fuel\ consumption\ \times\ CO_2\ factor}{Annual\ distance\ travelled\ \times\ Capacity}$$



ply with the CII limitations, she will be asked to revise before returning in service (Qi et al., 2021). As argued in Wang et al. (2021), ongoing research is essential to refine and improve the CII. This includes developing more sophisticated models and using real data to create versions of the CII that are effective in driving emissions reductions. This obviates the key role digital twining and industry dataspaces can play.

The first reporting year for the CII is 2023, this means that the first annual reporting will be at the end of 2023, and the first rating given will be in 2024. Reviewing the effectiveness of EEXI and CII will be required to develop further amendments. As has already been done for ships that their operational profile justifies the usage of correction factors and exceptions in the calculation of the attained CII value, as shown in MEPC 78 in the resolutions 352 to 355.

As shown in Figure 2, IMO expects a 20% reduction in emissions by 2030, a 70% reduction by 2040 (compared to 2008 levels), and the ultimate goal of achieving net-zero emissions by 2050.

METHODOLOGY

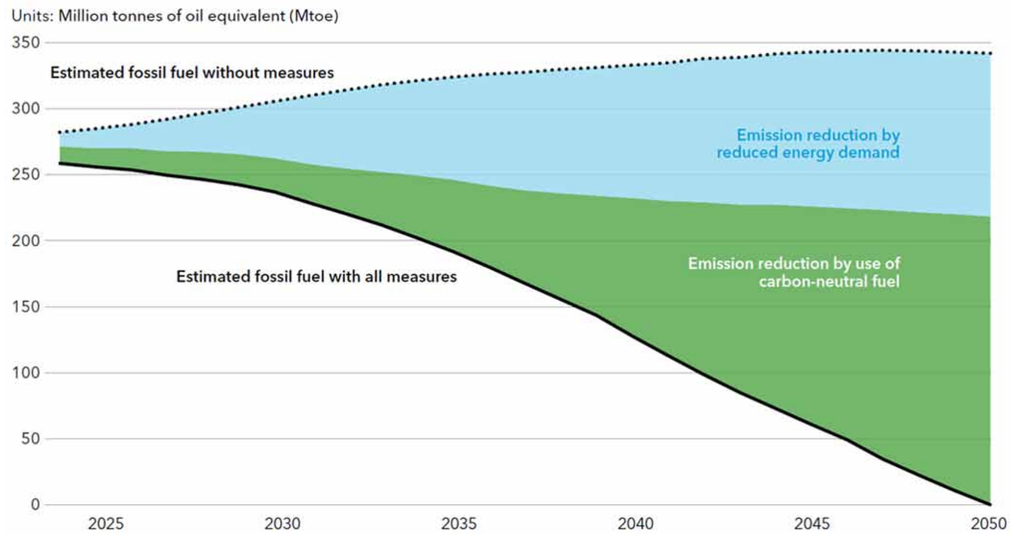
Rationale

The methodology for Digital Twin-aided assessment of decarbonization technologies and ship-specific solutions is based on a data-driven and proactive approach which selects and deploys decarbonisation solutions that takes into account technology options that match ship profiles and company strategies. By leveraging real-time data and simulations, ship operators and their consultants can make informed decisions, optimize performance, and contribute to a more sustainable and decarbonized shipping industry.

The approach is based on a classification of decarbonisation technologies, Table 1 shows a two-phase classification of decarbonisation technologies for retrofitting of the existing ships, and a single phase for the design of new zero-emission ships.

Figure 3 illustrates the potential contributions of different decarbonisation strategies, emphasising the early importance of energy efficiency and operational improvement, which are included into the emission reduction by reduced energy demand section, contrasted with the longer-term prominence of green fuels combined with new power and propulsion technologies, that can be summarised in the emission reduction by use of carbon neutral fuel section. For existing ships, phase 1 uses mainly the first two categories with minimal investment and importantly establishes a critical timing for the second phase intervention that ideally will enable the ship to operate to the end of her life in compliance with emissions regulations.

Figure 3. Contributions of different decarbonisation technologies to zero emissions transition



The triggering factor for phase 2 interventions, is maintaining level C in CII or alternative target. The CII computation is an important element of the approach, and its calculation is also presented in this section. Actual CII rating can be directly estimated by the DT, since the required parameters are inherently available within the DT. But most importantly, the digital twin can forecast the CII based on its decisions and adapt or optimize its decisions, accounting not only for other KPIs but also for the CII. In this way the combination of a DT and CII calculation method for real time and forecasted situations, can effectively support the transition to zero- emission shipping.

The classification of some of the possible decarbonisation technologies is detailed in Table 1, as mentioned above.

CII Calculation

In this section, the CII calculation is described, utilising a Digital Twin platform for real time, automated input from ship sensors' data streams, in contrast to the typical approach where usually manually measured and registered noon report data are used.

The information required for the calculation include the distance travelled, the type, quantity, and specifications of the fuel used. The latter holds especially in the case of a non-standard fuel (MEPC.308(73)) (IMO, 2018). Furthermore, for specific ship operation profiles more data is needed, as shown in MEPC.355(78) (IMO, 2022), in order to calculate the attained CII, taking into account any corrections or exemptions that are applied to the reporting vessel.

The CII calculation, can be utilised in various cases, such as:

- To assess the current CII rating, that includes data the beginning of the current year.
- To predict the CII rating for the next three years, assuming the same ship use, as required by regulations.

Table 1. Classification of decarbonisation technologies

Category	Subcategory	Technology	PH 1	PH 2	Range (%)
Energy Efficiency Improvements: technologies and design enhancements to improve fuel efficiency.	hydrodynamic and ship resistance enhancements	Design optimization of bulbous bows			1-5
		Advanced hull coatings Air lubrication			2-8
		Innovative propellers, energy-saving devices Desai et al (2022), Wang et al (2021); Song et al (2018); Belibassakis et al (2022)			1-12
		Waste Heat Recovery and Energy optimisation (Sinhg & Pedersen, 2022)			3-8
Operational decarbonisation improvements		Route Optimization - Weather routing			4-12
		Slow steaming			5-25
		Port call optimisation			1-8
		Cargo management - optimising intermittent fluctuation of power demand utilising onboard and port systems			1-6
		Predictive ship maintenance system (hull, machinery) sensor data, simulation, AI, and robotics to anticipate maintenance needs, optimize maintenance schedules			2-12
Carbon Capture and Storage (CCS) (Roussanaly,et al., 2021) metrics space, energy requirements, cost (Baroudi, 2021)		Amine Scrubbers (Chemical Solvents) and solid adsorbents			70-90
		Membrane-Based Systems where space constraints or weight limitations are a concern			50-70
		Hybrid Systems			80-95
Power and propulsion improvements metrics power capacity, cost, lifetime of fuel cell		Fuel cells (Perčić et al, 2022)(Abdelkareem et al.,2021) efficient energy converting devices with satisfying CO_2 capturing and/or conversion features SOFCs, MCFCs, that can use various fuel sources			20-100
		Electric battery-powered propulsion, batteries can be charged by shore-based power sources when in port or by onboard generators, hybrid-electric systems, fuel cells			Up to 100
		Wind-assist propulsion(Lindstad, E. et al. ,2022) (Flettner rotors, Suction Wings, rigid WingSails, DynaRigs and kites),			10-40
Zero-Emission Fuels (McKinlay et al.,2021) Of varying levels of maturity, potential availability, and costs		Hydrogen produced using renewable energy sources			100
		Ammonia -			100
		Biofuels, such as biodiesel and bioethanol drop-in blends with conventional fossil fuels in existing engines without significant modification (Watanabe et al., 2022)			20

- To estimate the future CII rating at the end of a certain period using data-driven models that calculate future fuel consumption and other factors for the CII calculation.

The methodology to calculate the CII illustrates the required data intensity, which is compatible with ship performance optimisation data. The aforementioned methodology can be broken down to the following steps:

STEP 1. The total consumption of each fuel is calculated and then it is converted to grams of CO_2 according to MEPC.308(73). The basic characteristics of the fuels, as described in MEPC.308(73), including representative values from ships participating in DT4GS, are shown in the Table 2 below:

STEP 2. Calculate the attained CII value using the MEPC.352(78), as shown in the equation bellow:

Table 2. Fuel characteristic according to MEPC.308(73)

Type of fuel	Reference	Lower calorific value [kJ / kg]	Carbon content	CF [tCO2/tFuel]
Diesel	ISO 8217 Grades DMX through DMB	42,700	0.8744	3.206
LFO	ISO 8217 Grades RMA through RMD	41,200	0.8594	3.151
HFO	ISO 8217 Grades RME through RMK	40,200	0.8493	3.114
LPG	Propane	46,200	0.8182	3
LPG	Butane	45,700	0.8264	3.03
LNG		48,000	0.75	2.75
Methanol		19,900	0.375	1.375
Ethanol		26,800	0.5217	1.913

$$CII_{ship} = \frac{\sum_j \left(M_j \cdot CF_j\right)}{C \cdot D_t} \left[\frac{g_{CO_2}}{t \cdot nm}\right]$$

where:

CII_{ship}: The CII attained from the specific voyage, according to MEPC.336(76), in $\frac{g_{CO_2}}{t \cdot nm}$

- M_j: The mass of the j type of fuel that has been consumed, in grams.
- CF_j: The carbon coefficient C_f of the j fuel according to MEPC.308(73)
- C: The capacity of the vessel as described in MEPC.353(78)
- D_t: The distance traveled by the vessel in the reporting period, in nautical miles (i.e., the trip that we want to calculate the CII)
- j: The different fuels that are consumed in the reporting period (i.e., the trip that we want to calculate the CII)

STEP 3. In case that the corrections and exemption of MEPC.355(78) are applicable for the reporting vessel, the attain CII (CII_{ship}) value can be calculated using the equation bellow:

$$CII_{ship} = \frac{\sum_j C_{Fj} \cdot \left\{FC_j - \left(FC_{voyage,j} + TF_j + \left(0.75 - 0.03y_i\right) \cdot \left(FC_{electrical,j} + FC_{boiler,j} + FC_{others,j}\right)\right)\right\}}{f_i \cdot f_m \cdot f_c \cdot f_{iVSE} \cdot Capacity \cdot \left(D_t - D_x\right)}$$

where:

- j: The fuel type.
- C_{Fj}: represents the fuel mass to CO2 mass conversion factor for fuel type *j*, in line with those specified in the 2018 Guidelines on the method of calculation of the attained EEDI for new ships

(resolution MEPC.308(73) as amended by resolutions MEPC.322(74) and MEPC.332(76)), as may be further amended);

- $FC_{voyage,j}$, D_x, TF_j, y_i: the factors for any potential exemption as described in the MEPC.355(78).
- f_i, f_m, f_c, f_{iVSE}: The corrective factors, as described in the MEPC.355(78).
- $FC_{electrical,j}$: The correction for $FC_{electrical,j}$ refers to 3 main categories:
  - Refrigerated Containers
  - Cargo cooling systems on gas carriers and LNG carriers
  - Electric cargo discharge pumps for tankers
- FC_{Boiler}: For cargo heating and discharge pumps on tankers
  - In the case of boilers used for cargo heating, the amount of fuel used by the boiler (FC_{Boiler}) should be measured by accepted means, e.g., tank soundings, flow meters.
  - For tankers which use steam driven cargo pumps, the amount of fuel used by the boiler (FC_{Boiler}) should be measured by accepted means, e.g., tank soundings, flow meters.

Note that boiler consumption should not include consumption during voyage adjustment periods.

- FC_{others}: For discharge pumps on tankers powered by their own generator, the amount of fuel used for the period that the discharge pumps are in operation (FC_{othera}) should be measured byaccepted means, e.g., tank soundings, flow meters.

STEP 4. Calculate the baseline CII (or reference) as dictated in the MEPC.353(78), for the year of 2022:

$$CII_{reference} = a \cdot capacity^{-c} \left[\frac{g_{CO_2}}{t \cdot nm} \right]$$

Where:

$CII_{reference}$: Is the baseline (or reference) CII rating, as dictated in the MEPC.353(78), in $\frac{g_{CO_2}}{t \cdot nm}$

- *capacity*: The capacity of the vessel as described in MEPC.353(78)
- *a,c*: Coefficients depended to the ship type, as described in MEPC.353(78)

Then we calculate the future (y year) baseline CII (reduction targets) as dictated in the MEPC.338(76):

$$CII_{reference,y} = \left(1 - \frac{Z}{100}\right) \cdot CII_{reference} \left[\frac{g_{CO_2}}{t \cdot nm} \right]$$

With Z the percentage required for reduction each year.

STEP 5. Calculate the limits for the different CII ratings, according to MEPC.354(78), where we multiply the required CII reference with the adequate set of factors (exp(d1), exp(d2), exp(d3), exp(d4)) according to the ship type. In this way, the upper limits for each CII rating are produced.

The same procedure is applied to calculate the corresponding limits for the y year in the future, but this time using the $CII_{reference,y}$ instead of $CII_{reference}$.

Furthermore, regarding the third use case, due to the continuous connection of the ship with the Digital Twin platform the user can have access to the running CII rating from the start of the reporting year till the present moment. The real added value that the Digital Twin platform can provide to the user, regarding the CII calculation, can be seen in the precise calculation of the attained CII value by the end of a trip and the ability to optimize future voyages of the ship considering the CII value.

STEP 6. Identify, in the long term (future 3-year plan), if the CII rating is projected to be below the C rate which will trigger selection, evaluation and deployment of one or combination of decarbonization technologies.

A Methodology for Developing and Deploying an Integrated Ship Performance Model for Reduced Emissions

According to Naito [in Tsujimoto & Orihara, 2019], ship performance is categorized as propulsive performance, safety performance, seakeeping performance, and manoeuvring performance. Among these, propulsive performance in actual seas is more prominent, since it affects fuel consumption and hence CGH (Tsujimoto & Orihara, 2019).

In our approach we define an Integrated Ship Performance Model as a model that includes the above types of performance parameters and their relation to decarbonisation technologies (DEs). A DE according to this approach impacts positively or negatively one or more performance parameters. The exact impact can be described using simulation and/or analytical models that are informed by the ship's DT data.

Therefore, the integrated ship performance model provides a holistic view of how discrete decarbonisation technologies and/or their combination affect critical ship performance parameters.

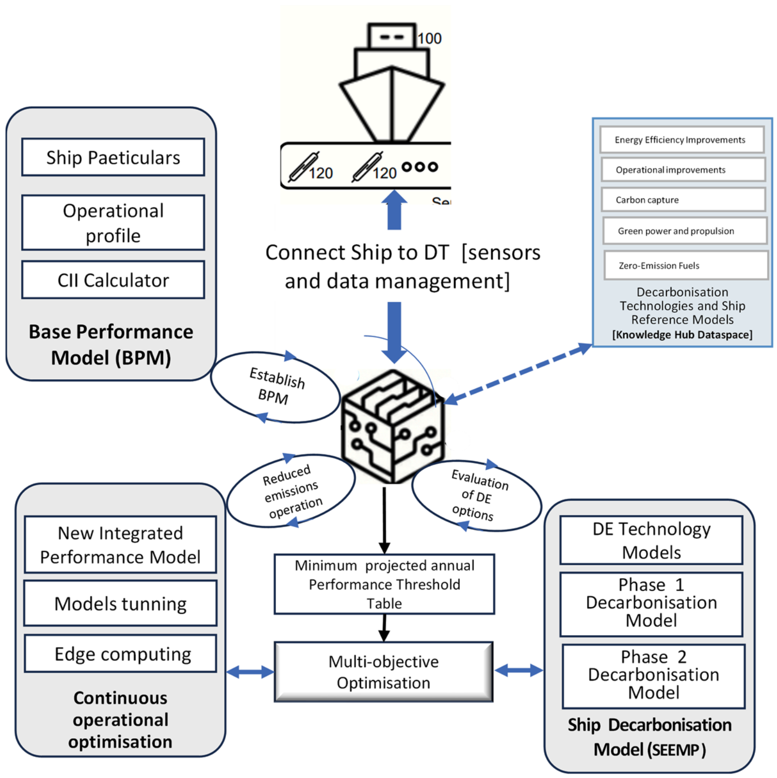
Key steps and components of this approach, depicted in Figure 4, are:

1. Connect the Ship to the Headquarters Digital Twin:
    a. Identify the already existing sensors on the ship and examine if they are adequate for the implementation. In that direction, additional sensors may be identified as required and deployed on the ship to enhance monitoring capabilities.
    b. Establishment of a digital connection between the ship and the shore-based office enables real-time data exchange, remote monitoring, and decision-making support.
    c. Data management services are set up to handle the vast amount of data generated by various ship sensors and systems.
    d. In case of retrofitting with installation of new decarbonisation solutions additional sensors will be introduced to monitor the performance of devices or applications.
2. Establish Ship Profile and Performance Model:
    a. Historical data is used to create a ship profile that includes routes, ports of call, cargo capacity, fuel consumption and CO2 patterns as well as typical weather conditions. In addition, the expected utilisation of the ship for its remaining lifecycle (locations and numbers of voyages, frequencies of voyages and planned maintenance activities) are also included.

   b. To establish a benchmark against which decarbonisation solutions and their combinations can be assessed, actual data is used to develop the ship's base performance model.
   c. Performance models from shared industry data spaces can be leveraged to increase development efficiency and possibly enhance accuracy.
3. Calculate Carbon Intensity Indicator (CII) and rating:
   a. A CII calculator is employed to calculate the ship's CII for the current reporting period and project the CII value and its respective rating after future voyages.
   b. This data is critical for guiding the decarbonization transition strategy.
4. Specify Decarbonization Transition Strategy:
   a. With reference to SEEMP Decarbonization Transition Strategy, based on the ship type, status, i.e., years in operation, expected remaining life, an annual minimum performance threshold table is created to set performance targets.
   b. Technologies of interest are identified for two phases, as mentioned in the section 3: Phase 1 involves minimal investment, while Phase 2 focuses on compliance with emission reduction regulations over the ship's lifespan.
   c. Multiple objectives are defined to achieve optimal ship performance, including efficiency, load factors, operating cost reduction, and emission targets.
5. Evaluation of Decarbonisation Technologies – produce Decarbonisation Strategy:
   a. Simulation is used to evaluate the impact of various decarbonization technologies, and their combinations, based on ship profiles and base performance models.
   b. Evaluation criteria may include the ability to meet performance thresholds, cost-effectiveness, technological maturity, and crew acceptance.
6. Create an Integrated Performance Model:
   a. A Knowledge Graph (see Chapter 3 of this book) is utilized to represent the interdependencies of all ship subsystems affecting performance variables.
   b. This integrated model provides a holistic view of how control variables interact and affect ship performance.

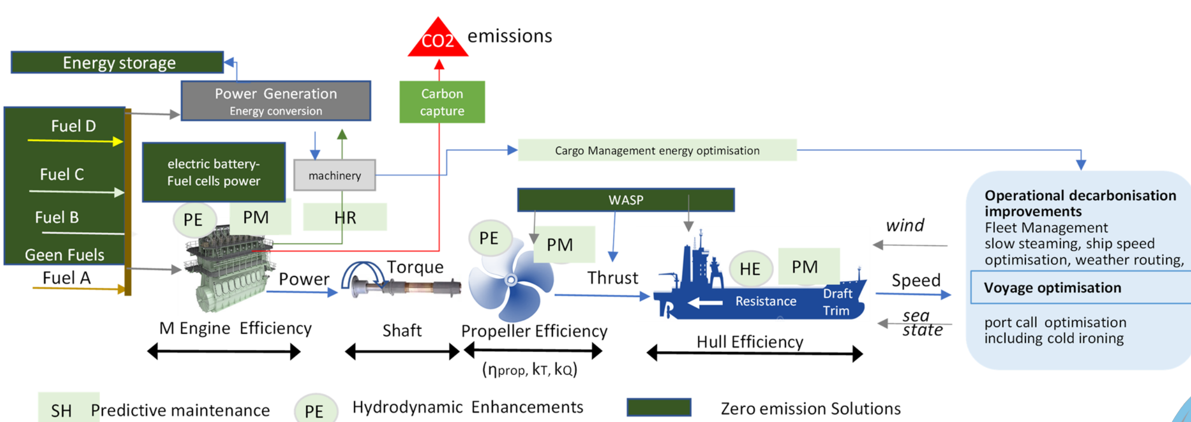
The Integrated Performance Model depicted in Figure 4 is designed to optimise the ship's propulsive performance (i.e., in terms of GHG emissions) given as control inputs the different decarbonisation technologies adopted, (described as a Decarbonisation Strategy) in the diagram. The control objective therefore is to select an optimal mix of decarbonisation technologies that when applied to the Base Performance Model, as shown in 2b above, yield a performance improvement above a given threshold, while satisfying the constraints imposed by the other performance parameters. The controller is therefore model based and more specifically incorporates the Integrated Performance Model of the ship that includes the main interactions between the ship model parameters (including environment parameters such as financial: CAPEX, OPEX. The Integrated Performance Model therefore, integrates the ship's characteristics, operational data, and the performance parameters, energy consumption, propulsion performance, and emissions, of selected decarbonisation options and is supplied with data obtained from the Ship's Digital Twin. The multi-objective optimisation process is applied both for the design of the Decarbonisation Strategy and in support of continuous operational ship optimisation. The formulated mathematical optimisation program is set in a rolling time-horizon. This means that the optimization process considers real-time data and adapts to changing externalities over time. This enables the system to make informed operational and maintenance decisions based on up-to-date information.

Figure 4. Schematic overview of the methodology



Moreover, a Reference Integrated Performance Model for Low Emissions Ship Operation can be found bellow, providing mapping of decarbonisation technologies in a ship performance model is shown in Figure 5. The multifaceted problem of managing the transition to zero emission shipping is illustrated in this mapping, having multiple different aspects of ship's operation and technologies included such as

Figure 5. Mapping decarbonisation technologies to ship subsystems



Performance Efficiency, Power Management, Hydrodynamic Enhancement, etc.., as well as alternative/bio fuels, carbon capture, etc.

Implementation Performance Validation and Tuning

After the new decarbonisation technologies have been fitted/retrofitted to the ship and the ship returns to operation. The Digital Twin is updated with the corresponsive newly integrated decarbonisation technologies' models, thus, keeping it up to date.

Additionally, feedback is provided to the Dataspace Knowledge Hub (discussed in the next section) with the experiences (collected from the physical ship and uploaded to the DT). While operating under the new configuration, more data regarding the ship's behaviour under different operating conditions are collected, having as a direct outcome the enrichment of the Dataspace, i.e., more valuable. This in turn, has impact to the models, used in the DT, that becomes more refined and updated, through the iterative feedback, correction and fine tuning of the models. Furthermore, the applications that utilise these 'updated' models continue to improve as the accuracy and precision of predictions pertaining to ship optimisation decisions gets increasingly reliable.

Developing and Maintaining a Knowledge Hub and Dataspace for Shipping Decarbonisation

Industry Knowledge Hubs and Dataspaces provide evidence-based insights to guide decision-making, inform policy development, and support the implementation of effective measures to achieve climate goals and a sustainable future.

Global decarbonization studies often highlight the importance of international cooperation and coordination to address transboundary challenges. They assess the potential for technology transfer, financial support, and knowledge sharing among countries to accelerate decarbonization efforts on a global scale. This section considers how the information provided earlier can be used, extended and refined in a dataspace to support the shipping decarbonisation transition.

A shipping Dataspace can be defined as "*A data ecosystem, specified by a shipping community, whereby decentralised infrastructure enables trustworthy data sharing with commonly agreed capabilities*". Thus, a Dataspace is produced by an ecosystem of actors that interact through the sharing of data and is the main objective of initiatives like the International Data Spaces (IDS) association, and GAIA-X.

Moreover, a Dataspace of shipping decarbonisation models, can have a pivotal role in the achieving of the shipping decarbonisation targets, providing tools for the alignment of the efforts of different actors from the broader ship operation domain. In this direction, the Dataspace of shipping decarbonisation models can offer the basic means of industry knowledge transfer, utilising data available in the interconnected Digital Twins (DTs). Interconnected DTs represent:

- Ships equipped with one or more decarbonisation solutions or
- Decarbonisation equipment test facilities or related DTs.

The interface of the nodes are connectors complying to international standards such as the IDS reference architecture, ensuring the sharing of useful data in a uniform and secure way. Each DT dataset provides an insight of its specific "experience" in an adopted decarbonisation solution, special condition encountered, etc. The accumulated data are used to produce new models or to refine existing ones which become available to the participants who have the right to access the Dataspace and its resources. Only models are shared, guaranteeing data confidentiality, and providing the shipping industry collective knowledge. Therefore, through the dataspace, each DT can project the application of a decarbonization technology conducted on another physical vessel onto its own case.

In addition to the knowledge generated by each DT instance, the Knowledge Hub is trained by internet resources on trends in decarbonization and provides perspectives that can be consumed within the dataspace.

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A Dataspace of shipping decarbonisation models provides the basic means of industry knowledge transfer, utilising data available in the interconnected Digital Twins (DTs). Interconnected DTs represent 1) ships equipped with one or more decarbonisation solutions or 2) decarbonisation equipment test facilities or related DTs. The interface of the nodes are connectors complying to international standards such as the IDS reference architecture, ensuring the sharing of useful data in a uniform and secure way. Each Digital Twin (DT) dataset provides an insight of its specific 'experience' in an adopted decarbonisation solution, special condition encountered, etc. The accumulated data are used to produce new models or to refine existing ones which become available to the participants who have the right to access the Dataspace and its resources. Only models are shared, guaranteeing data confidentiality, and providing the shipping industry collective knowledge. The initial set of reference models are provided by projects such as DT4GS (https://dt4gs.eu).

As more data about the ship's behaviour under different operating conditions are collected, the Dataspace becomes enriched, i.e., more valuable. Owed to this, the applications that utilise 'updated' models continue to improve as the accuracy and precision of predictions pertaining to ship optimisation decisions gets increasingly reliable.

Overall, a repository of green shipping solutions and data sources is essential for reducing the environmental impact of shipping, complying with regulations, saving costs, and improving reputation and brand image. It can help the shipping industry move towards more sustainable and environmentally friendly practices, while also benefiting companies financially and socially. Generally, Information hubs are platforms designed to store and distribute information related to a particular field or topic. They can take many forms, such as online databases, digital libraries, or information portals. However, simply storing information is not enough to create a valuable resource that supports informed decision-making and promotes sustainability. To achieve this, information hubs must evolve into knowledge hubs.

Knowledge hubs take the information stored in information hubs and add value by organizing, synthesizing, and analysing it to create knowledge that can be used to solve problems, make decisions, and drive innovation. By transforming information hubs into knowledge hubs, users can gain a deeper understanding of the data and its implications, identify patterns and trends, and apply this knowledge to real-world challenges.

As an illustration, consider an information hub that stores data related to a particular field or topic. While this information is valuable, it may not be enough to fully understand the implications of the data or apply it to real-world challenges. By transforming this information hub into a knowledge hub, the data can be analyzed, synthesized, and organized to create knowledge that can be used to support informed decision-making and drive innovation. By synthesizing and analyzing data from various sources, knowledge hubs can provide a comprehensive and up-to-date understanding of these issues and support the development of effective solutions. Moreover, knowledge hubs can help bridge the gap between research and practice by translating complex research findings into actionable knowledge that can be used by policymakers, practitioners, and other stakeholders. This can lead to better decision-making, improved outcomes, and ultimately, a more sustainable future.

However, the effectiveness of knowledge hubs depends on the quality and reliability of the data and analysis they provide, as well as their accessibility and usability for different stakeholders. Ongoing collaboration and dialogue between knowledge hub developers and end-users are crucial to ensuring that knowledge hubs meet the needs of different users and support informed decision-making in various fields.

To implement an information hub that can evolve into a knowledge hub, several technologies can be utilized, including:

1. Semantic Web Technologies: These technologies, such as RDF (Resource Description Framework), OWL (Web Ontology Language), and SPARQL (SPARQL Protocol and RDF Query Language), enable the creation of a semantic data layer that allows for more meaningful data connections and relationships.
2. Knowledge Graphs: Knowledge graphs are a type of graph database that use a network of nodes and edges to represent data and relationships between data points. They enable the creation of a more interconnected and contextualized understanding of data.
3. Machine Learning: Machine learning can be utilized to identify patterns and relationships within data, which can then be used to generate insights and predictions. This can be particularly useful in identifying correlations between different data.
4. Natural Language Processing: Natural language processing can be used to extract meaning and context from unstructured data sources, such as text documents, social media posts, and news articles.
5. Data Visualization: Data visualization tools can be used to create meaningful and easily understandable representations of complex data sets, making it easier for stakeholders to interpret and the data.

These technologies can be used to support knowledge representation, inference, and reasoning within knowledge hubs, enabling more sophisticated analysis and decision-making. For example, ontologies can help to standardize and organize domain-specific concepts and relationships, while knowledge graphs can help to identify patterns and connections within complex data sets.

Moreover, these technologies can be integrated with other data management systems such as PostgreSQL to support the storage, retrieval, and analysis of data within knowledge hubs, depending on the specific requirements of the information hub. For example, RDF data can be stored in PostgreSQL using the RDF data model and queried using SPARQL. Natural language processing and machine learning algorithms can be implemented within PostgreSQL using programming languages like Python and integrated with the database using the PL/Python extension. Data visualization tools can also be integrated with PostgreSQL to provide users with interactive dashboards and reports.

Creating a knowledge hub for green shipping information requires an effective system to manage and organize the large amounts of data that need to be stored and accessed. PostgreSQL, a powerful RDBMS, provides an excellent solution for this task. With its robust features, PostgreSQL can efficiently handle and manage large amounts of data, while maintaining the integrity and consistency of the information. In addition to its data management capabilities, PostgreSQL provides strong security features to protect sensitive data. It includes various authentication mechanisms, such as SSL and Kerberos, and supports encryption to ensure data confidentiality. PostgreSQL's advanced security features ensure that sensitive data remains secure and protected from unauthorized access. Another advantage of PostgreSQL is its flexibility and scalability. It can be customized to meet the specific needs of the knowledge hub and can adapt to changes in requirements over time. PostgreSQL supports a variety of programming languages and provides a wide range of extensions and plugins that can be used to enhance its functionality.

Overall, PostgreSQL is an excellent choice for creating a knowledge hub for green shipping information. Its reliability, scalability, and strong security features make it a preferred choice for managing and organizing large amounts of data while maintaining the integrity and confidentiality of the information.

PostgreSQL organizes data into tables consisting of rows and columns, with each table representing a different type of data or entity in the system. Relationships can be defined between tables to represent how different entities are related to each other. For example, in a green shipping knowledge hub, tables can be created for ships, routes, and ship_routes.

The creation of a knowledge hub with information on green shipping solutions involves several essential steps, with determining the taxonomy being the first step. To achieve this, entities that require classification such as different types of ships, green shipping solutions, or emission factors need to be identified. Categories and subcategories can then be defined based on the entities identified, such as having a top-level category for ships with subcategories for cargo ships, tankers, and passenger ships, or a top-level category for green solutions with subcategories for renewable fuels, energy-efficient designs, and sustainable materials. Once the taxonomy has been determined, the next step is to create a schema in the PostgreSQL database that reflects the categories and subcategories identified in the taxonomy. This is done to create a logical container for tables that share a common purpose, making it easier to organize and manage data within the database. For example, a schema called "green_shipping" can be created to hold all tables related to the knowledge hub. Within the schema, tables for each category or subcategory are created, such as "cargo_ships" with columns for ship name, size, fuel type, and emissions data, or "renewable_fuels" with columns for fuel type, emissions data, and availability. The tables can be further organized into subcategories as needed, such as "electric_cargo_ships" or "biofuels."

By creating a schema that reflects the taxonomy, it will be easier to navigate and manage the database, especially as it grows in size and complexity. It also ensures consistency and accuracy in the data, as each table will be focused on a specific category or subcategory. This approach can ultimately lead to more efficient queries and analytics, and a more effective and impactful knowledge hub. The relationships between the tables are then defined based on the taxonomy determined. This involves creating a table called "ship_solutions" with columns for ship ID and solution ID to represent the relationship between different ships and the green solutions they use.

After defining relationships, the tables are populated with data obtained from research and analysis of green shipping solutions, best case user, and emission factors of ships. SQL queries can be used to insert data into the tables. Queries can also be used to retrieve specific information from the database, such as all cargo ships that use renewable fuels and have low emissions, or all green solutions that have been proven to reduce emissions in real-world applications.

Finally, it is crucial to maintain and update the database over time as new information becomes available to ensure that it remains relevant and accurate. This involves regularly reviewing and updating the data to ensure its integrity, as well as adding new data sources and refining the schema and tables as necessary. By maintaining the database over time, it can remain a valuable resource for stakeholders in the shipping industry, providing up-to-date and comprehensive information to support informed decision-making and promote sustainability. Overall, creating a knowledge hub with PostgreSQL involves determining the taxonomy, creating the schema and tables, defining relationships, populating the tables with data, querying the data, and maintaining and updating the database over time.

Consumers are increasingly aware of environmental issues and are more likely to support companies that prioritize sustainability. Having a repository of green shipping solutions and data sources can help companies demonstrate their commitment to sustainability and improve their reputation and brand image. This can, in turn, lead to increased business opportunities and competitive advantages for these companies.

CASE STUDY: ONBOARD ENERGY PRODUCTION, DISTRIBUTION, MANAGEMENT AND RECOVERY PROCESS SIMULATOR

In this section, we present an overview of a simulator integrated into the ship's Digital Twin (DT) framework. This simulator serves the crucial role of modelling and analysing a wide spectrum of onboard processes, including energy production, distribution, management, and recovery. It harnesses the inherent advantages of the digital twin concept, ensuring robust data availability and, in relevant scenarios, even offers a means of control over vessel systems.

It is noted that the described structure of the simulator has an open, modular, object-oriented architecture, which is adaptable to current and future ship propulsion-power plant configurations. Currently there are two typical power paradigms in merchant ships:

- Diesel paradigm, where the propulsion-power is provided by one or two slow-speed diesel engines and the electric power for shipboard services is provided by a set of diesel generators, and
- Diesel-Electric paradigm, where the propulsion shaft is driven by two electric motors and the electric power for both propulsion and shipboard services is provided by a set of diesel generators (Hoang, 2020). This aforementioned paradigm is widely used for the cruise ship.

In both cases the main power source is a large slow-speed or mid-speed diesel engine with a thermal efficiency of about 50%, meaning that for each kW of utilizable shaft power, equal power is dispersed as heat and a smaller part in the friction.

Therefore, especially for vessels with high installed power (such as large container vessels and cruise ships), there is a large potential margin for fuel consumption reduction and consequently of emissions reduction, from the recovery of the waste heat. This can be done either directly in the form of thermal power or indirectly in the form of electric power.

It is estimated that an optimized high-efficiency Waste Heat Recovery (WHR) Plant may recover up to 10% of the main Diesel Engine / Generator shaft power. Cruise ships, being characterized by a Hotel Load for the Electric Users almost as large as the Propulsion Load as well as by an important direct heat request from the Heat Users, may benefit the most from WHR strategies. The section places special emphasis on Waste Heat Recovery (WHR) systems, a technology that, although not new, continues to hold promise and has the potential to deliver significant efficiency enhancements.

Benefits and Requirements of DTs in Energy System Optimization

The Digital Twin provides enhanced capabilities for optimization purposes through the lifecycle of the object: design, operation, retrofitting, retire. Among other reasons, this is achieved by considering in detail a multitude of parameters beyond those associated solely with the specific system under examination.

Another advantage of employing energy system optimization within a DT framework is the utilization of its structured information about regarding subsystem and components availability and overall configuration.

The primary scope of the Digital Twin based simulator is the benchmarking of the energy efficiency of different WHR configurations, modelled through a limited set of design parameters, over a large set of service conditions representative of the operational profile of the ship.

The WHR simulation aims to evaluate the overall electric / heat energy balance of the ship and as such it will be able to manage production, distribution and consumption of Fresh Water, Steam and Electric power.

In general, there are two types of simulators that can be used:

- Disregarding transient states, a logical state-machine solving a system of algebraic equations with given known terms to determine the resulting balance state.
- Modelling in real-time the internal processes occurring in each involved system and the regulation feed-back loop of the relevant mass flows and associated temperatures implemented to achieve the dynamic equilibrium; time-domain simulation solving a system of differential equations driven by initial conditions to analyse the dynamic evolution of the energy processes.

Focusing on the steady state option, each simulation considers a static set of operational conditions denoted as a “voyage condition”, which could either represent a stay in port or a navigation leg. A chain of sequential voyage conditions will therefore represent a typical “voyage” of the ship whereas a chain of voyages will represent the “operational profile” of the ship that is the set of operational / environmental conditions which the ship will likely encounter during a year of standard service.

In this context, the information concerning loads in terms of power requested for propulsion and the electric load must be seen as input for the energy simulation, indeed, the requested values must be fulfilled in the different operative condition.

Hence, knowing the requested of powers the user can modify the layout of onboard devices to assess the change a ship energy performance.

In detail, the operation profile, consists of:

- a navigation leg to be completed within an expected time.
- a set of environmental conditions (i.e., sea / wind / current) likely to be encountered.
- the service load expected in the leg.

The service load will have in general the following breakdown:

- propulsion power (in case of Diesel-Engine propulsion); electric power requirements; propulsion load (in case of Diesel-Electric propulsion)]; hull & engine services load; hotel load
- Fresh Water requirements
- Cooling Water requirements
- Steam requirements

In particular, the voyage simulator provides Power requested to the Main Propulsion Plant and the Electric Power requested to the Power Generation Plant to the WHR simulator. Based on this, the WHR simulator estimates the Waste Heat produced by the Power Generation Plant and by the Main Propulsion Plant (in case of Diesel-Engine propulsion), which will be used as an input to the WHR Plant model.

Based on this input (and the prevalent internal / external environmental conditions), the WHR Plant model provides an estimate of the electric power and thermal power recovery. However, it must be considered that, when electric energy recovery from the waste heat of Diesel Generators is implemented, the recovery process should be analyzed iteratively as the resulting reduction in the electric load will in turn reduce the waste heat and thus the recovery.

Modular Model High Level Description

As there is a diversity of possible WHR Plant configurations, depending on ship types and operational profile, it is of primary importance for the simulation tool to be easily configurable, even in automated way controlled by the DT.

For this purpose, the components registered in the DT as power producers or consumers are modelled in terms of thermodynamic interaction (mass and energy, input and output). Indicatively, such components are the following:

- Generation units
    - Diesel Engines
    - Alternators
- Recovery units
    - Heat Recovery Units
    - Electric Recovery Units
- Users
    - FW Users
    - CW Users
    - Steam Users
- Similarly, in the context of DT as decarbonization methods, thermal and electrical recovery units are considered, all falling under the category of waste heat recovery units. These units can be modelled in the energy simulator and include: Steam Economizers
- HW Economizers
- Evaporators
- Heat Exchangers for Heating / Re-Heating / Pre-Heating of FW
- Absorption / Adsorption Chillers Units
- Organic Rankine
- Steam Power Turbines

- Gas Power Turbines

CASE STUDY: HULL CONDITION PREDICTION SIMULATOR

In this section it is demonstrated how typical procedures that are currently used, e.g., for hull condition assessment can be enhanced by incorporating them into DTs and, on the other side, how the DT can facilitate their application. The basis of the study is the ISO 19030 (ISO 19030-1, n.d.) (ISO 19030-2, n.d.) that accounts for the hull and propeller performance assessment. It pertains to the comparison of performance of a specific ship to herself, over a certain period of time. This can be conceived through the relation between the ship's underwater condition and the power needed to move the ship through water at a specific speed. For a given speed, variation in the needed power may be observed, due to changes in the underwater hull and propeller condition, leading to increased hull resistance and alterations in the propeller efficiency.

It is important to highlight that data-driven methods are well-suited for hull assessment within a DT. Nevertheless, model-driven ('white-box') approaches continue to hold value, especially when used in conjunction with data-driven methods, giving rise to grey-box methods.

Flows Data Requirements

In a ship's Digital Twin (DT), the top priority is to gather all available data from navigation instruments (GPS, echo sounder, speed log, anemometer, gyro and ruder indicator), draft sensors, and shaft power meters or flow meters. These sources provide the fundamental information needed to construct an accurate representation of the ship's operational status. In addition, the DT is typically integrated into a dataspace with weather and oceanic data providers. Lastly, in the DT, various constructive, geometrical, and hydrodynamic particulars and references are documented, as these are essential for creating a comprehensive digital representation of the vessel. This includes data such as the height of the anemometer, the relationships between draft, trim, list, and displacement and sea trials.

On the other side, the ISO 19030 procedure primarily considers the ship's speed through water and the delivered power as its key parameters. Additionally, it takes into account several secondary parameters, including the ship's speed over ground, relative wind speed and direction at the height of the anemometer, significant wave height, direction, and spectrum (for wave resistance corrections), swell height, direction, and spectrum (for wave resistance corrections), water depth, water temperature and density, loading conditions, dynamic floating conditions, and rudder angle/frequency of rudder movements.

Furthermore, the digital twin typically relies on advanced data collection and processing techniques, leading to filtered, normalized, and synchronized data. According to the ISO 19030 the measurement procedures consist of data acquisition, data storage and data preparation, in terms of ensuring the same sample rate. The next crucial part of this first, preparatory stage, is the data filtering process, during which outliers and invalid data is excluded from the calculations thereafter. To this end, and exploiting Statistic's theory, the document of ISO 19030 dictates the use of Chauvenet's criterion, which is based on the calculation of the probability for the occurrence of any value within the data. The process prescribes the calculation of the mean values and standard deviation of consecutive, non-overlapping subsets of data.

It is evident that the typical data availability and data processing tools within the typical Digital Twin exceeds the requirements of ISO 19030, making its application significantly more straightforward and accessible.

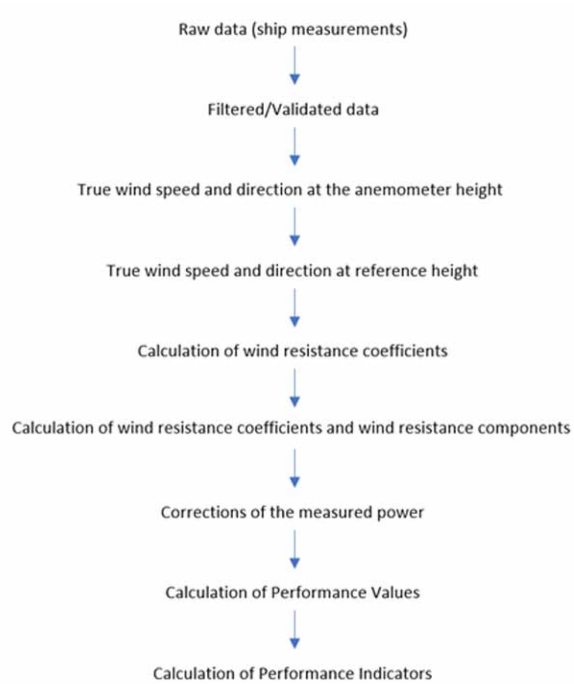
Brief Model Description

After the stage of filtering and validating the raw data obtained from the ship and ensuring uniform sample rate, the next step of the described process is the calculation of true wind speed and direction, at the height of the anemometer, which in turn allows the calculation of the relative wind speed and direction at reference height. The latter are exploited directly for the calculation of the wind resistance coefficients, which are utilized to derive the components of the wind resistance components and therefore for the corrected delivered power The described process is graphically shown with the aid of Figure 6, which is literally the backbone of ISO 19030.

Wind Resistance Calculation

The relative wind speed and direction at the current loading condition of the vessel, serve as input for the corrections of the measured power (ΔP_w). The wind resistance corrections eventually lead to the subtraction of that component of the delivered power that is required to overcome the wind resistance. The wind resistance correction is calculated by the equation:

Figure 6. Process for the assessment of hull-propeller performance, as described in ISO 19030



$$\Delta P_w = \frac{(R_{rw} - R_{0w}) \cdot v_g}{\eta_{D0}} + P_D \cdot \left(1 - \frac{\eta_{DM}}{\eta_{D0}}\right)$$

where R_{rw} is the wind resistance due to relative wind, R_{0w} is the air resistance in no-wind condition, v_g is the ship speed over ground, ηD_0 is the propulsive efficiency coefficient in calm condition and ηDM_is the propulsive efficiency coefficient in actual voyage condition. Rrw_and R0$w_a$re given by the following expressions:

$$R_{rw} = \frac{1}{2} \cdot \rho_a \cdot v_{wr}^2 \cdot A \cdot C_{rw}\left(\psi_{wr,ref}\right)$$

$$R_{0w} = \frac{1}{2} \cdot \rho_a \cdot v_g^2 \cdot A \cdot C_{rw}(0)$$

where ρa is the air density, A is the transverse projected area in current loading condition, C$r_{w(}$Ψw$_{r,ref)}$ is the wind resistance coefficient, dependent on wind direction of relative wind and finally C$r_{w(}$0) is the wind resistance coefficient for head wind (0°). We can directly notice that wind resistance expressions follow the general form of any resistance-component expression.

Speed Loss Calculation

The next step of the process is the calculation of the percentage speed loss (V_d). It is calculated as the relative difference between the measured ship speed through water V_m and the expected speed through water (V_e). The latter is obtained by a speed power reference curve. In detail, these non-dimensional parameters are given by the equation:

$$V_d = \frac{V_m - V_e}{V_e} \cdot 100$$

where, V_m is the measured vessel speed through water and V_e is the expected speed through water. For the calculation of V_e, the well-known Admiralty Coefficient can be also exploited. Besides, the speed-power reference curve of the ship, as well as data from the trim and stability booklet of the ship are indispensable.

Definition of the Reference Periods

The evaluation of the hull condition is carried out by comparing its performance with reference conditions. These reference conditions are extracted from intervals where the following criteria are simultaneously met:

- water temperature greater than 2°C, given that the vessel does not navigate in ice

- the true wind speed must be between 0m/s and 7.9m/s (or equivalently 0 and 4 BF)
- the water depth must hold: $h > max\left(3\sqrt{BT_M}, 2.75 \cdot \frac{V_s^2}{g}\right)$, where h is the water depth, B is the ship breadth, T_M is the draft at midship, or mean draft, V_s is the ship speed and g is the gravitational acceleration

Calculation of the Performance Indicators

There are four performance indicators (PIs): the first one assesses the effectiveness of a dry docking, while the second determines the in-service performance, through the assessment of the effectiveness of the underwater hull and propeller solution (e.g., hull coatings), including any maintenance activities. The third and fourth PIs refer to the crucial issue of the maintenance of the ship structure, particularly whether it is necessary or not to trigger a maintenance activity and to evaluate the effectiveness of a possible maintenance activity.

Specifically, for the dry-docking performance, the period following directly after the latest dry-docking is the evaluation period. The period following directly after the previous dry-docking is the reference period. All periods are to be of the same length of 1 year. For the in-service performance, the period following directly after the latest dry-docking is the reference period. The period following the reference period until the end of the same dry-docking period is the evaluation period. The reference period and the evaluation period shall both be of minimum 1 year. For the maintenance trigger, the period following directly after the latest dry-docking is the reference period. A period after the reference period in the same dry-docking interval is the evaluation period. The reference period and the evaluation period shall both be a minimum of 3 months. Finally, for the maintenance effect, the period following directly the maintenance event is the evaluation period. The period preceding the event is the reference period. The reference period and the evaluation period shall both be a minimum of 3 months.

From the mathematical point of view, a PI is defined as the difference between the average percentage speed loss of the reference period and the evaluation period. The average percentage speed loss over the reference period, is calculated from:

$$\bar{V}_d^{ref} = \frac{1}{k}\sum_j^k \frac{1}{n}\sum_i^n V_d^{j,i}$$

where k is the number of reference periods, j is the reference period counter, n is the number of data points in the processed data set under reference conditions in the reference period j, i is the counter of data points in reference period j, $V_d^{j,i}$ is the percentage speed loss for data point i in reference period j and $\bar{V}_d^{ref}$ is the average percentage speed loss over the reference period. Regarding the average percentage speed loss over the evaluation period:

$$\bar{V}_d^{eval} = \frac{1}{n}\sum_i^n V_d^{eval,i}$$

where, n is the number of data points in the processed data set under reference conditions in the evaluation period, $V_d^{eval,i}$ is the percentage speed loss for data point i in a data set of the evaluation period and $\bar{V}_d^{eval}$ is the average percentage speed loss in data set of the evaluation period. Finally, the corresponding PI is obtained by the equation:

$$k_{HP} = \bar{V}_d^{eval} - \bar{V}_d^{ref}$$

The results are always anticipated to describe both qualitatively and quantitively the hull and propeller degradation. Specifically, plotting the extracted PI versus time allows a visual representation of the continuously decreasing ship performance. Besides, it enables the involved entities to identify what the exact decrease of the ship's performance is (in %) and to evaluate whether a dry-docking is needed or, for example, what the effectiveness of any possible underwater maintenance activities was.

CONCLUSION AND FUTURE OUTLOOK

The diverse array of decarbonization technologies at various stages of maturity, necessitates the use of decision support tools to aid in the selection of the most suitable combination of technologies for a specific ship profile, time period and decarbonisation requirements.

The use of Digital Twin-based decision support tools streamlines the process of evaluating and selecting decarbonization technologies, making it possibly more efficient and accurate. By leveraging real-time data, simulations, and optimization algorithms, Digital Twins enable the maritime industry to navigate the complexity of decarbonization and transition toward a sustainable, low-emission future.

It is important to note that the maturity, potential availability, and cost of zero-emission fuels are subject to ongoing research, development, and market dynamics. Government policies, regulations, and incentives will also play a significant role in shaping the future landscape of zero-emission shipping technologies and fuels.

The proposed methodology for assessing and deploying decarbonisation technologies emphasises the following:

- Gather data on the ship's operational profile, including routes, ports of call, cargo capacity, fuel consumption and CO2 patterns and produce the ship Base Performance Model to be used in simulations that can provide insights into areas for improvement.
- Produce decarbonisation models, to meet decarbonisation goals / strategies utilising industry knowledge hubs that maintain a comprehensive database of available decarbonization technologies, including alternative fuels, energy-efficient systems, waste heat recovery, and emission reduction solutions.
- Use of an Integrated Performance Model to assess the ship's performance and emissions under various operational scenarios, considering different technologies and fuel options.
- Use of the DT to continuously monitor the effectiveness of decarbonisation solutions to continuously optimise ship operations, while sharing experiences and data within the Shipping Industry.

Chapter 3
Shipping Digital Twin Data Management With the Use of Knowledge Graphs

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ABSTRACT

This chapter explores the data management challenges inherent in a digital twin framework and elucidates the pivotal role of knowledge graphs in meeting these demands. The author introduces a functional metamodel designed to semantically convert scenarios related to the green transition into a standardized format. This metamodel emerges as a vital instrument for both business and technical stakeholders, streamlining the intricate interplay among operational requisites, environmental factors, optimization strategies, and decarbonization technologies. It adeptly encapsulates the ship's environmental and economic performance indicators. In synergy with the metamodel, a knowledge graph (KG) encodes industry-specific parameters, laying a robust groundwork that depicts the vessel's functionalities, variables, and operational processes, and serves as a repository for model metadata. This facilitates the automation of shortest path computations, effectively bridging the divide between overarching platform operations and the complex nuances of maritime assets and activities. The utility of the metamodel and knowledge graph in translating real-world issues into a digital twin-compatible format is exemplified through a case study focusing on the application of variable frequency drives for enhancing the efficiency of the high-temperature cooling system. The chapter concludes by summarizing the data management hurdles encountered in maritime digital twins and offering a perspective on future developments.

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BACKGROUND

In the ever-evolving landscape of industryes, the fusion of digital technologies has been a catalyst for transformation. Among these digital innovations, the emergence of Digital Twins (DTs) has stood out as a powerful paradigm. DTs represent a bridge between the physical and digital artifacts. They are digital reflections of physical assets, systems, or processes, replicating their behaviors, characteristics, and interactions. The significance of DTs is underscored by their capabilities to enable real-time analysis, predict potential challenges, and bolster decision-making through insights rooted in real-world data.

In the maritime domain, a DT embodies a real-time, digital duplicate of a vessel, port, or a maritime process (Madusanka et al, 2023). This chapter primarily focuses on DTs representing ships and their operational functionalities. A ship DT, in essence, is a virtual mirror of the vessel, reflecting every component, system, and operation. This includes not only the ship's structural features but also its operations, maintenance processes, and even its behavior in diverse maritime conditions. Within this context, DTs allow stakeholders to monitor, simulate, and optimize operations in a virtual environment, offering potential to enhance operational efficiency, optimize maintenance, and improve decision-making. Even before the physical ship takes shape, its DT can be instrumental in refining its design through virtual prototyping and simulations, thus sidestepping hefty real-world expenditures.

Once a ship is operational, DTs become indispensable in real-time oversight of equipment efficiency, fuel usage, and emission metrics. By analyzing this data, potential problems can be anticipated before they manifest, reducing unplanned downtime and ensuring optimal ship performance. In addition, DTs can aid in the development of optimal routes based on weather conditions, cargo weight, and fuel consumption. They can also assist in training the crew by simulating real-life scenarios, thus minimizing human error.

DT applications have already been deployed in maritime in areas such as ship-building, the offshore oil and gas Industry, marine fishery, and the marine energy industry (Zhihan et al, 2023).

(Coraddu et al, 2019) have developed a data driven Digital Twin of the ship that leverages the large amount of information collected from the on-board sensors, and is used for estimating the speed loss due to marine fouling. The authors claim that their approach has better speed loss prediction accuracy than the one obtained by the ISO 19030, thus allowing reducing the fuel consumption due to fouling.

However, the management of the data that underpin a digital twin is challenging. Such data management challenges include data variety, volume (Big Data) and dynamicity (Singh et al, 2021). While the potential of DTs is promising, its realization hinges on the quality and management of data. In particular, as vessels generate a vast amount of data from sensors, onboard systems, and external sources the data management of shipping digital twins becomes more prominent. Data streams obtained from ship sensors must be collected, stored, processed, and analyzed in a structured manner, to derive meaningful insights. These data streams, comprising operational parameters, environmental conditions, and machinery performance, need to be collected, stored, processed, and analyzed effectively. Robust data management frameworks are essential to ensure data accuracy, integrity, security, and accessibility.

Moreover, the different models that comprise the digital twin's simulation environment require access to the aforementioned data streams. This can become feasible only in a common data environment that hides the heterogeneity of the data and satisfies the data consumption requirements of the different models.

To overcome the above challenges, we propose a mechanism that connects the models to each other as well as to each other for complex digital twin simulations. Specifically, we introduce a model built on Knowledge Graphs (KGs) as a promising solution to address the above discussed concerns. In this Chapter we present the organization of the Knowledge Graph in terms of concepts, links between concepts and abstraction mechanisms such as classification and hierarchies to deal with data and model heterogeneity. Finally, we discuss Knowledge Graph search techniques for connecting models to data and to each other for coordinated model executions.

The Chapter is organized as follows. Section 2 introduces the data management requirements in shipping digital twins and the application of knowledge graphs.

Section 3 introduces a metamodel designed to connect the digital twin infrastructure with domain-specific knowledge and requirements.

Section 4 discusses the application of knowledge graphs in shipping DTs. Knowledge graphs serve as the system's data management structure, performing multiple roles, encompassing vessel components/functions, variables, and measurements, as well as operating as a semantic intermediary between ship structural models and operational models.

Section 5 illustrates a practical application of the suggested approach on the application of variable frequency drives for enhancing the efficiency of the high-temperature cooling system.

Finally, Section 6 discusses further evolutions of the integration of knowledge graphs and digital twins.

DATA MANAGEMENT AND KNOWLEDGE GRAPHS IN SHIPPING

Data Management in Shipping

As in other areas of industrial activity, in maritime, the spotlight increasingly turns to data management, marking it as the keystone of operational efficiency. As the shipping industry produces an intricate tapestry of data, it generates demand not just for storage but for transformative solutions that can distill, secure, and leverage this data into actionable insights. At the confluence of these demands, a suite of technological innovations is emerging, each tailored to address specific challenges and opportunities inherent to the shipping sector. These state-of-the-art solutions, while diverse in their applications and mechanisms, collectively aim to reshape and elevate the digital twin paradigm in the shipping industry, ensuring a future that's both connected and informed.

Given the complexity of ships and the maritime environment, effective data management solutions become crucial to unlock the complete potential of these digital representations. In the current section, we outline the general data management requirements for Shipping DTs and introduce the state-of-the-art technologies in this domain. Subsequently, we discuss available frameworks specific to shipping digital twins.

For the implementation of the digital twin technology, effective data management forms the bedrock of accurate and real-time representations of physical systems. This process begins with the collection and verification of data in real-time from an array of sensors, equipment, and external sources. Given the vast diversity in the origins and types of data, the integration of this data emerges as a central challenge. This challenge is further compounded in the maritime sector where mainly older ships, rely on legacy systems. Hence, modern digital twin solutions must not only be compatible with state-of-the-art systems but also adept at interfacing seamlessly with these legacy systems.

Once collected, data demands a sophisticated storage and processing infrastructure. Contemporary approaches favor the utilization of cloud platforms and distributed databases, which are chosen for their inherent scalability and prowess in efficient data processing. However, mere storage and processing are insufficient. The transformation of raw data into actionable insights necessitates the deployment of advanced analytics tools. Furthermore, to facilitate a clear understanding of these insights, especially when dealing with complex datasets, visualization methods become indispensable. These methods serve the dual purpose of representing data coherently and aiding stakeholders in making informed decisions.

Beyond visualization, digital twinning ventures into the territory of active scenario modeling. By constructing a detailed and accurate digital model of the physical system, researchers and practitioners can conduct simulations and scenario analyses. Such simulations, conducted in a controlled digital environment, grant the ability to optimize operations, test varied strategies, and predict outcomes without risking real-world assets or operations.

The pinnacle of this technological journey is reached with the application of predictive and prescriptive analytics. By harnessing the capabilities of machine learning and artificial intelligence, digital twin systems can predict future events, from maintenance needs to potential operational anomalies. More than just predictive, these systems can also prescribe optimal solutions, guiding performance and resource allocation towards desired outcomes.

Knowledge Graphs

Knowledge graphs can be seen as semantic network knowledge bases with a directed graph structure (Qui et al, 2017). By extracting information from semi-structured or unstructured data to form triples such as (subject, predicate, object), a knowledge graph can support knowledge retrieval and reasoning (Yan et al, 2018). It can display the complicated relations between domain knowledge, connect fragmentary knowledge, and it can support knowledge retrieval, knowledge question and answer, knowledge recommendation, knowledge visualization, and other applications.

While the primary and initial application of knowledge graphs is to infer knowledge from large datasets, now it is increasingly used in the semantic web community and providing a standard for information retrieval and utilization.

Knowledge Graphs have been deployed in diverse industrial applications such as planning maintenance planning of complex industrial equipment (Xia et al, 2023), and for predictive maintenance of hydraulic systems (Yan et al, 2023).

In the shipping and maritime domain, knowledge graphs have been used for ship collision accident reports and the improvement of maritime traffic safety (Gan et al, 2020).

(Zhang et al, 2020) have constructed a knowledge graph of maritime dangerous goods aimed to simplify the retrieval process of dangerous goods knowledge, realise the automatic judgment of cargo stowage and segregation, and promote the intelligent transportation of dangerous goods.

Langxiong et al (2023) have created a Ship Collision Accident Knowledge Graph and used it to discover the internal relationship of the accident and could be used to expedite the judicial process, which simplifies the process of marine accident investigation.

Knowledge graphs have emerged as a pivotal innovation in enhancing the capabilities of DTs. By modeling entities, relationships, and attributes in a structured manner, knowledge graphs offer a dynamic way to organize and connect information in the DT. Applied to the maritime sector, knowledge graphs enable a holistic representation of a vessel's ecosystem, encompassing equipment, maintenance schedules, historical data, and regulatory requirements. This interconnected knowledge facilitates predictive analytics, risk assessment, and scenario simulations. By connecting real-time data streams with historical information, knowledge graphs facilitate predictive maintenance, allowing for the timely identification of potential issues.

Therefore, owing to the inherent characteristics of knowledge graphs, specific functionalities are naturally extended to shipping DT applications:

Visual Representation: Knowledge graphs can visually represent the interconnections between different ship components. For instance, how the engine's performance might influence the propeller's speed or how a malfunction in one subsystem can cascade into another.

Semantic Search: With knowledge graphs, operators can search for information contextually. For example, instead of just searching for "engine malfunction," they can query "effects of engine malfunction on ship's speed during stormy conditions."

Intelligent Analysis: Knowledge graphs can help in understanding patterns and correlations within data. This could lead to uncovering insights that would otherwise remain hidden. For example, recognizing that a certain type of cargo influences the ship's balance in specific weather conditions.

In the approach discussed in the present chapter, knowledge graphs are utilized mainly to support DT system operation, specifically data management in a way that enhances interoperability between DT data sets and models.

In this context, a knowledge graph can be utilized for the following purposes:

- Providing a unified representation of vessel assets, operational condition and performance.
- Providing the functionality of the DT, storing measured and simulated values for a particular time or interval, depending on the DT application.
- Providing a semantic layer for the user and encoding shipping domain concepts in a format that can be consumed by the IT system.
- Providing a common registry for DT software components, to support system functionality.
- Use as a tool to store and explore data about vessel subsystems and the corresponding simulation models.
- Use for the optimal execution sequence for discrete simulation models.
- Use for sharing DT knowledge.

BRIDGING DIGITAL TWINS WITH DOMAIN REQUIREMENTS

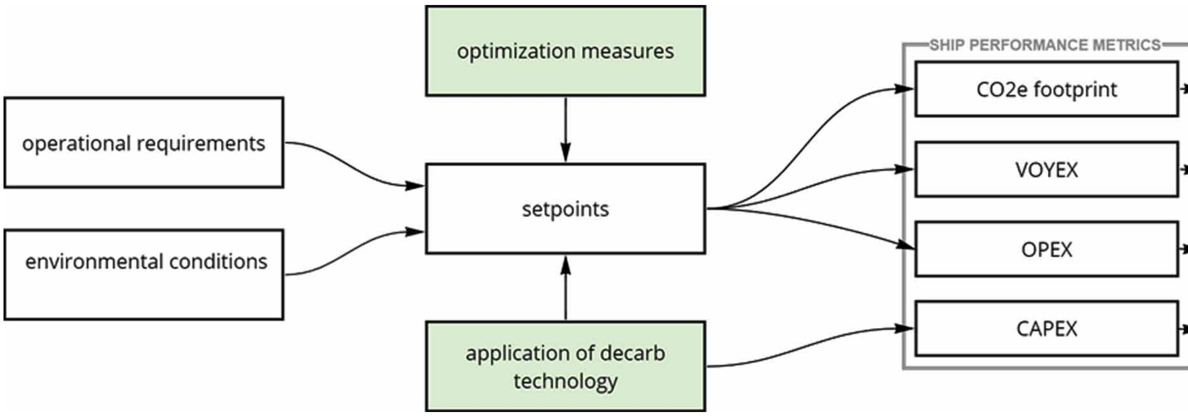
Introducing the Operational Metamodel

An operational metamodel is a structured framework that defines the fundamental concepts, relationships, and rules governing the operation of a system. It provides a standardized way to depict how components interact, how processes are executed, and how data flows within a given context. This metamodel serves as a reference point for designing, analyzing, and comprehending the operational aspects of systems, facilitating effective communication and implementation across diverse applications or use cases.

Given the diverse range of applications that a Digital Twin (DT) can encompass, there arises a necessity to establish a foundational "principle of operation" that can be applied to various use cases. To accomplish this, we propose the adoption of an operational metamodel, as illustrated in Figure 1, which outlines the fundamental functioning of the system.

The operational metamodel serves as a semantic layer between the high-level use cases description and the actual system operations. The user/business perspective is the causal relationship between the operational requirements, environmental conditions, applied optimization measures and installed decar-

Figure 1. The operational metamodel



bonization technologies on the one side and the ship's environmental and economic performance indexes on the other. These parameters along with three operational mechanisms that compose the system, i.e., model execution engine, convergence checker and optimization engine are described in the following paragraphs.

The proposed metamodel should be consistent in various use cases of the system, with respect to aspects such as:

- Temporal context, for example examining a voyage segment, a whole voyage, a reference condition (e.g., scantling draft at Maximum Continuous Rating (MCR)) or even examining the whole lifecycle of the vessel.
- Different users, such as the ship owner, the ship operator, the charterer and the other stakeholders of ship digital twin ecosystem. For example, system user can be a fund that intends to build a green fleet of autonomous vessels and uses digital twins to investigate the perspectives.
- All levels of vessel functionalities, eg low level such as machinery operation or high level such as cargo carrying capacity vs cost

In addition, it should support two modes of operation: real-time operation, where recommendation for optimized operation is automatically produced, by continuously adapting system to external and internal conditions and operation of the digital twin as a decision support tool, executing what-if scenarios.

MAIN CONCEPTS OF THE OPERATIONAL METAMODEL

Ship Performance Metrics

A simple definition of ship performance is the rate of fuel consumption required to move the vessel through the water for the given conditions, which may be operational (speed or draught) or environmental (wave height, wind speed, etc.) (Kim et al, 2021), (Armstrong, 2013). However, the quantification of vessel performance in shipping digital twin should account both for environmental and financial metrics. For example, using a green fuel may result to reduced CO2 footprint but increased operational cost. Building a vessel with a dual fuel engine, may result to lower CO2 emissions and increased initial capital but the operational costs are to be estimated.

The parameters currently considered are the CO2 footprint in CO_{2e} g/ton-mile, VOYEX (costs directly related to a voyage), OPEX (operational costs that do not depend on voyage), and CAPEX (capital expenditures). With these arrangements both real time operation and lifecycle analysis can be implemented. Vessel performance assessment is differentiated for each user type. By applying the appropriate weights to the above parameters, indicators applicable to different type of stakeholders can be produced.

Operational Requirements

"Operational requirements" is the basic input. An interpretation of this term is "how the vessel should behave". Operational requirements include:

- regulatory obligations, such as ballast treatments or emissions constraints
- contractual or business obligations, such as arrival time, FOC or vessel speed and
- other operational constrains, such as required stoppage for bunkering, crewing, supplies, maintenance, etc.

Environmental Conditions

Apart from the operational requirements another input is the environmental conditions which are the external factors such as weather conditions and bunker prices. Depending the context, these parameters can be acquired for the present time from an external data source or can be based on a forecast (e.g., for the weather), can be variables of a scenario, or can be assumed.

Setpoints (Operational Conditions)

Operational requirements, along with environmental conditions determine the setpoints, which are parameters that describe machinery operation. Setpoint are the settings to achieve the operational requirements, given the environmental conditions. Engine speed is a fundamental operational condition.

Optimization Measures

Optimization measures is the set of available measures to optimize vessel performance and reduce CO_{2e}. Such measures include:

- JIT arrival
- Trim optimization
- Weather routing
- Under Water Cleaning and/or Propeller Polish
- Modifying maintenance frequency
- Determining fuel type
- Optimizing bunkering location/quantity

Application of Decarbonization Technologies

While optimization measures consider existing vessel assets, the application of decarbonization technologies refer to the application of an addition or retrofit.

Such measures may include:

- M/E retrofit to utilize different fuel or fuel blend
- Wind assist
- Carbon Capture / Fuel cells
- Application of coating
- Installation of energy saving devices (duct, fin, etc.)

KNOWLEDGE GRAPH FOR SHIPPING DIGITAL TWINS

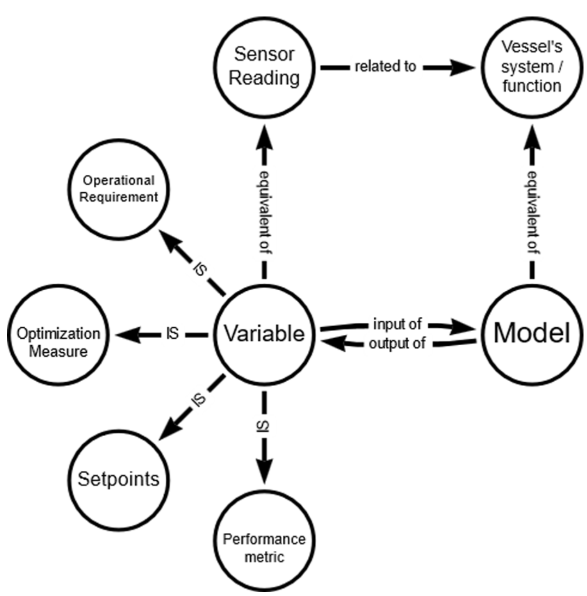
Linking Physical Assets, Digital Assets, and Domain Concepts

In the following sections it is provided a detailed description of the KG. However, in higher level, the underlaying schema of the knowledge graph and it's linkage to the operational metamodel, is shown in Figure 2

Main classes of the knowledge graph are the predictive models and the corresponding vessel's systems, in two "parallel" structures. In addition, variables, that are model's inputs and outputs are correlated to actual vessel sensor reading, composing the digital twin and the digital shadow, respectively.

Despite that the functional metamodel, described in section 3, is a conceptual model, it is applicable to lower, functional levels being part of the knowledge graph. Each node, such as operational require-

Figure 2. The underlaying schema of the knowledge graph



ments, optimization measures, etc are classes of variables which are interconnected to Model's inputs/outputs and vessel sensor reading. For example, vessel speed is an operational requirement, connected to the corresponding sensor's reading and input/output of one or more prediction models.

The knowledge graph is also used to detect which models should be utilised and their execution sequence in order to conduct a calculation given the provided inputs and requested outputs. For this functionality model library includes all required model properties to enable automated model selection. This functionality provides a solution to address the diversity of model that may exist in a library especially within the context of co-simulation.

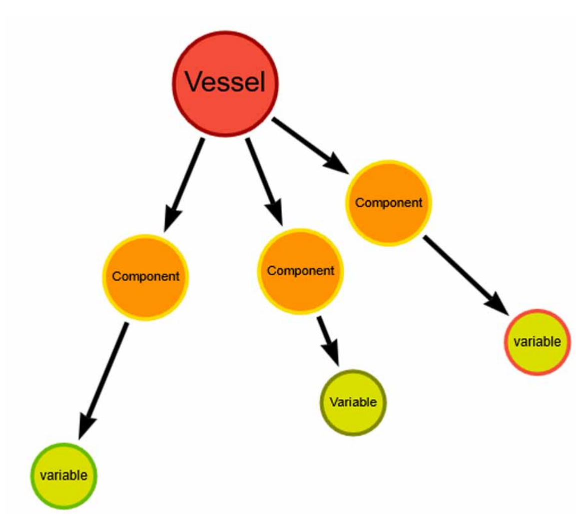
The Vessel Domain Model

Data used to build the digital twin, needs to be based on some reference schemas. Standardization speeds up the adoption of digital twinning. Standard industry-wide schemas need to be introduced, while for data types that are shared within different domains (e.g., geospatial data) existing models can be utilised. Ship data models are used by classification societies and provide an important baseline in this area. A notable example is the DNV Functionally Oriented Vessel Data Model (DNV n.d) based on a hierarchical ship's functions structure, a library of components and interrelations between functions and components, adhering to ISO 15926A (ISO, 21003) principles.

Ontologies have become a standard for knowledge representation across several domains (Rodríguez-Revello et al, 2023). In maritime in particular, ontologies have been utilized for solving collision situations at sea (Hatlas-Sowinska, 2023) and for knowledge extraction for shipyard fabrication workshop reports (Hiekata et al, 2010).

In our approach, we define an ontology layer to represent vessel functions and their corresponding variables, and secondarily, other domain-related concepts such as fuels, weather, voyages, and more. This ontology layer is also encoded in the Knowledge Graph, aiming to support interoperability between DT models.

Figure 3. Vessel components/functions and variables ontology layer



Vessel Components and Functions Metamodel

The term "Functions" refers primarily to 'vessel functions', i.e., the ability to perform or prevent certain actions. Examples are structural integrity, anchoring, propulsion, navigation and fire prevention. However, the term Function is also used in a broad sense covering elements such as administrative items and compartments. While building a DT, we consider for a collection of every function that we are interested in, such as pumping, the main engine, the auxiliary engines, but also green functions such as heat recovery, wind assistance, etc.

Some functions may be applicable to decarbonization solutions. For example, hull coating (silicon hull paints) or energy saving devices (Gaggero &Martinelli, 2021), such as propeller boss cap fins can be characterized as decarbonization technology. This information is included in the knowledge graph either as a property or preferably by linking the relevant nodes.

Variables

Associated to each function, there are variables that describe the condition, performance, or status of the functionality. For example, the exhaust gas heat recovery function is described by gas mass rate and temperature, exchanger inlet and outlet temperature etc. There exist variables that instead of being related to a "function/component" node, are related to elements of the graphs described below, for example "significant wave height" of the weather-related graph, or "required speed" of the "Charter Party Agreement" graph.

Vessel Particulars

Vessel geometrical properties, tanks sounding tables, deadweight scale, and other information that is required input for simulation models.

Operational References

This aspect of the knowledge graph encodes various reference conditions related to vessel operation, categorized by component, i.e., M/E, DGs, boilers, hull and by source:

- Official Tests
    - Shop test
    - Sea trials
    - Maker reference
- User reference
    - Based on trials
    - Based on data analysis
- System
    - Model weights
    - Constants library

Fuel Information

Graph including available fuel types, properties, prices and ports availability.

Shipping Sector Information

- Commercial practices
  - Charter Party Agreement (CPA) terms
  - Company common practices
  - Ports – vessel interaction (required paperwork, info exchange).
- Voyage particulars
  - events/operations
- Regulations
  - CO_2 SOx NOx emissions metrics
  - Discharged water/wastes
  - ECAs
  - Safety
  - Ballast treatment
- Cargo related information
  - Cargo categorization, locations, and freights
- Infrastructure
  - There exists relationship with other classes for example, bunkering locations are also referenced in the fuel graph.
  - Terminals (container, refinery, passengers, vehicles)

Weather

Weather services providers and linkage to the weather related variables.

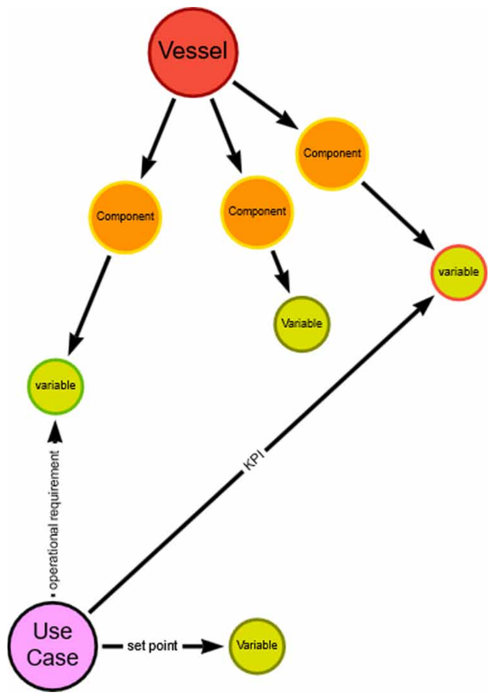
Encoding Use Cases Into the Knowledge Graph

As per the operational metamodel, a use case comprises requirements, setpoints, and metrics. Figure 4 illustrates the encoding of use cases in the knowledge graph. Relevant variables are associated with the use case using corresponding relationships such as “operational requirement”, “setpoint”, etc.

The Models Layer of the Knowledge Graph

In a digital twin framework, the ability to simulate various operational and environmental scenarios plays a crucial role. This dynamic digital representation requires the integration of advanced simulation models to mirror the real-world behavior of vessels, their interactions with the environment, and the myriad of operational conditions they encounter. By registering simulation models into the framework, the system can predict outcomes, optimize operations, and enhance decision-making processes with accuracy and efficiency.

Figure 4. The relationships of a use case with the variables of the ontology encoded in the KG



The knowledge graph is used to store the available models metadata and more importantly, the relation of model inputs and outputs with the variables of the vessel domain model, presented previously. shows the graph related to the operational phase where the model is used to predict component operation.

Figure 5 shows a model that has as an input a variable and its output is fed as input to another model estimating the final variable. It is also shown an alternative model that estimates the final variable, using only the first variable, ignoring variables related to the component in the middle. In Figure 5 (b) and (c) is shown model instantiation for a vessel, which is discussed in the next section.

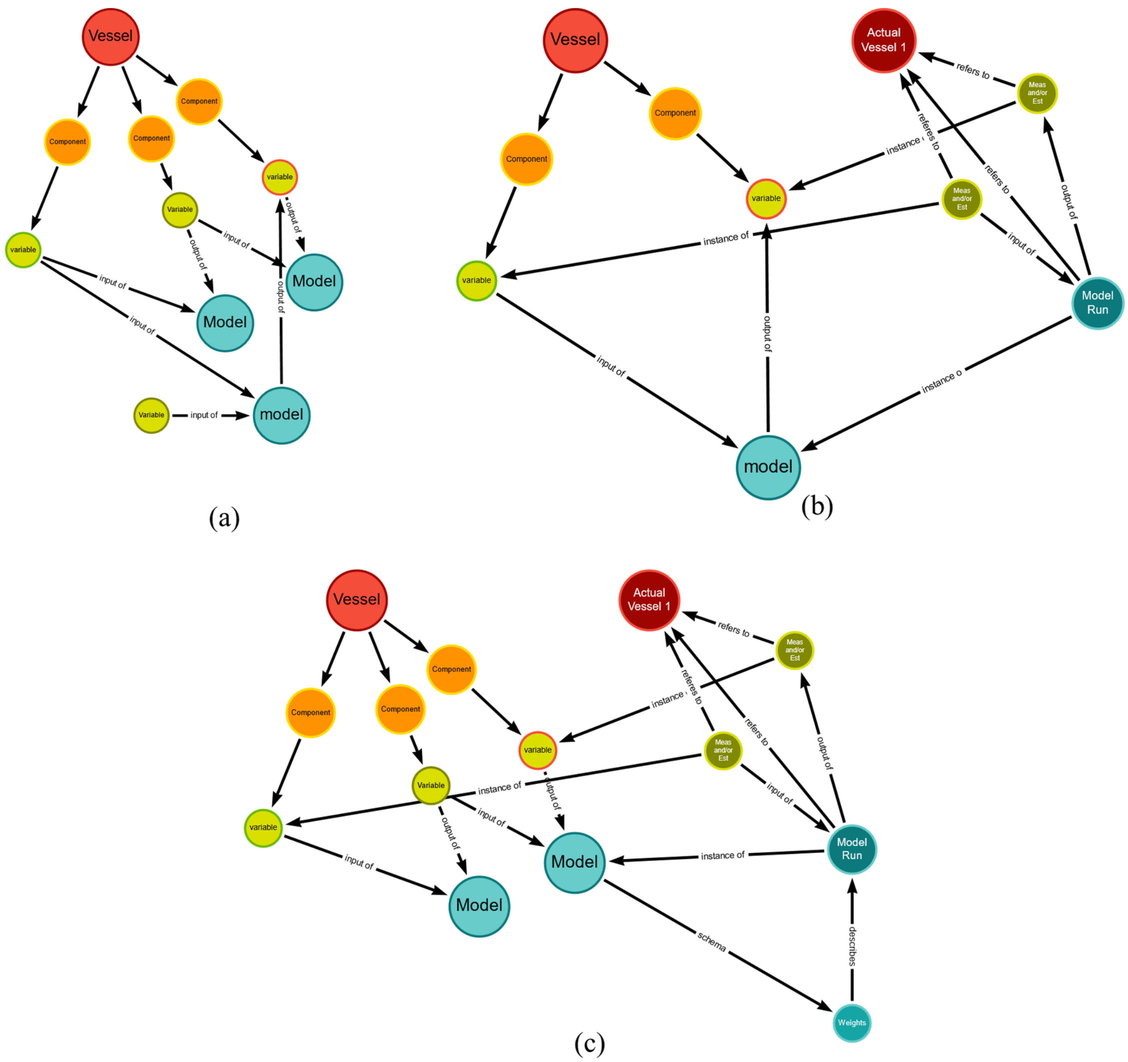
The Layer of Vessel Instantiation: The Incorporation of the DT

The vessel domain model may include all vessel functions and variables that can be considered. However, these may not be applicable to every application of vessel. On the other side one vessel may have multiple instances of a single item.

In this position it is introduced the instantiation of a vessel. A new node, shown in dark red in Figure 5, representing the actual vessel is created in the knowledge graph. New entities, shown in dark green represent the actual measurements, instances of the variables of the generic model.

The focus so far has been on the theoretical components, e.g. variables not related to a specific vessel or measurements. Now, we shift our attention to an instantiation, which involves a specific vessel equipped with various components. Measurements that describe the operation of these components are explicitly linked to relevant variables in the knowledge graph. This establishes a reliable reference for understanding the nature of these measurements.

Figure 5. Models and their relationships within the KG (a) Connections with the ontology layer, (b) instantiation of a model for a specific vessel, (c) automated modification of models' instantiation after change of vessel assets

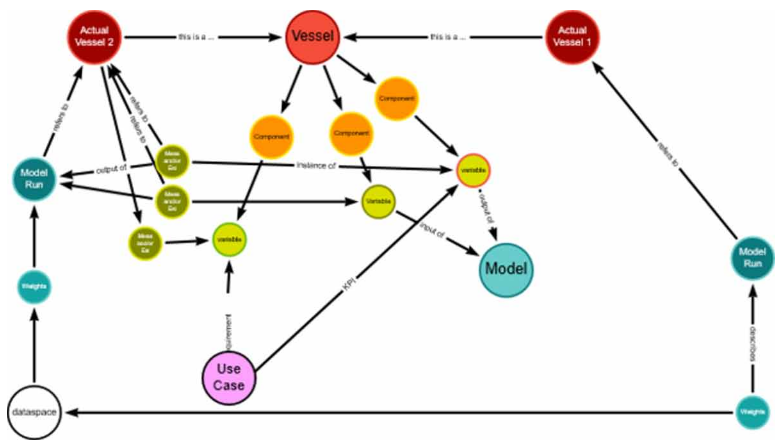


The nodes within the scope of the DT serve a dual purpose: they house both the actual measured values and the simulated values, that stem from the execution of the corresponding model.

Knowledge Graph for Digital Twin Linking

The utilization of the knowledge graph, which connects different aspects and instances through the ontology layer, offers a notable advantage in terms of transferring knowledge across DT.

Figure 6. Knowledge transfer in terms of simulation model weights in different vessel via the dataspace



In the example of Figure 6, there are two vessels, one of which is equipped with a new green technology. A simulation model is tuned to accurately predict the effect of this technology on vessel performance, based on the specific use case. The knowledge graph provides the opportunity to identify interdependencies and enables the conditional utilization of the model weights in the second vessel, which is not equipped with the green technology. This 'knowledge transfer' allows for the evaluation of the green technology on the second vessel.

Model Pipeline Creation Using the Knowledge Graph

Part of our research objective is the development of a framework capable to accommodate a wide context in terms of decarbonisation technologies and applications, intended to provide a unified representation of vessel operational aspects.

To achieve these two objectives, it is required to constantly produce and consume the available knowledge. However, this is complicated, especially when considering the models that are available. A solution suggested to address these difficulties is using knowledge graphs at the metalevel of the models. Including model blueprints into the knowledge graphs and connecting model inputs/outputs with the variables of the ontology layer it is achieved to provide a semantic layer to the user and tune system operation by detection of the shorter model execution path.

The knowledge graph stores a register of variables and a library of models used in the DT. Model inputs/outputs are related to the variables of the register. Vessel measurements are also related to variables of the register and models are instantiated for specific vessels.

When the DT is required to simulate vessel operation, it is required to determine a model pipeline, in other words model sequence, which will be executed for the estimation of the required variables (outputs) using the available variables (inputs). The input and output variables are determined by the use case described in previous sections.

For the detection of the model pipeline, the knowledge graph is employed. Since the models are connected to the ontology variables with "input of" and "output of" relationships, the interconnections between models can be inferred. In the knowledge graph is stored which variables have a known value and which are the outputs. Therefore, a special query at the knowledge graph can return the model sequence required to calculate the outputs based on the available inputs.

In addition, it is possible to assign a computational cost metric and accuracy metric. Technically, the metrics are attributed to the relationships rather that nodes. Then, a query can be applied to provide the "shortest path" considering the weights defined by the application (accuracy vs execution time).

A SAMPLE APPLICATION OF THE APPROACH

The Application of Variable Frequency Drives for Cooling System Optimization

Historically, the design and construction of marine vessels did not prioritize the energy efficiency of auxiliary systems, leading to the implementation of systems on existing ships that lack optimization for reduced fuel consumption. This trend persists, with many ships still being constructed without a significant focus on energy-efficient solutions. Furthermore, shipyards often overlook the long-term ownership costs associated with vessels. In the absence of specific owner demands for incorporating certain technologies into the design specifications, the energy efficiency potential of these ships remains underutilized, despite the fact that investing in additional equipment could result in substantial savings within a year. Currently, many marine installations adjust for environmental fluctuations using inefficient methods like 'throttling' and 'by-pass loops'.

Shipboard systems that offer significant opportunities for enhancing energy efficiency include those with large pumps and fans, which do not need to operate continuously at maximum capacity. Equipping electric motors with Variable Frequency Drives (VFDs) can lead to more efficient operation of pumps and fans under partial load conditions, such as during reduced-speed sailing or when there is less need for ventilation. The electrical power usage of a pump correlates with its volumetric flow rate as per the affinity laws. Decreasing the pump's speed results in a squared reduction in system pressure (Head) and a cubed decrease in electrical power consumption. For instance, reducing the pump's speed by 10% can lead to a 27% reduction in power usage (Inal et al,2023).

The cooling water system aboard a vessel, primarily composed of pumps, stands as a significant energy consumer on ships. Seawater serves as the primary coolant for the machinery within the engine room. A typical oceangoing merchant vessel's central cooling water system is divided into three subsystems: the seawater (SW) cooling system, the low-temperature fresh water (LTFW) cooling system, and the high-temperature fresh water (HTFW) cooling system. The SW system uses seawater to cool the LTFW system's fresh water, while the LTFW system, in turn, cools the HTFW system. Each of the three systems—SW, LTFW, and HTFW—has two dedicated pumps, all of which are electrically powered. The pump capacity is dictated by the ship's size and the main engine's power output.

Ship systems must operate within a highly dynamic environment, with the central cooling water system particularly affected by this variability due to fluctuations in engine load, seawater temperatures, and LTFW side cooler temperatures. Engine load variations are often a result of maneuvering conditions, such as when navigating at full speed or slowing down in narrow passages, channels, straits, and during berthing. Additionally, since ships traverse international waters, they encounter a wide range of climates and seawater temperatures, directly impacting the central cooling water system.

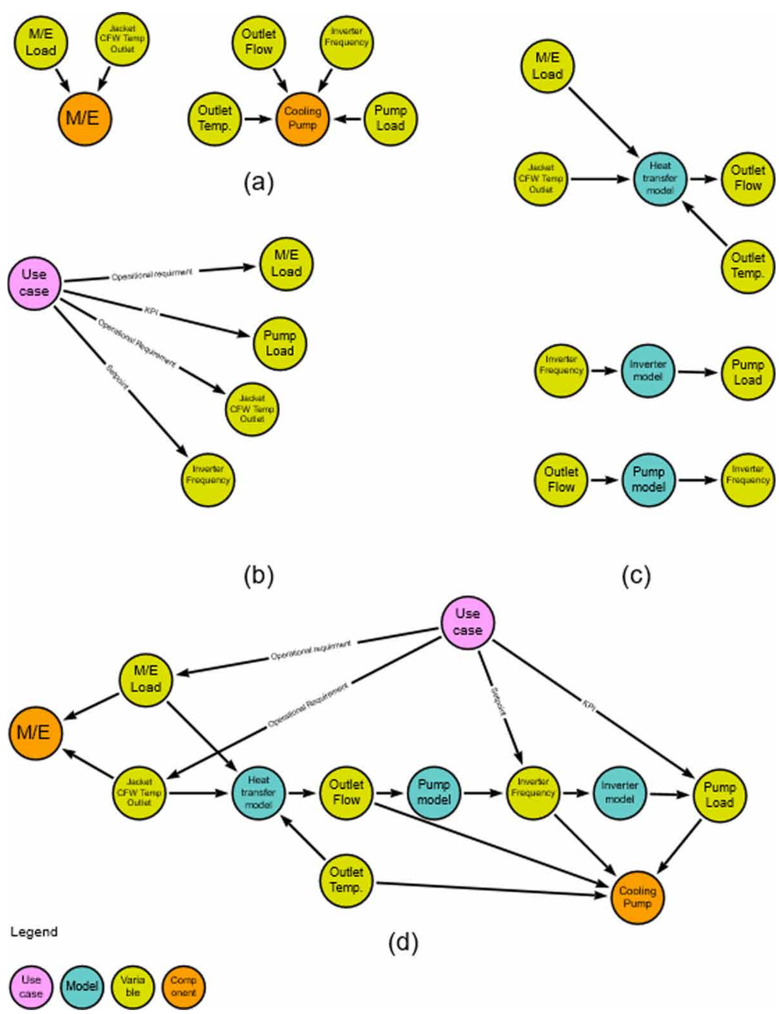
The cooling system of a ship is engineered to function under extreme conditions for safety reasons. Under these design conditions, the pumps operate at full capacity, constant speed, and constant mass flow rates regardless of the ambient conditions. From an energy efficiency standpoint, this results in suboptimal performance when conditions are not tropical. Typically, temperature regulation of the fresh water in varying environmental conditions is managed by bypassing the water. However, adjusting the mass flow rate of the seawater pumps in response to changing seawater temperatures can lead to substantial energy savings. Implementing variable speed seawater pumps could achieve this efficiency.

Knowledge Graph Entries for Cooling System Optimization

The foundational layer of the knowledge graph is dedicated to the vessel domain model, encompassing the components and functions being analyzed, as well as the variables necessary to characterize their operations.

Concentrating on the High Temperature Fresh Water Cooling System, to enable Digital Twin adaptation it is essential to incorporate into the knowledge graph the Main Engine (M/E) and variables such

Figure 7. Knowledge graph nodes related to the cooling system optimization use case



as the engine's load and the jacket cooling water temperature, Figure 7(a). Given the Main Engine's critical role within the vessel, it is likely that the M/E, along with a wide array of variables detailing its functioning, would be cataloged within the knowledge graph for many other use case as well. Apart from the M/E, Cooling pump and variables such as outlet flow rate, outlet temperature, load, and operational frequency (define by the VFD) should be registered into the knowledge graph.

Next, we encode the use case into the knowledge graph, as illustrated in Figure 7(b). This involves integrating specific operational scenarios or examples into the knowledge graph structure. For the mentioned use case, the "M/E load" and the "jacket cooling water temperature" are identified as operational requirements. This means that the specified values for these parameters—such as a certain load level for the engine and a specific temperature for the cooling water used in the engine's jacket—need to be adhered to or maintained within certain limits during the operation of the vessel. The resulting load of the pump is the "KPI" and the operating frequency is the "setpoint". In other words, this use case outlines a scenario where the objective is to determine the optimal frequency for an inverter to minimize the pump's load while ensuring that the Main Engine operates at a specified load and the temperature of the jacket cooling water remains below a predetermined threshold.

Finally, we register the simulation models required to conduct these calculations. We have (i) a heat transfer model that correlates engine power with coolant water inlet and outlet temperature (ii) a mode for the Variable Frequency Driver and (iii) a mode for the pump.

Model Pipeline Creation for the Cooling System Optimization Use Case

Upon integrating the "use case," "model," "variables," and "component" nodes into the knowledge graph, the system employs resolvers to link these nodes through common connections and relationships, effectively weaving a comprehensive network as depicted in Figure 7(d). This enriched graph facilitates the identification of the most efficient pathways between nodes, enabling the formulation of a shortest path query that delineates the optimal sequence of models necessary for computational analysis. The outcomes of this query are then channeled into the model execution orchestrator. This orchestrator manages the simulation models, ensuring flow of data by coordinating the exchange of input and output variables among the models, thereby driving the simulation process towards achieving the calculations.

DISCUSSION AND FUTURE OUTLOOK

The Chapter has introduced a new approach to managing issues of heterogeneity and integration in DTs, using knowledge graphs. Heterogeneity pertains to both data and models used for simulations and underpinning the behaviour of DTs. In other words, data need to be connected to the right models. And models to each other in order to achieve dynamic and realistic behaviour of the DT. The Chapter has demonstrated that knowledge graphs can support the above, due to their flexibility and technology neutrality.

DT data can be correctly linked to class nodes in the knowledge graph and then be discovered by the data consuming models by following links. Different models can be interlinked via input-output data linked via the knowledge graph. Therefore, the knowledge graph acts as a semantic integrator of data and models in the DT.

In DT research and despite the promising potential of DTs in shipping, several challenges persist. Key among these are issues related to data standardization, ensuring different systems can work together (interoperability), and achieving a uniform data language among various parties involved. Tackling these challenges is crucial, and the focus of this chapter is on them. (Fonseca & Gaspar, 2021) discuss the challenges involved when creating a DT, from a data modeling perspective. Amongst such challenges they highlight the lack of digital twin ship data standardization and of open data platforms. They argue that as similar to how web services were standardized, a neutral core data standard for digital twins could be defined and used as the basis for an ecosystem of heterogeneous tools, and platforms and connection to external services and applications. Additional obstacles to the creation of a cohesive DT for ships include the tradition of siloed software systems and the general data handling practices in the maritime sector.

Another challenge pertains to the construction and utilization of the Knowledge Graph. More specifically the challenge refers to the effort required to construct a large scale and ship specific Knowledge Graph. General-purpose knowledge graphs are characterized by large scale, wide breadth, and a high degree of automation and openness. However, their depth is shallow, their accuracy is relatively low, and the degree of reasoning is weak, so it is difficult to directly use them for a specific industry. (Zhang et al, 2019)

Towards creating a domain specific knowledge graph automatically, or semi-automatically, some research approaches have been proposed. Diamantini et al (2023) present an approach where an ontology describing the fundamental elements involved in Industrial Internet of Things (IIoT) and their relations, is used for the construction of a Process-aware IIoT Knowledge Graph, where raw sensor data are enriched with information about process activities and the physical production environment.

Ontologies therefore can play a pivotal role in constructing domain specific knowledge graphs. For instance, in (Zhang et al, 2018) an ontology is developed to model knowledge of ship behaviour. However, integrating different ship ontologies (represented as knowledge graphs) and their concepts also presents its unique challenges. Therefore, approaches for the synthesis of multilevel knowledge graphs (Man et al, 2023) could be employed. Also, tools such as the one described in (Rodríguez-Revello et al, 2023) that extract concepts from existing ontologies and automatically construct draft ontologies could be utilised.

In summary, this Chapter has highlighted the potential of knowledge graphs to underpin the management of digital twin data and shipping and support the pipeline execution of heterogeneous ship models, thus paving the way for an industry wide adoption of DT technologies.

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Chapter 4
Towards Intelligent Ship-Edge Computing Enabling Automated Configuration of Ship Models and Adaptive Self-Learning

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ABSTRACT

Edge computing is a solution that prioritizes data processing for low-latency and specialised applications, particularly those involving complex and mission-critical processes. An ideal example of an edge device is a ship, which heavily relies on its onboard computing capabilities to autonomously perform various navigation tasks. The transportation sector, including shipping, has witnessed the emergence of software-defined vehicles where sensor data, analytics, and algorithms play a pivotal role in optimising operations such as propulsion, cargo handling, energy management, communication, and human-machine interactions. This chapter delves into the significance of edge computing in the shipping industry, outlining its ability to enhance operational efficiencies. It explores the specific user requirements for an effective edge computing solution and highlights the role of AI in enabling scalable and continuous computation. Additionally, the chapter provides a comprehensive overview of edge infrastructure, platform requirements, and considerations pertaining to data and AI at the edge. The discussion incorporates the Mayflower autonomous ship as a case study, illustrating the criticality of edge computing for the future of shipping.

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INTRODUCTION

Edge computing is an architecture rather than a specific technology. It provides a framework for distributed computing that aims to bring enterprise applications closer to data sources such as local edge servers or IoT devices. By being in close proximity to data sources, edge computing provides several benefits, including faster insights, improved response times, and improved bandwidth availability. It is a response to the increasing demand for large-scale data processing at the edge, and the need for resilience to network disruption.

While this data-centric approach offers many mission-critical benefits, it is crucial for edge computing to exist as part of a cloud continuum that allows stakeholders to interact with data and processes it in a unified way. This ensures that edge computing is integrated seamlessly into existing cloud infrastructure, enabling a unified and cohesive approach to data processing and management.

EDGE COMPUTING OVERVIEW

Edge computing minimises latency by bringing computational workloads closer to the data source and the location where actions need to be taken – removing the distance between collecting data, processing it, and making those results available for use in decision making. Data is generated from diverse sources and at different scales, encompassing equipment, devices, individuals, and processes.

The concept of edge computing is closely intertwined with cloud-native development and decisions regarding where computational tasks should be executed. It prompts considerations on which data should be transmitted back to the cloud for further processing.

Telecommunication providers often refer to the network edge, which offers a chance to deploy edge infrastructure and leverage communication capabilities, particularly with technologies like 5G. This presents an opportunity to enhance edge capacity and optimize the utilization of communication resources.

The integration of compute capabilities into modern industrial equipment has opened up new possibilities for performing a wide range of tasks. For instance, cameras on assembly machines can be utilized for quality control analytics. Production processes can be optimised, comprehensive management of distribution centres becomes feasible, and software containers can be deployed in a suitable runtime environment enabling elastic scalability.

However, managing these deployments poses significant challenges. With an estimated 15 billion devices worldwide, enterprises must oversee the provisioning, deployment and ongoing management of thousands of devices, each with different specifications, purposes, operating systems, and workloads. While the provisioning process can be done in a controlled environment to ensure full compliance, security becomes a major concern as these devices operate outside the traditional confines of IT data centres. They lack the typical safeguards found in hybrid cloud environments, such as physical barriers and the uniformity required for certification. Ensuring the integrity and preventing tampering of edge devices becomes paramount.

To support the growing role of edge computing, it is crucial to build an ecosystem that facilitates its development. The impact of edge computing on enterprise computing is expected to be substantial, comparable to how mobile technology has transformed the consumer sector.

Cloud vs. Edge Computing

The primary difference between cloud computing and edge computing is the location where data processing occurs. In cloud computing, data is processed on a central cloud server, which is usually located far away from the source of information. Traditionally compute took place on centralized cloud services such as Amazon EC2 instances. Hybrid cloud is a mixed computing environment where applications are run using a combination of computing, storage, and services in different environments—public clouds and private clouds, including on-premises data centres or edge locations.

Hybrid cloud computing approaches are widespread because almost no one today relies entirely on a single public cloud. Hybrid cloud solutions offer the flexibility to seamlessly migrate and manage workloads across diverse cloud environments, empowering organizations to tailor their infrastructure to meet specific business requirements. By adopting hybrid cloud platforms, organizations gain the ability to lower costs, mitigate risks, avoid vendor lock-in, and leverage existing cloud-native developer skills and CI/CD pipelines to drive successful digital transformation initiatives.

In today's landscape, the hybrid cloud approach has become a prevalent infrastructure setup. As organizations undergo cloud migrations, hybrid cloud implementations naturally emerge, enabling a gradual and systematic transition of applications and data. With hybrid cloud environments, enterprises can continue utilizing on-premises services while harnessing the advantages of public cloud providers like AWS, Azure, and GCP, which offer flexible options for data storage and application access (Google, n.d.).

Edge computing extends the hybrid cloud paradigm to address the unique requirements of enterprise and consumer applications. Although they possess individual traits, edge computing and hybrid cloud can collaborate to establish a comprehensive and adaptable computing infrastructure. A notable aspect of contemporary edge computing solutions is their adoption of cloud native development practices specifically designed for the edge. By leveraging cloud native development practices, applications can be built and deployed using the same skills and tools that have been honed for developing cloud native applications in hyper-scale cloud environments or private data centres. This allows for the seamless extension of these practices to the edge, enabling organizations to leverage their existing expertise and resources for edge computing deployments.

Hence, aspects such as distributed computing, data processing, management, and integration, as well as workload placement and optimisation are enabled in an accelerated and scalable manner.

Concept and Technology

Edge architecture encompasses all the active components of edge computing, including devices, sensors, servers, and clouds, spread throughout the network wherever data is processed or utilized. By bringing processing closer to the data source, edge architecture significantly reduces latency and cost: applications and programs running at the edge can swiftly and efficiently respond to user interaction and data without the need for transferring data across a wide area network, resulting in an enhanced user experience and optimal overall performance.

The definition of the "edge" is flexible and context-dependent. For example, in the case of a shipping company, the edge may encompass activities at docks where shipments are loaded and unloaded, or it may include on-board processing of ship systems and operations. In both scenarios, processing and analysis occur in near real-time, leading to data-driven decision-making. While the company's headquarters with the main data centre may be located miles away, the edge represents the crucial point where data is collected, processed, and managed to derive insights, irrespective of latency challenges.

Why Edge Computing in the Maritime Industry

Ship transport accounts for over 80% of global trade in goods and raw materials, making the efficiency and speed of large container ships critical to the value chains and production processes of countries worldwide. However, the environmental impact of shipping, including emissions, fuel efficiency, and noise pollution, is becoming more apparent. To address these concerns, emerging technologies like artificial intelligence (AI) and digital twin are being leveraged to improve the efficiency, management, and environmental sustainability of shipping routes.

Whilst digitalisation of the transport sector is key to unlocking efficiencies, this is currently hindered by data silos, technological limitations, and barriers of complexity. DT4GS promises to enable stakeholders in shipping to actively embrace the full spectrum of Digital Twins innovations to support smart green shipping in both the upgrade of existing ships, as well as the building of new vessels.

These solutions will be deployed across the cloud continuum from centralized public cloud services to decentralized edge computing devices. At one end, ship owners and stakeholders can leverage public cloud services provided by major cloud providers that offer centralized computing power and storage resources that can be accessed from anywhere. On the other end, edge computing will be deployed closer to where the data is generated to provide compute at every step of the ship system. This provides unique benefits and advantages in terms of data sovereignty and security, resilience to outages and connectivity constraints, innovation opportunities and flexibility to different providers, as well as inherent autonomy that are critically important to shipping.

There are multiple complexities inherent to ship operations and decision making. Whilst the central complexity may be the difficulty and uncertainty inherent in decision making in the ocean, there are multiple technological challenges to overcome:

- Scale: There are thousands of ships with limited or no technical expertise on board. The solutions implemented must be self-healing and turn-key, requiring minimal intervention and maintenance.
- Heterogeneity: Each ship represents a dynamic and unique environment, making it challenging to find a one-size-fits-all model. Solutions need to be adaptable and flexible to cater to the diverse needs and characteristics of each vessel.
- Data Gravity: Ships and their instruments generate vast amounts of logs, events, and metric data, often in different formats. Additionally, the sensitivity of some of this data adds another layer of complexity. Handling and processing this data in a secure and efficient manner is crucial.
- Resource Constraints: Ships serve as the ultimate edge nodes, characterized by limited communication, computational, and energy resources. These constraints must be considered when designing solutions, ensuring they can operate effectively within the ship's resource limitations.

Fundamentally, edge and cloud technologies promise a solution that seamlessly infuse AI and simulation across the entire spectrum of shipping operations. Agnostic of connectivity or compute capabilities, it provides a continuously available digital assistant to guide all aspects of decision and automation.

AI can assist Captains and crew to make better decisions by seeing things humans overlook or don't fully recognize; by assessing alternatives they may not have considered; by evaluating and optimizing choices with more mathematical precision than can be accomplished by the human mind alone; by reacting to events in real-time and at a rate that is much higher than is humanly possible. Perhaps the AI can pre-empt these crises from emerging. And the holy grail of these potential advantages is to inspire decision-makers to ideas they might not have produced on their own.

Doing so promises to improve decision-making, which in turn will improve operational efficiency, safety, and decrease burden. With AI we can reduce the current carbon footprint of transporting goods across the oceans. We can incur fewer accidents, limit cargo damage and loss, and most importantly make maritime travel less risky.

To do this, we need to harness the power of AI to recognize dangers, evaluate alternatives, and present recommendations in the decision-making process. We need to incorporate AI into the human decision processes. In essence, the AI needs to act as another member of the crew, offering interpretation, advice, and warnings as appropriate to provide meaningful contribution to how crew leaders and the Captain make their decisions. Easier said than done.

A prominent example in this regard is the Mayflower Autonomous Ship (MAS400) (Kıcıman et al., 2023; MAS, n.d.). The MAS400 vessel was built without any provision for humans on board and must make all navigational decisions on its own. It uses an array of visual and other signal input to sense its environment. AI is used to perceive and interpret what it "sees". It classifies a wide range of objects and determines whether they are an obstacle to its current course. It establishes potential strategies for navigating around them, and evaluates each for their safety, conformance to regulations, and optimization. And then, of course, it puts those decisions into action – controlling rudder and speed to achieve the outcome it has determined.

However, a potentially larger and more immediate use of this technology is not for vessels that drive themselves all over the world, but rather to assist sea Captains in their own navigational and ship operations responsibilities. One of the lessons from the Mayflower project is that sometimes you do need a human on-board – to fix a broken manifold coupler to the auxiliary engine, or to repair the electrical connection that has frayed and causing a short. And with human lives at risk, you need humans that have the authority and responsibility for protecting those lives – for making the critical decisions necessary to fulfil their mission safely.

STATE OF THE ART IN EDGE COMPUTING

A forecast by International Data Corporation (IDC) estimates that there will be 41.6 billion IoT devices in 2025, capable of generating 79.4 zettabytes (ZB) of data (Hojlo, 2021). The latency advantages of edge computing provides obvious appeal to extract insight from these vast volumes of data. However there are also multiple other considerations driving edge adoption including security, operational costs, resilience, and flexibility (Rathore et al., 2022).

The global edge computing industry is experiencing rapid growth, driven by advancements in technologies such as 5G, IoT, and the Industrial Internet (Rathore et al., 2022). Edge computing entails extending a consistent computing environment from the core datacentre to physical locations in close proximity to users and data. Similar to a hybrid cloud strategy that enables organizations to run workloads across their own datacentres and public cloud infrastructure, an edge strategy expands the reach of a cloud environment to numerous additional locations. This approach allows for a more widespread and distributed computing infrastructure, bringing computing capabilities closer to the edge for enhanced performance and responsiveness.

There are three categories of edge use cases (Schabell, 2022):

- The first is called enterprise edge, and it allows customers to extend application services to remote locations. It has a core enterprise data store located in a datacentre or as a cloud resource.
- The second is operations edge, which focuses on analysing inputs in real time (from Internet of Things sensors, for example) to provide immediate decisions that result in actions. For performance reasons, this generally happens onsite. This kind of edge is a place to gather, process, and act on data.
- The third category is provider edge, which manages a network for others, as in the case of telecommunications service providers. This type of edge focuses on creating a reliable, low-latency network with computing environments close to mobile and fixed users.
- For industry applications, edge computing capabilities can be decomposed into two categories:
- **Edge Server**: This typically refers to IT equipment specifically designed for computing tasks at the edge and operating as an extension to the computation tasks performed in the cloud. It can take the form of a half rack comprising 4 or 8 blades, or it can be an industrial PC. Essentially, it is a piece of IT equipment dedicated to edge computing operations.
- **Edge Device**: An edge device is a piece of equipment built for a specific purpose, such as an assembly machine, a turbine, or a car. While these devices were initially designed for their primary functions, they also possess computing capacity. In fact, many devices that were traditionally considered IoT devices now incorporate increased computational power. For instance, an average car today is equipped with approximately 50 CPUs. These devices often run on the Linux operating system, allowing for the deployment of software containers, and enabling edge computing applications to be executed directly on the devices themselves.

Deploying workloads across both cloud and edge resources presents several fundamental challenges for technology solutions:

- Consider the scale of the challenge at hand. With an estimated 15 billion devices in the world today, enterprises are faced with the task of managing thousands of devices within their operations.
- Heterogeneity at the edge poses another significant factor to address. These devices come in various forms, each serving a different purpose and running on different operating systems. Managing the diverse range of devices and the specific tasks they perform can be a complex endeavour.
- Security is a critical concern when dealing with edge devices. Unlike traditional IT data centres, these devices operate outside the confines of controlled environments. They lack the physical barriers, uniformity, and consistency typically found in hybrid cloud environments that aid in ensuring security. Protecting edge devices from tampering and unauthorized access becomes a priority.
- Building a robust ecosystem is essential. The role of edge computing is rapidly expanding and will have a profound impact on enterprise computing, much like how mobile technology has influenced consumer behaviour. Establishing a comprehensive ecosystem that integrates and supports edge devices and their functionalities will be crucial for organizations to maximize the benefits and potential of edge computing.

- Maintenance and ongoing support presents some unique challenges. Software and AI components are complex and require period patches and updates. Software performance can also be impacted by environmental conditions. Having a rigorous approach for software life-cycle management and drift detection is essential to achieve optimal performance and avoid catastrophic failure where nearby IT support personnel is not available.
- Ensuring data privacy throughout the deployment process is essential to safeguard sensitive information against data breaches, regulatory compliance, and to enhance public trust within organisations. As workloads are distributed across diverse and interconnected environments, ranging from public clouds to edge devices, the potential attack surface widens significantly. Adhering to stringent data privacy measures becomes imperative to mitigate risks associated with unauthorized access, data leakage, and malicious activities.
- The strategic placement and optimization of workloads play a pivotal role in maximizing performance, minimizing latency, and optimizing resource utilization. The deployment of workloads across diverse environments, encompassing cloud data centres and edge devices, presents unique challenges and opportunities. By harnessing the power of intelligent workload orchestration, organizations can unlock the full potential of their computing infrastructure, ensuring optimal performance and resource allocation while seamlessly catering to the unique requirements of individual workloads.

FULL STACK EDGE SOLUTION

Edge solutions require multifaceted capabilities, including the orchestration of heterogeneous workloads, creation of a scalable, extensible, and robust data management pipeline, and seamless deployment of data inference and AI on the edge. The latter consideration is especially critical as many organisations become AI-driven enterprise and infuse generative AI capabilities across their operations (Yusuf, 2023). The requirements of workload orchestration, data operations, and AI infusion, include:

- **Edge orchestration:** A fundamental requirement is to enable seamless deployment of containerised applications to multicloud and edge environments. Deploying on 1000s of nodes in a scalable, replicable manner requires deep automation for advanced management of 1000s of different software applications across 1000s of compute nodes distributed across the entire footprint of an organisation's operating remit. Solutions such as Open Horizon (Open Horizon, 2023) enables the autonomous management of more than 10,000 edge devices simultaneously. Core architecture considerations include:
  - The provisioning of Open Horizon includes the management hub that runs in an instance of OpenShift Container Platform installed in the data centre. The management hub is where the management of all remote edge nodes (edge devices and edge clusters) occurs.
  - Managed edge nodes can then be installed in remote on-premises locations to make application workloads local to where critical business operations physically occur, such as docks, ships, factories, warehouses, retail outlets, distribution centres, and more.
- **Data Operations (DataOps):** Edge consist of disparate devices such as engines, propellors, hulls, berths, shipping containers, etc., that are all generating data. Resilient edge solutions require robust data management and organisational strategies for collecting and handling data, ensuring

compliance with data sovereignty regulations, and providing flexible data quality solutions facilitating the training and deployment of AI models. Further, cognisant of data latency restrictions, data processing on the edge must translate from vast volumes of raw data to digestible subsets of high-quality, high-value features that can be used for AI model finetuning and prediction. As an example, computer-vision based hull monitoring solutions generate large volumes of data, while only small subsets of this data may be relevant for guiding hull cleaning and maintenance.

- **AI Operations (AIOps):** AI-backed decision making will play a critical role in improving the sustainability, safety, and efficiency of shipping. Ship captains and stakeholders can use AI to process large data volumes and make decisions related to route selection, navigation, port arrival and logistics, weather-enforced disruption and mitigation. Further, many aspects can be fully automated such as power management, HVAC system optimisation, cargo and inventory management, predictive maintenance, crew management, and risk analytics. As AI begins to play a central role in shipping, it is critical that 1) ships possess the compute infrastructure to fully exploit these advantages and 2) the AI layer provides reliable inference monitoring mechanisms to assess model performance, detect potential errors or uncertainties, and instil confidence in the decision-making process.
- **Network Operations (NetOps)** plays a crucial role in the seamless deployment of workloads across the cloud to edge continuum. NetOps makes sure the network infrastructure is properly configured, optimized, and secured. It involves activities like network surveillance, traffic control, performance enhancement, security setup, and troubleshooting. Ship owners may ensure effective data transmission, low latency, and dependable connectivity across cloud and edge settings by utilizing NetOps principles, enabling the smooth deployment and execution of workloads. Additionally, NetOps aids in resolving issues with network resilience, scalability, and resource allocation, enabling businesses to fully utilize the cloud to edge continuum. Ultimately, NetOps serves as a crucial link that makes it possible for workloads to be seamlessly integrated and run across a range of computer platforms, improving flexibility, performance.

Edge Infrastructure and Compute

Recent years has seen the evolution and maturation of IoT technology from primarily a data collection and transmission approach, to devices with significant compute capabilities and the ability to deploy workloads to the data. In traditional IoT setups, data generated by connected devices were often transmitted to the cloud for processing and analysis. This approach worked well for certain applications but introduced challenges like latency, network congestion, and increased reliance on cloud connectivity. Edge computing emerged as a solution by bringing data processing closer to the source, enabling real-time analysis and quicker response times.

As edge matures, a critical concern for stakeholders is infrastructure considerations such as server selection for different workloads, security of distributed devices, and loading necessary software onto hardware devices to support various edge applications such as visual inspection, voice interaction, and inference.

Compute capabilities within the shipping and logistics space is an evolving state. While container ships may have some computing equipment for basic tasks such as monitoring and controlling ship systems, these capabilities are generally limited in scope and processing power. The computing infrastructure on a container ship is designed to support essential functions like engine control, navigation, communication, and safety systems.

However, it's worth noting that with the increasing adoption of digital technologies and automation in the shipping industry, there is a growing trend towards incorporating more advanced computing capabilities on certain types of vessels. For example, larger and more advanced container ships may have additional computing systems for tasks like cargo management, route optimization, and fuel efficiency monitoring.

Overall, while there may be some level of compute capability on a typical container ship, it is typically limited and focused on specific operational requirements rather than extensive computing tasks. The bulk of compute-intensive tasks, data processing, and analytics are more commonly performed in onshore data centres or edge computing systems that support the shipping operations.

Several companies offer edge solutions that provide integrated hardware and software for edge computing deployments. Some examples include:

- Dell EMC Edge Gateway provides a compact and ruggedized device designed for edge computing. It comes with off-the-shelf, pre-configured, pre-certified, ready-to-use products, for different industries or applications (Dell, 2023).
- Intel NUC Edge is a compact edge device that promises an out-of-the-box solution ideal for running any critical applications on-premise with immediate high availability (Scale Computing, n.d.).
- Microsoft Azure Stack Edge is a solution that combines hardware and software to bring AI, analytics, and IoT capabilities to the edge. It includes an on-premises appliance that can be deployed in disconnected or low-connectivity environments and integrates with Azure services for seamless cloud-edge integration (Microsoft Azure, n.d.).

When one considers compute infrastructure for shipping, it is important to consider the types of compute capabilities that may be deployed: edge servers and edge devices (described in more detail in Section 1).

Edge Platform and Orchestration

Edge, by its very nature, generally involves 1000s of devices. Hence, concepts from the data centre do not translate directly to the edge. Instead, it requires software capabilities to monitor and update a limitless number of edge devices from across the world and new security technology and protocols to keep everything safe (Hines, 2023).

An edge computing platform contains many components. These include:

- **Edge Management and Orchestration:** This component handles the management, configuration, and physical deployment of edge devices and placement of applications that will run on them. It ensures efficient resource allocation, software updates, and monitoring of edge infrastructure.
- **Security and Authentication:** Edge computing software incorporates security measures to protect edge devices, data, and communications. This includes authentication, encryption, access control, and threat detection capabilities.

- **Edge Gateway:** The edge gateway serves as a bridge between the edge devices and the central cloud or data centre. It provides connectivity, protocol translation, and data aggregation capabilities.
- **Containerization and Virtualization:** To enable portability and ease of deployment, containerisation of software workloads is critical. Software containers or virtual machines encapsulate applications and their dependencies, making them easier to manage and deploy at the edge.

Edge management and orchestration are critical components of edge computing. Edge management refers to the management of edge devices, including device provisioning, configuration, and monitoring. Edge orchestration refers to the management of network resources across an edge network by controlling how network resources flow between devices and applications in an edge environment to produce a more responsive and smartly optimized network.

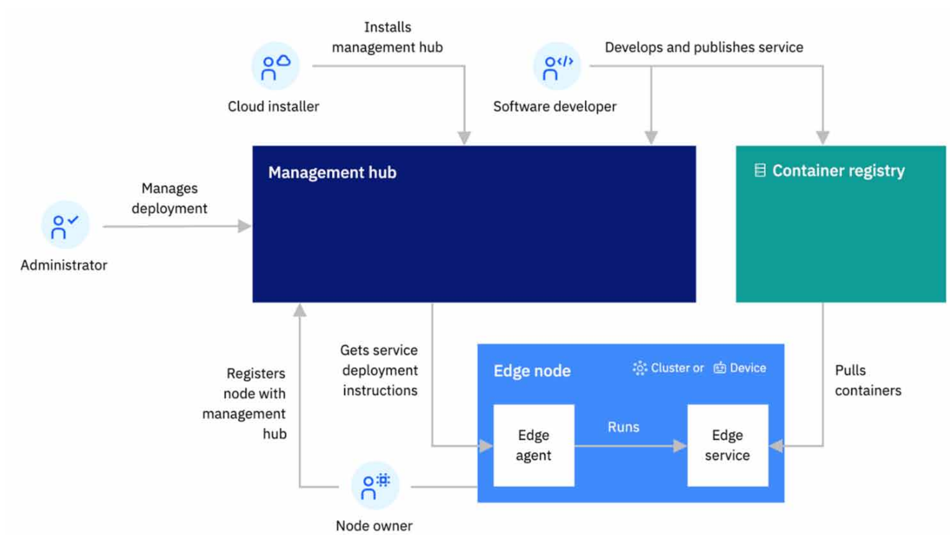
As an example, Open Horizon deploys an orchestrator called "management hub" in an instance of OpenShift Container Platform installed in the data centre. The management hub is responsible for controlling the placement of containers to all remote edge nodes, both edge servers and edge devices.

Figure 1 provides a typical edge computing architecture. The two most critical responsibilities of the orchestrator are the deployment and monitoring of workloads.

Fundamentally, the edge deployment is based on containerisation of workloads. A Cloud Operations team installs the management hub components. Specific applications are developed by data scientists and domain experts and containerised, which are then published to the management hub edge library. Administrators define the deployment policies that control where edge services are deployed.

Edge orchestrators use various monitoring techniques to ensure that edge devices are functioning correctly and that network resources are being used efficiently. Some examples of monitoring techniques used by edge orchestrators include:

Figure 1. High-level topology for a typical edge computing setup
Taken from https://open-horizon.github.io/



- Device monitoring: Monitor the status of edge devices to ensure that they are functioning correctly. This includes monitoring device health, connectivity, and performance.
- Application monitoring: Monitor the performance of applications running at the edge of the network to ensure that they are meeting performance requirements.
- Network monitoring: Monitor network traffic to ensure that network resources are being used efficiently and that there are no bottlenecks in the network. This can also include monitoring of network traffic for security threats and vulnerabilities.
- Data monitoring: Edge orchestrators monitor data flows between devices and applications to ensure that data is being processed correctly and that there are no data integrity issues.

These monitoring techniques help edge orchestrators to identify issues before they become critical and to optimize network resources for better performance. In the context of shipping, it is critical to consider "Day 0/Day 1/Day 2" of the software lifecycle:

- Day 0 activities encompass the initial definition, design, procurement and provisioning of the hardware and software solution. For factory pre-install, this stage includes the initial installation and testing of the hardware and software in the factory prior to shipping it to its final destination. Additional testing are also performed when the device is wired into the network at its final destination and powered up.
- Day 1 marks the actual deployment or launch of the software solution. It represents the first day of production use or operation. On Day 1, the software is made available to users or customers, and the system goes live. This phase involves activities such as testing, data migration, user onboarding, and initial training. The goal of Day 1 is to successfully deploy software created during Day 0 and transition from the development phase to the operational phase and ensure that the software meets the required functionality and performance standards.
- Day 2 refers to the ongoing operational phase of the software after it has been deployed and is in active use. It represents the period of maintenance, support, and continuous improvement. During Day 2, organisations focus on tasks such as monitoring, troubleshooting, bug fixes, performance optimization, regular updates, and feature enhancements. The emphasis is on managing and maintaining the software to ensure its stability, reliability, security, and efficiency throughout its lifecycle.

In the case of shipping, the vast number of deployed edges and the geographical location of each deployment generally makes it prohibitively expensive to provide local IT support at each location to monitor, maintain and update these deployments. Instead, edge technologies must provide a comprehensive solution for administration, managing, monitoring, and securing an almost limitless number of edge servers and devices.

The deployment of thousands of Edge devices means that each of those devices are potential entry points for hackers and security breaches. There are some critical considerations to security on the edge. Some of these include (Iyengar, 2023):

- The enterprise should have the ability to check whether the edge nodes are operating properly by comparing the current configuration of various resources against the desired state.
- The communication between an edge agent and management hub should be signed and encrypted.

- Each container run on an edge endpoint should be verified against the official container to check for tampering.
- Each container should be running in its own "docker" network with self-regulated (application dependencies) connectivity between the components.
- Each edge agent should check that it is running the latest version of the container when the endpoint is connected to a network.
- The enterprise should create a cryptographic signing key pair and have a plan to rotate them.

In the shipping industry, security plays a vital role as any unauthorized access or control over a vessel's ecosystem can have catastrophic consequences. Ensuring robust security measures is of utmost importance to prevent potential threats and protect the safety and integrity of maritime operations.

In contrast to typical centralized Internet of Things (IoT) platforms and cloud-based control systems, the edge control plane is mostly decentralized. Each role within the system has a limited scope of authority so that each role has only the minimum level of authority that is needed to complete associated tasks. No single authority can assert control over the entire system. A user or role cannot gain access to all nodes in the system by compromising any single host or software component. For Open Horizon, the control plane is implemented by three different software entities (IBM, 2021):

- Horizon agents: Outnumber all of the other actors in Open Horizon. An agent runs on each of the managed edge nodes. Each agent has authority to manage only that one, single, edge node. The agent advertises its public key in Horizon exchange, and negotiates with remote agbot processes to manage the local node's software. The agent only expects to receive communications from the agbots that are responsible for deployment patterns within the agent's organization.
- Horizon agbots (agreement robots): Are processes that can run anywhere. By default, the processes run automatically. Agbot instances are the second most common actors in Horizon. Each agbot is responsible for only the deployment patterns that are assigned to that agbot. Deployment patterns consist primarily of policies, and a software service manifest. A single agbot instance can manage multiple deployment patterns for an organization. Deployment patterns are published by developers in the context of an Open Horizon managed user organization. The deployment patterns are served by agbots to Horizon agents. When an edge node is registered with Horizon exchange, a deployment pattern for the organization is assigned to the edge node. The agent on that edge node accepts offers only from agbots that present that specific deployment pattern from that specific organization. The agbot is a delivery vehicle for deployment patterns, but the deployment pattern itself must be acceptable to the policies that are set on the edge node by the edge node owner. The deployment pattern must pass signature validation, or the pattern is not accepted by the agent.
- Horizon exchange: Refers to a centralized, but geographically replicated and load balanced, service that enables the distributed agents and agbots to join and negotiate agreements. Horizon exchange also functions as a shared database of metadata for users, organizations, edge nodes, and all published services, policies, and deployment patterns.
- The switchboard in Open Horizon serves as a central communication hub, facilitating coordination and orchestration between edge devices and the management infrastructure. It ensures efficient workload placement, dynamic updates, and seamless communication, optimizing resource utilization and enabling effective deployment of workloads.

- The MMS/Sync service in Open Horizon is responsible for synchronizing and managing edge devices within the ecosystem. It ensures devices stay updated with the latest configurations, policies, and workloads from the central management hub, enabling efficient and secure communication. By keeping devices in sync, it enables seamless coordination and orchestration of workloads, enhancing the scalability and performance of edge computing deployments.

To maintain anonymity, the agent and agbot processes share only their public keys throughout the entire discovery and negotiation process. All parties within Open Horizon treat each other party as an untrusted entity by default. The parties share information and collaborate only when trust is established, negotiations between the parties are complete, and a formal agreement is established.

Edge-in-a-Box

Edge-in-a-box takes a full stack approach to deploying Machine Learning and AI models on the edge in order to provide a high level of resiliency and semi-autonomous operations. It defines a delivery model and associated tools and capabilities for users who want to run complex analytics on premises, and closer to where the data is generated. Enterprises today face a number of challenges in scaling Edge deployments to numerous locations. Two main hurdles encountered are:

- *Time/cost to deploy*: Each deployment consists of several layers of hardware and software that need to be installed, configured and tested prior to deployment. Today, a service professional can take days or even weeks when installing complex AI solutions *at each location* - severely limiting how fast and cost effectively enterprises can scale up their deployments.
- *Day-2 Management:* The vast number of deployed edges and the geographical location of each deployment could often make it prohibitively expensive to provide local IT support at each location to monitor, maintain and update these deployments.

To address these challenges, Edge-in-a-box uses a hub-and-spoke approach for (a) zero-touch provisioning of each edge server, (b) continuous monitoring of its state and (c) capabilities to manage & push software/security/config updates to numerous edge locations - all from a central location. Automation of the provisioning process is accomplished using configuration policies that are developed and tested in the factory and ensure that all elements of the stack including compute nodes, storage, operating system, applications and all their dependencies work properly together. As such, prior to installation, each managed edge-in-a-box cluster is attached to the hub and is assigned a placement tag. The placement tag determines what policy set is applied to the attached cluster and, in turn, triggers the installation of all the software components that are associated with the configuration policies in the policy set.

DataOps at the Edge

DataOps is an approach that combines practices, processes, and technologies to enhance data analytics by focusing on quality, speed, collaboration, and continuous improvement. It leverages agile methodologies and automation from software engineering to deliver high-quality data quickly and securely. DataOps extends the concept of DevOps, which integrates software development and IT operations, to the realm of data analytics.

In the era of data-driven enterprises, DataOps has gained significance as organizations recognize the strategic value of utilizing their data assets to make informed decisions. The objective of DataOps is to transform data from a mere liability requiring storage and management into a valuable asset that improves decision-making processes. While centralized cloud solutions face challenges in implementing DataOps, data lake solutions aim to address these challenges. In decentralized edge deployments, data management and mining become more complex, requiring comprehensive solutions to maximize the value of data.

Ships generate vast amounts of data related to systems, engineering metrics, sensor logs, employee information, camera and audio data, as well as external weather and supply chain information. Ideally, a scalable data unification policy is desired to merge these diverse data sources across key business entities such as ship operations, components, navigation, crew, cargo, customers, and suppliers. Traditional approaches relied on simple extract, transform, load (ETL) systems and rule-based merging schemas. However, as the data ecosystem grows larger, more complex, and heterogeneous, machine learning-based tools become essential for effective data utilization in enterprises.

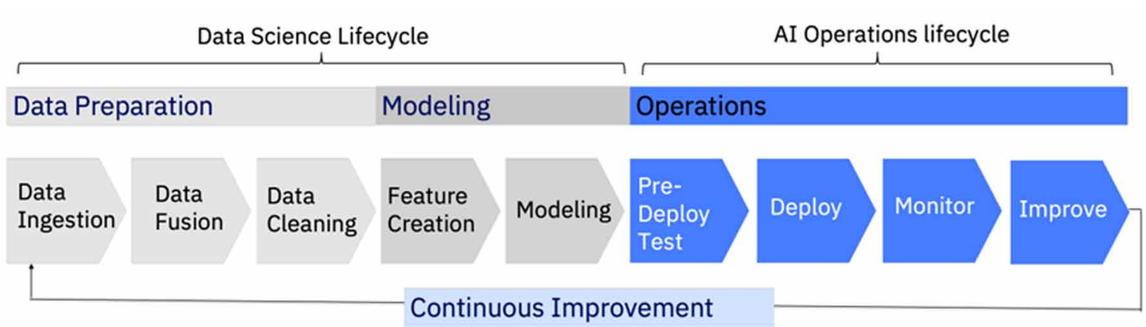
In distributed edge deployments, it is inefficient to transfer all data to the cloud. Instead, data is typically stored locally, processed on edge devices, and only intelligent subsets or insights are communicated to the cloud. DataOps implementation must also comply with relevant regulations and ensure the protection of sensitive data by automating and integrating data governance, data quality, and policy management. In the shipping industry, this consideration extends to adhering to country-specific regulations across different nodes of the system.

AIOps at the Edge

Coined by Gartner, AIOps—i.e. artificial intelligence for IT operations—is the application of artificial intelligence (AI) capabilities, such as natural language processing and machine learning models, to automate and streamline operational workflows. The AI lifecycle consists of multiple stages, including data preparation, modelling, and operations. Figure 2 illustrates a typical model development and deployment pipeline (Arnold, 2020). While significant attention has been devoted to the initial data science stages of the lifecycle, the subsequent stages of AI operations are frequently disregarded or overlooked altogether, despite their essential role in effectively deploying AI models in real-world scenarios.

After deployment, ensuring the generation of reliable predictions by AI models and promptly identifying any erroneous outputs is crucial. This plays a vital role in instilling confidence in the decision-

Figure 2. End-to-end AI lifecycle



making process of the model. In essence, AIOps focuses on the continuous monitoring and improvement of deployed models. AIOps uses big data, analytics, and machine learning capabilities to automate some aspects of the following (IBM, n.d.):

- Collect and aggregate the huge and ever-increasing volumes of data generated by multiple IT infrastructure components, application demands, and performance-monitoring tools, and service ticketing systems
- Intelligently sift 'signals' out of the 'noise' to identify significant events and patterns related to application performance and availability issues.
- Diagnose root causes and report them to IT and DevOps for rapid response and remediation —or, in some cases, automatically resolve these issues without human intervention.

AIOps encompasses data engineering, machine learning engineering, systems engineering, and reliability engineering, aiming to deliver comprehensive AI solutions tailored to specific use cases. It enables the deployment of AI models in production environments and facilitates rapid updates to adapt to evolving conditions. Initially designed for data centre deployments, AIOps plays a crucial role in edge deployments that face increased exposure, limited protections, and greater isolation from support staff and software updates.

AI on the Edge

In recent years, the field of AI has experienced a tremendous surge in interest and development. It has been described as reaching its "Netscape moment," indicating a significant breakthrough (Kahn, 2023). This has led to the rapid development and deployment of large AI models by organizations, with a focus on automating and enhancing various aspects of their operations.

Foundation models, also known as pre-trained language models, have emerged as a fundamental component in this AI revolution (Bommasani, 2021). These models serve as the building blocks for a wide range of natural language processing (NLP) tasks. They are trained on extensive amounts of text data from the internet and are specifically designed to comprehend and generate human-like text.

Built on transformer architectures, foundation models excel at capturing contextual relationships between words, enabling them to generate coherent and contextually relevant responses. They serve as the starting point for developing task-specific models, thus earning the term "foundation." While they have gained recognition for their performance in language-related tasks, they can also be customized for various domains beyond NLP, including computer vision, IT operations, and industry applications. For instance, IBM Research has developed a geospatial foundation model that learns from raw satellite imagery to create customized maps of natural disasters and environmental changes (Raghavan & Shim, 2021). This pre-trained model can be fine-tuned for downstream applications like disaster response, supply chain logistics, and agriculture.

By leveraging foundation models, developers and researchers can save significant time and resources that would otherwise be required to build and train models from scratch. These models provide a robust starting point with generalizable capabilities, which can be further refined and adapted to specific applications or industries.

Prominent examples of foundation models include OpenAI's GPT (Generative Pre-trained Transformer) models, notably GPT-3. These models have garnered attention for their remarkable language generation capabilities and their versatility across a wide range of NLP tasks.

Foundation AI for Shipping

AI can assist Captains and crew to make better decisions by seeing things humans overlook or don't fully recognise. However, it requires the ability to make robust decisions in a complex and chaotic environment. Nearly all contemporary examples of AI at best perform a form of inductive reasoning — recognizing examples of prior knowledge. AI excels at recognizing ships and buoys, rocks and paddle boards, but only because it has been taught what those things look like from training data that exemplifies them. Prior knowledge.

AI struggles to deduce what it is seeing actually means — that when it sees a person on paddle board and then suddenly that person disappears that that means they have fallen and are probably still in the water. It is difficult for AI to extrapolate causal relationships that we all take for granted. We understand that people don't just simply disappear in thin air. We understand that waves can hide things from view. We have an intuition of the laws of physics. We can deduce that when a paddle-boarder suddenly disappears they are likely just low to the water, hidden by waves, and probably haven't drifted far from where they fell.

The renowned computer scientist and philosopher, Judea Pearl emphasizes the significance of causation in the context of AI and deep learning. He argues that causation is essential for the success and advancement of deep learning models because it enables them to move beyond mere pattern recognition and make more accurate and reliable predictions (Pearl, 2009).

According to Pearl, traditional machine learning methods, including deep learning, focus primarily on correlation. They excel at identifying patterns and relationships in data but struggle to determine the cause-effect relationships that underlie those patterns. This limitation restricts their ability to provide explanations or interventions based on a true understanding of how variables interact and influence each other (Pearl, 2009).

To overcome this limitation, Pearl advocates for integrating causal reasoning into deep learning models. By incorporating causal knowledge and understanding the cause-effect relationships in the data, models can go beyond prediction and generate more meaningful and reliable insights. Causal reasoning enables deep learning models to answer "what if" questions, perform counterfactual reasoning, and make interventions in complex systems (Pearl & Mackenzie, 2018).

By embracing causality, deep learning models can achieve a higher level of interpretability, transparency, and robustness. They can provide explanations for their predictions, handle situations where training and test data distributions differ, and generalize better to unseen scenarios. Incorporating causal reasoning into deep learning opens up new possibilities for more reliable decision-making, understanding complex phenomena, and addressing challenges such as bias and fairness in AI systems.

Despite significant advancements in the field of causality over the past two decades, its practical application in real-world scenarios still falls short compared to deep learning-based methods. However, the emergence of foundation models that are pre-trained on extensive datasets and then fine-tuned for specific domains, such as shipping, has shown promise in deciphering causal relationships. Although these models do not possess innate causal reasoning abilities, experimental results demonstrate that large language models, when fine-tuned, outperform existing causal algorithms in benchmark tasks related to causal discovery.

The true potential for AI to revolutionize shipping is contingent on creating solutions that are explainable, interpretable, and where there are strict protocols guiding how data is used to train and fine-tune models.

Mayflower Autonomous Ship and Lessons Learned

With the completion of the Mayflower Autonomous Ship voyage from England to United States, ProMare has proven that AI can completely and safely navigate a ship across the oceans autonomously – without crew or remote control (Kıcıman et al., 2023; MAS, n.d.).

This and other similar experiments will likely usher in a new era of fully autonomous vehicles at sea. You can quickly imagine, for example, a fleet of self-driving vessels trawling the oceans for weeks and months at a time, collecting data for marine science – from assessing the impact of climate change, improving weather predictions, monitoring sea life and marine chemistry, to supporting exploration of our deep-water ocean frontiers – all at a fraction of the cost and risk of outfitting a vessel full of sailors and scientists manually collecting that same data. At some point in the future, no doubt cargo will be transported across the oceans without any crew — just load it, point, and set it on its way.

However, a potentially larger and more immediate use of this technology is not for vessels that drive themselves all over the world, but rather to assist sea Captains in their own navigational and ship operations responsibilities. One of the lessons from the Mayflower project is that sometimes you do need a human on-board – to fix a broken manifold coupler to the auxiliary engine, or to repair the electrical connection that has frayed and causing a short. And with human lives at risk, you need humans that have the authority and responsibility for protecting those lives – for making the critical decisions necessary to fulfil their mission safely.

The MAS experiment provides valuable insight to guide how technology and AI can be used to revolutionize shipping:

- Data quality matters. Ships can encounter a vast array of conditions during their voyage. The Promare team used an off-the-shelf computer-vision algorithm from IBM to do some of its image segmentation and object detection, but to get the AI to classify those objects it had to develop a bespoke dataset. The team created a training set of millions of images of things that float in the sea, from buoys to boats to crab pots, taken in all kinds of weather and lighting conditions to train its algorithm (Kahn, 2021). Replicating this effort is clearly unsustainable. Instead, intelligent data must be married with powerful foundation models that are fine-tuned to different use cases. For example, Meta recently released "Segement Anything" a foundation model trained with over 1 billion masks on 11M images (Kirillov, 2023).
- There are advantages to treating the ship as a series of interconnected components. Each component fulfils a specific role: one handles computer vision from MAS's cameras, another analyses radar data, another utilizes GPS for navigation, and yet another optimizes power consumption among the various components drawing power from the battery. On top of this stack lies a decision-making engine responsible for determining the boat's course and controlling the engine throttle. The key benefit here is that this decision-making captain can continue functioning even if one of the underlying systems it relies on for perception and location data fails. Moreover, the

decisions made by the AI captain are explainable. Engineers have the ability to retrospectively review the inputs, their relative importance, and the resulting actions taken by the ship. Unlike a single neural network, it is not an opaque black box.

- Guardrails are vital: Adherence to essential regulations is crucial, as ships must always abide by important rules such as the International Regulations for Preventing Collisions at Sea (COLREGs) and the International Convention for the Safety of Life at Sea. When it comes to intelligent ship systems, they must consider real-time data to enhance decision-making processes while ensuring compliance with maritime regulations.
- Humans + AI solutions: The Mayflower AI Captain held a distinctive position, assuming complete control of the ship. However, the true potential of AI solutions lies in their capacity to assist ship captains and other stakeholders in processing vast amounts of data generated onboard. These AI tools can then suggest optimal decisions across various domains, including route selection, navigation, engine performance, HVAC systems, crew scheduling, and maintenance requirements. While AI can acquire contextual understanding and situational awareness, along with the algorithms to evaluate and determine effective options, it must still establish the most effective means of influencing decisions and executing actions. Ultimately, AI must earn the trust of its users, necessitating interaction with users, providing explanations for its reasoning behind certain decisions, and collaborating with users iteratively to arrive at the best possible choices.

Modern ships are characterized by their advanced technology, featuring an extensive array of sensors, devices, and servers that contribute to their day-to-day operations. To enhance the efficiency, sustainability, and reliability of the shipping industry, the integration of AI throughout the ship's operational systems is crucial. This entails incorporating AI into various aspects such as data acquisition, mechanical performance, logistics and supply chain management, port interactions, route selection, navigation management, and accounting for external factors like weather disruptions and geopolitical events. To create robust, reliable, actionable, and explainable decisions, a diverse set of routines are required. It is vital to ensure that the system can withstand IT outages, data contamination, model errors, and potential malicious actions. Additionally, each component must be designed to optimize human-machine interactions and ensure that the system's recommendations are easily understandable and applicable for stakeholders involved.

Foundation models have the potential to transform enterprise operations, showcasing impressive performance across various domains like natural language understanding, image generation, virtual assistants, data analysis, and healthcare. For the shipping industry, the crucial aspect is harnessing the power of these pre-trained models, adapting them to specific applications, and seamlessly deploying them either on-premises or in the public cloud. While foundation models introduce a new wave of AI capabilities, the underlying frameworks to enable them remain consistent. Considerations such as compute hardware, security-focused systems, intelligent workload orchestration, cloud-native applications, and robust development protocols involving DevOps, DataOps, and AIOps are essential factors to be addressed.

CHALLENGES AND RESEARCH DIRECTIONS

Rathore et al. (2022) review some of the challenges and future opportunities for edge computing, including:

- Security: The distributed architecture, mobility support, and data processing in edge computing raise security concerns. Thorough testing, access control systems, trust management, privacy measures, and intrusion detection systems are crucial. Security protocols, artificial intelligence, and encryption techniques can enhance protection, but fatal defects need to be addressed.
- Cost: Configuring, deploying, and maintaining edge computing devices can be expensive. Backup servers for fault tolerance and machine learning-based systems may incur additional costs. Developing cost-effective devices with low communication and computation expenses is essential.
- Power: Providing cloud-like remote services in remote areas requires high-power processors, voltage, and three-phase electricity, posing challenges.
- Data: Optimizing data usage is vital as edge computing devices process subsets of data, potentially overlooking additional data or wasting raw data. Effective data segregation and sharing across devices are crucial for efficiency. Computation-aware networking can enhance distributed systems.
- Heterogeneity: Resolving the heterogeneity of data and the ecosystem within edge computing networks is a challenge. Collaboration between different vendor systems, load balancing, synchronization, resource sharing, data privacy, and interoperability contribute to the complexity.
- Trust: User trust in edge computing systems is tied to security and privacy. Developing consumer trust models that foster confidence in adopting edge computing devices is an ongoing challenge.

Shipping stands out as a prominent example of edge deployment due to its unique characteristics, including restricted latency, inherent geographic distribution, autonomy demands, substantial data generation capacity, and the necessity for resilience, fault tolerance, and regulatory compliance. Further the shipping industry has ambitious decarbonisation ambitions which impacts all aspects of decision making (IMO, n.d.).

CONCLUSION

There have been many evolutions in computing from transistor computing to microprocessors, to networking and the internet. The past two decades have seen the rise of cloud computing and the many instances of these from public cloud to private cloud to hybrid and multi-cloud solutions. Edge computing is considered an extension of the cloud continuum because it complements and expands the capabilities of cloud computing. While cloud computing excels at handling massive data storage, complex data analysis, and resource-intensive tasks, edge computing focuses on processing data locally, enabling quick responses, and reducing the need for data transmission to the cloud. These two computing paradigms work together to provide a holistic and scalable solution.

By bringing computational power closer to the data sources, edge allows for faster processing and real-time decision-making, enhancing the overall efficiency of the system. The importance of edge enabled capabilities for shipping is obvious. Realizing the potential of edge computing is contingent on two factors:

- Extending cloud-centric development frameworks such as DevOps, DataOps, and AIOps to the Edge so that developers can seamlessly develop, deploy and improve new solutions within a single user framework.
- Leveraging new AI technologies such as foundation models rapidly on the edge. Deploying these powerful capabilities allows the industry to unlock sophisticated natural language understanding, image generation, data analysis, and decision capabilities at a fraction of the effort.

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Chapter 5
Shipping Green Fuel Strategies and Benchmarking Supported by Digital Twins

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ABSTRACT

The chapter is concerned with the potential of alternative fuels, i.e., any other fuel than conventional fossil fuels, for powering ships. The alternative fuels surveyed in this chapter include liquefied natural gas (LNG), methanol, hydrogen, ammonia, as well as synthetic fuels (e-fuels). The chapter explains how digital twin's simulation capabilities, can be used to model complex energy systems and alternative fuels and compute emissions, power consumption/output, etc., virtually. The chapter provides a comparison of alternative marine fuels, in terms of storage requirements and energy converters (e.g., combustion engines, fuel cells) suitability. Finally, the chapter discusses the role of digital twins in supporting further research and development towards the evolution of alternative fuels.

INTRODUCTION

Alternative fuels include fuels that can be used as drop-in fuels, like biodiesel, as well as hydrogen, ammonia, methanol, and Liquified Natural Gas (LNG) to replace currently used fuels such as heavy fuel oil (HFO), marine diesel oil (MDO), and marine gas oil (MGO). Alternative fuels do not impact global CO2 emission levels (Sustainable Ships-a), i.e. they are 'carbon neutral', or have CHG emissions that are significantly lower than fossil-based fuels. Biomass (the source of biodiesel) for instance, absorbs CO2 directly from the air. This biomass is then transformed into fuel, using a variety of processes, that

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is burned releasing the carbon again in the form of CO2. This is then again, absorbed by the biomass, creating a repeated cycle without adding to the total amount of CO2.

Both alternative and fossil-based fuels are used for the powering of ship engines They are consumed within fuel cells, as liquids or gases in internal combustion engines and in external combustion engines. Ship fuels differ from each other in a variety of ways, as their chemical and physical characteristics may be completely different. Furthermore, their environmental impact, renewability and sources can be significantly different.

A fundamental aspect to be considered in the use of alternative fuels for marine use is their flashpoint. According to the IMO International Convention for Safety of Life at Sea ("SOLAS"), "low-flashpoint fuel" means gaseous or liquid fuel having a flashpoint lower than permitted under SOLAS regulation II-2/4.2. Typically, bunkers with a flashpoint below 60˚C are deemed unsafe. The usage of marine fuels below 60˚C is already prohibited under SOLAS.

Furthermore, the IMO International Code of Safety for Ships Using Gases or Other Low-flashpoint Fuels (IGF Code) provides industry standards for ships that use fuels with a flashpoint of less than 60°C. The IGF Code seeks to regulate the safety changes from the carriage and use of gas fuel, in particular liquefied natural gas (LNG) and other low-flashpoint fuels. The IGF Code sets out mandatory provisions for the arrangement, installation, control and monitoring of machinery, equipment and systems that use low-flashpoint fuels. Currently the IGF Code addresses in detail the requirements for the safety of ships using LNG as fuel. Draft Guidelines have been issued (for fuel cells, LPG and methyl/ethyl alcohol) or are in preparation (for hydrogen, ammonia, low-flashpoint fuel oils) and it is expected that – after a period of non-mandatory application to gain experience – the relevant provisions will be included as new mandatory sections of the IGF Code.

Although the usage of alternative fuels is an essential part of the strategies to comply with the stringent IMO and EU requirements targeting the progressive decarbonization of maritime transport, the real focus of the new IMO regulations and draft interim guidelines is on the safety of ships using such alternative fuels, to address and manage the additional risks introduced by their flammability, toxicity and corrosivity.

In parallel, IMO is also revising the regulations addressing the transport of such alternative fuels as cargo for their transport in global trading routes, e.g., the IMO Code for the Construction and Equipment of Ships Carrying Liquefied Gases in Bulk (IGC Code).

These international regulations have a significant impact on the use and the costs (CAPEX and OPEX) of the alternative fuels on all kind of vessels and – more in general – waterborne transport, including inland navigation. The main characteristic of alternative fuels is that they are, in most cases, renewable, meaning that they don't run out and can be replenished naturally over time, which contrasts with the nature of fossil fuels that have been formed from decaying plants and animals, over millions of years and thus they exist in finite resources. Alternative fuels, generally, emit fewer greenhouse gases (GHG) than their fossil counterparts, even having net zero footprint for the environment, while, in contrast, the burning of fossil-based fuels produces significant amount of greenhouse gases (GHG). That difference can be even more significant, especially if the alternative fuels have been produced from renewable green sources ('green fuels') and utilizing Carbon Capture and Utilization (CCU). In this aspect we must underline the fact that the usage of alternative fuels contributes also to the reduction of the air pollution in general, as the alternative fuels generally emits less, or even zero, air pollutants such as like sulphur dioxide, nitrogen oxides, and particulates.

The impact of the replacement of fusil-based fuels with alternative ones has a geopolitical angle, as most of the proposed alternative fuels can be domestically produced by most countries, resulting in reduction to imports from foreign countries and contributing to energy security. Moreover, as the alternative fuels can be created from a wide range of different sources, such as biomass, water, sunlight and even waste products, contrasting with the fossil-based ones, that derives from a single source of origin, as most of the fossil-based fuels are produced from a limited range of sources (coal, petroleum, and natural gas). This difference also contributes to the diversification of the energy sources, which also in turn contributes to the energy security.

However, there are issues that must be investigated, regarding the advantages of the fossil-based fuel, as the technologies for their production and usage are in a well-developed stage, being widely deployed, while their alternative counterparts require further research and development regarding their production distribution and storage. Although the technology related to the production, transport and use of some alternative fuels is already known and applied in land-based applications and industrial fields (e.g. using ammonia, hydrogen, methanol), marine standards and “marinization” requirements are still at an infancy stage, and therefore the cost of production and infrastructure scale-up, is higher. As the technologies used for fossil-based fuels are mature and the infrastructure extensive and well developed, the cost of using fossil fuels is comparatively lower than that of alternative ones.

Moreover, fossil-based fuels are, in general, characterized by high energy density, making them very efficient for transport and energy storage, while the alternative fuels have variable energy densities, and large deviations in their energy content and energy density both energy density by volume and energy density by mass (e.g., hydrogen). Compatibility with the existing engines might also be a problem for the alternative fuels, as there are fuels that can be directly used in existing engines as drop in fuels, or as blends, with minimal or even no modifications required in the engine, while others might need extensive modifications, specialized engines, or delivery systems. In contrast, as the existing technology has been developed and designed around fossil-based fuels, they are completely compatible with the existing engines and infrastructure.

Considering the public perception, it is evident that the public favours alternative fuels, in general, due to their environmental benefits over the traditional fossil-based fuels. Moreover, there is strong governmental support in the development of alternative fuels and renewable energy, especially in EU, which for years has been importing fossil fuels from other countries, as the geopolitical and energy security factor becomes more critical. Furthermore, as the global climatological change becomes more and more evident, more actions will be taken in the direction of alternative fuels.

As argued in (Mofor et al., 2015). the development of renewable energy solutions for shipping has been hampered by over-supply of fossil fuel-powered shipping and weak investments. The main problems that renewable technology faces in order to increase its usage in the maritime sector is essentially the lack of commercial viability and higher costs well-to-wake. At the same time, the motivation for a fuel shift is very high. There is a compelling need for all stakeholders to decarbonize maritime transport to comply with the progressively stricter emission limits from now to 2050. Therefore, in addition to slow steaming and energy saving/energy recovering on board, alternative fuels are the third–and probably the most effective way to seek regulatory compliance.

This Chapter aims at a thorough survey of alternative fuels for shipping, their evaluation and comparison, and a critical analysis of their current status of use and future potential. The Chapter is organized as follows. The next section provides a taxonomy of alternative fuels and focuses on green methods for their production as well as technologies for their storage. Section 3 discusses the key alternative fuels with a high potential for the shipping industry as replacements to fossil-based fuels. Section 4 contains a comparison of alternative fuels in terms of energy densities, emissions and requirements for storage and additional technologies for their utilization such as converters. Section 5 discusses the role of digital twins in producing and evaluating alternative fuels, as well as for improving the processes for their storage, transportation and utilization. Finally, Section 6 discusses the current state of maturity of alternative fuels and their possible future developments taking into account financial and technical considerations.

PRODUCTION AND STORAGE OF ALTERNATIVE FUELS

Green production methods for alternative fuels are particularly important, as the whole lifecycle of the alternative fuels must be considered, rather than simply the phase where the fuel is used (burned). Main green production techniques of alternative fuels include:

- Electro fuels (E-fuels) mainly hydrogen derived using water electrolysis powered by renewable electricity sources.
- Biofuels from sustainable biomass (forestry residue, agricultural waste, etc.) producing different carbon-neutral fuels such as bio-MGO (Marine Gasoil), bio-LNG and bio-methanol.
- Blue fuels from fossil energy by capturing the CO2 during the production process and using carbon capture and storage (CCS) technology, producing mainly 'blue' ammonia and 'blue' hydrogen.

Another green method of production includes renewable energy technologies such as photovoltaics, wind turbines and wave energy devices in offshore areas such as natural and man-made platforms, that produce green electricity, which in turn can be used to produce green fuels using different methods, for example electrolysis to produce green hydrogen. However, renewable energy can also be used directly in waterborne assets. Several potential energy sources have been proposed, including wind, solar, biofuels and wave. The adaptation of the renewable energy sources can be implemented for the existing ships or fleets through refitting and retrofitting, and for the newbuilds through optimised ship designs.

Renewable energy can be used to produce green fuels, like green hydrogen via electrolysis of sea water with electricity provided by offshore or onshore wind turbines. In that direction there are numerous investments like that of Siemens Gamesa and Siemens Energy (Mallouppas & Yfantis, 2021). Furthermore, there are various examples of implementation of wind assisted propulsion (WASP), for various WASP solutions, from which, one very interesting example being that of the SEA-CARGO's SC CONNECTOR which utilizes Flettner rotors in order to achieve 25 to 70% propulsive thrust.

Fuel Cells

Fuel cells (FCs) are efficient energy converting devices which use pure hydrogen or hydrogen derived from a reforming process of hydrogen-rich fuels, which can be integrated into the fuel cell power installations. Therefore, fuel cells are emerging as a promising technology for ship applications, offering a clean and efficient alternative for onboard power generation. The electricity is produced in the fuel cells, electricity through an electrochemical reaction. Among the different types of fuel cells, proton-exchange membrane fuel cells (PEM), solid oxide fuel cells (SOFCs), and molten carbonate fuel cells (MCFCs) for higher power output, are the most promising options for maritime applications based on metrics for energy efficiency, power capacity and sensitivity to fuel impurities. Overall, the main performance metrics for applying fuel cells to maritime applications are the power capacity, the cost and the lifetime of the fuel cell stack. With MCFC, waste heat recovery systems are applied to improve the overall efficiency, possibly coupled with organic Rankine cycles due to the low-grade temperatures.

Large capacity hydrogen fuel cells (200kW) are currently deployed to power industrial and transport machinery and have the capacity to provide energy for ship propulsion in suitable configurations (FC-Wave,2022). Currently, some cruise ships have also installed PEM fuel cells, using reformed methanol, to produce energy in the range of 300-350 kW for non-essential ship services of accommodation areas.

TYPES OF ALTERNATIVE FUELS

Biofuels

Biofuels are produced from organic waste such as plant and animal waste (International Transport Forum, 2018). As of now, the main sources of biofuels are from plant-based sugars and oils, such as palm, soybean and rapeseed (Hsieh and C. Felby, 2017). There are 3 generations of biofuels, with the second and third generations regarded as “advanced biofuels”. The categorization of the biofuels is based on the source of carbon used.

The European Biofuels Technology Platform defines first, second and third generation biofuels as follows (Mofor et al., 2015), (Mallouppas & Yfantis, 2021):

1. First Generation: “The source of carbon for the biofuel is sugar, lipid or starch directly extracted from a plant. The crop is actually or potentially considered to be in competition with food.”
2. Second Generation: “The biofuel carbon is derived from cellulose, hemicellulose, lignin, or pectin. For example, this may include agricultural, forestry wastes or residues, or purpose-grown non- food feedstocks (e.g., Short Rotation Coppice, Energy Grasses).”
3. Third Generation: “The biofuel carbon is derived from aquatic autotrophic organisms (e.g., algae). Light, carbon dioxide and nutrients are used to produce the feedstock, “extending” the carbon resource available for biofuel production.”

Advanced biofuels are a very promising and viable solution as a main energy source (Mofor et al., 2015) and they meet the requirements for Very Low Sulphur Fuel Oil (VLSFO) and for Ultra Low Sulphur Fuel Oil (ULSFO) (Hsieh & Felby, 2017). The problem with biofuels in shipping sector refers to the little experience and knowledge on handling and applying biofuels as part of the fuel supply chain, the required volumes of biofuel to fulfil the needs of the shipping sector and the concerns about the storage and oxidation stability of biofuels, as well as the blending different sources and variety of biofuels, leading to the need of further research in that sector (Hsieh and C. Felby, 2017). Another worth mentioning aspect is the fact that sustainable biofuel production is limited considering food price, natural resources (such as availability of land) and social conditions (International Transport Forum, 2018).

In a SWOT analysis provided by (Hsieh & Felby, 2017), biofuels have higher prices than fossil fuels, and the situation is expected to remain for at least a medium-term horizon, but with the right policies, regulations, initiatives and technology and infrastructure improvements, there will be a healthy market for biofuels (Hsieh & Felby, 2017). In that direction, market-based measures can be used to accelerate the adoption of biofuels in the maritime sector, as part of the decarbonization strategy of the shipping industry (Lagouvardou et al., 2020)

Biogas

Biogas can be either methane or hydrogen. Biogas is produced from anaerobic digestion within an enclosed environment which consists of microbes that break-down organic material (Vanek et al., 2012), after that, biogas can be further processed to remove impurities like hydrogen sulphide and moisture (Mofor et al., 2015). The produced methane can be liquified in the form of Liquified Bio-Methane (LBM) (Mofor et al., 2015), which can be used for deep decarbonization in the long-term of the shipping industry, as it is produced from renewable sources, in contrast with LNG which is favoured right now but is often considered as a transitional fuel rather than a terminal solution (Mallouppas & Yfantis, 2021).

Methanol

Methanol, due to the lower investment cost and the relative simplicity of handling - being liquid in normal ambient conditions may be an attractive solution as an alternative fuel compared to hydrogen and ammonia, moreover, its availability and competitive price (FCEnergy, 2018) (Doedee, 2023) makes it a promising alternative to conventional fuels. Furthermore, methanol provides a 25% drop in CO_2 emissions compared to HFO coupled with reduction in SO_x, NO_x and PM by 99%, 60% and 95% respectively (Mallouppas & Yfantis, 2021). Regarding its drawbacks, the fact that is toxic may introduce some additional risks, but on the other side due to the fact that is plentiful, available globally, readily miscible in water, biodegradable and it can be 100% renewable, makes it a very interesting option. Another worth mentioning aspect is that life-cycle environmental footprint of bio-methanol is “greener” compared to LNG (Mallouppas & Yfantis, 2021). The environmental benefits, technology readiness and economic feasibility of methanol as marine fuel are studied in (IMO, 2021). As mentioned, and above and in a study by (FCBI Energy, 2018) methanol is plentiful, available globally and potentially 100% renewable, compliant with short/mid-term emissions reduction regulations, although not carbon-free, while the current bunkering infrastructure needs only minor modifications to handle it with relatively modest costs compared to potential alternative solutions.

Liquified Natural Gas (LNG)

Liquified Natural Gas (LNG) is already in use in maritime industry and is the cleanest available fuel for shipping available right now in meaningful volumes (Shell, 2020). LNG is stored in -162° Celsius and provides a 20-30% reduction of CO_2 emissions compared to HFO, while having lower NO_x and PM emissions and 90% drop in SO_x emissions. The problem with LNG is that due to the methane slip, the environmental benefits are moderate, hence (excluding green LNG from Carbon Capture and renewable energy sources), LNG is considered by many like a transitional fuel rather than a terminal zero-carbon solution. In this point it must be mentioned that right now the only comparable in cost with HFO fuel is LNG, while other fuels such as bio-methanol and biofuel are compatible in price with HFO only when a tariff of 300 USD/ton CO_2 is applied on HFO consumption (Mallouppas & Yfantis, 2021).

Hydrogen

Hydrogen, on the other hand, can be used in internal combustion engines and in fuel cells, as described above. A recent study by CE Delft (Delft, 2020), has investigated the availability and costs of LBM and Liquified Synthetic Methane (LSM), also known as e-methane. In this study the LSM is assumed to be produced from CO_2 and H_2, where hydrogen is produced from renewable energy sources and CO_2 is recycled from carbon capture (Delft, 2020). The study has shown that the future projected supply of LBM and LSM can exceed the future demand of the maritime sector, if biomass will be used to produce methane and sufficient investments are made in renewable electricity production (Delft, 2020). Furthermore, the cost of the production of LBM and LSM may not be significantly higher or even be comparable to the production costs of other low- and zero-carbon fuels (Delft, 2020). Finally, if the costs of bunkering infrastructure and ships are comparable as well, then LSM and LBM fuels may be viable candidates to achieve decarbonization in the shipping sector (Delft, 2020) (Mallouppas & Yfantis, 2021).

As of 2020, the majority of hydrogen (~95%) is produced from fossil fuels by steam reforming of natural gas, partial oxidation of methane, and coal gasification. These methods produced, so-called 'blue hydrogen'. Other methods of hydrogen production include biomass gasification and electrolysis of water according to Wikipedia (https://en.wikipedia.org/wiki/Hydrogen_production).

Hydrogen, even though in many cases it can be proved advantageous, as it produces no CO_2, particulate matter (PM) or SO_x, when burned, presents many challenges to be addressed mainly about the refuelling, safety, storage (embrittlement of materials) as well as the production and usage (especially in Internal Combustion Engines - ICEs). Most of the hydrogen produced today comes from fossil fuels, making it impactful for the environment. The solution might be the so-called "green" hydrogen, which, in contrast with all the other hydrogen's types of production (Brown, Grey, Yellow, Blue, Pink), is produced solely from renewable energy sources, like solar, wind, etc., but at a higher cost than any other method of production. Another issue is that although hydrogen includes more energy per kilogram than any other proposed solutions, excluding nuclear power, it has very low volumetric energy density (Energy Transitions Commission, 2019). The answer to this problem may be liquid hydrogen (LH_2), which is stored in high pressure and very low temperatures (-253 Celsius), or compressed hydrogen (CH2) at high pressure (300-700 bar), but this obviously creates some new challenges, which can technically and financially be overcome, as it was shown by a project by Kawasaki Heavy Industries, using liquified hydrogen as cargo (Kawasaki, 2010)

Hydrogen is already in use to power offshore crane vessels (Sustainable-ships.org-c, 2021) and inland vessels (Sustainable-ships.org-e, 2021). Infrastructure for hydrogen production has begun development in various locations such as the green hydrogen refinery in Rotterdam (Sustainable-ships.org-d, 2021) and in BP's Lingen Refinery in northwest Germany (Sustainable-ships.org-f. 2021), as well as in planned off- shore platforms (Sustainable-ships.org-I, 2021). The European Commission estimates that €13-15 billion will be invested in electrolysers to increase hydrogen production capacity to 40 GW by 2030 (Charbonneau, 2021).

The European Maritime safety Agency (EMSA) commissioned and published in 2023 a very comprehensive study on the "Potential of Hydrogen as Fuel for Shipping", which details the technical issues, regulatory frameworks, and state of play for application of hydrogen as a fuel.

Ammonia

Ammonia doesn't need to be in cryogenic conditions to be stored in liquid state (it needs to be in -33.4 Celsius in contrast with the -252.9 Celsius for hydrogen) making ammonia a suitable hydrogen carrier for fuel cells (FCs). Even though ammonia can be used, similarly with hydrogen, as a drop-in fuel in ICEs, its properties compared with those of hydrogen and the disadvantages that it inherently has, mainly the toxicity, corrosiveness and the higher NO_x emissions, making hydrogen more suitable for ICE application (Mallouppas & Yfantis, 2021). Moreover, the method of ammonia's production must be addressed, because similarly with hydrogen its production relies heavily on the fossil fuels, in fact 90% of its production comes from fossil fuels, while the production of "green" ammonia, from renewable energy sources has been investigated by several global initiatives (Mallouppas & Yfantis, 2021). Under this scope, it is crucial to note that in order to produce lower carbon emissions than Heavy Fuel Oil (HFO) in ships, the carbon intensity of electricity needed for production of ammonia must be below 200 gCO_2/kWh, while for hydrogen, respectively, the limits are 150 and 175 gCO_2/kWh (Energy Transitions Commission, 2019).

Similarly to hydrogen, as mentioned above, EMSA has also commissioned and published in 2023 a very comprehensive study on the "Potential of Ammonia as Fuel for Shipping", which details the technical issues, regulatory frameworks, and state of play for application of ammonia as a fuel.

GREEN FUEL COMPARISON

Green fuels are often classified as green hydrogen and e-fuels. E-fuels are produced from hydrogen and CO2 and include e-Methane, e-Methanol, e-Diesel, e-Gasoline or e-Jet fuel. They have the potential to replace fossil fuels, although their climate effectiveness, high costs and uncertain availability (Falko et al., 2021) hinder their future potential. They can be blended gradually with fossil fuels until they fully replace fossil fuels as a primary energy source (Siemens, nd). It is estimated that the right incentives for e-fuels, the demand could reach up to 7% of the EU shipping fuel mix already by 2030 (Transport & Environment, nd). This would give the sector the kickstart needed to deploy renewable fuels and ultimately achieve net- zero emissions by 2050. To compare e-fuels with other green fuel options it is important to establish detailed models for understanding use options, and impact assessment on ship performance KPIs. This is the scope of this section.

Fuels and Fuel Tanks Characteristics

To be able to compute some regulatory indicators (FuelEU GHG II) and for a complete emissions analysis of the impact of the use of a given fuel, it is important to consider its emissions across the entire lifecycle ("from Well to Tank") in addition to the ("Tank to Wake") ones. Indeed, emissions for production, and transportation might not be negligible even if the considered fuel is not carbon based.

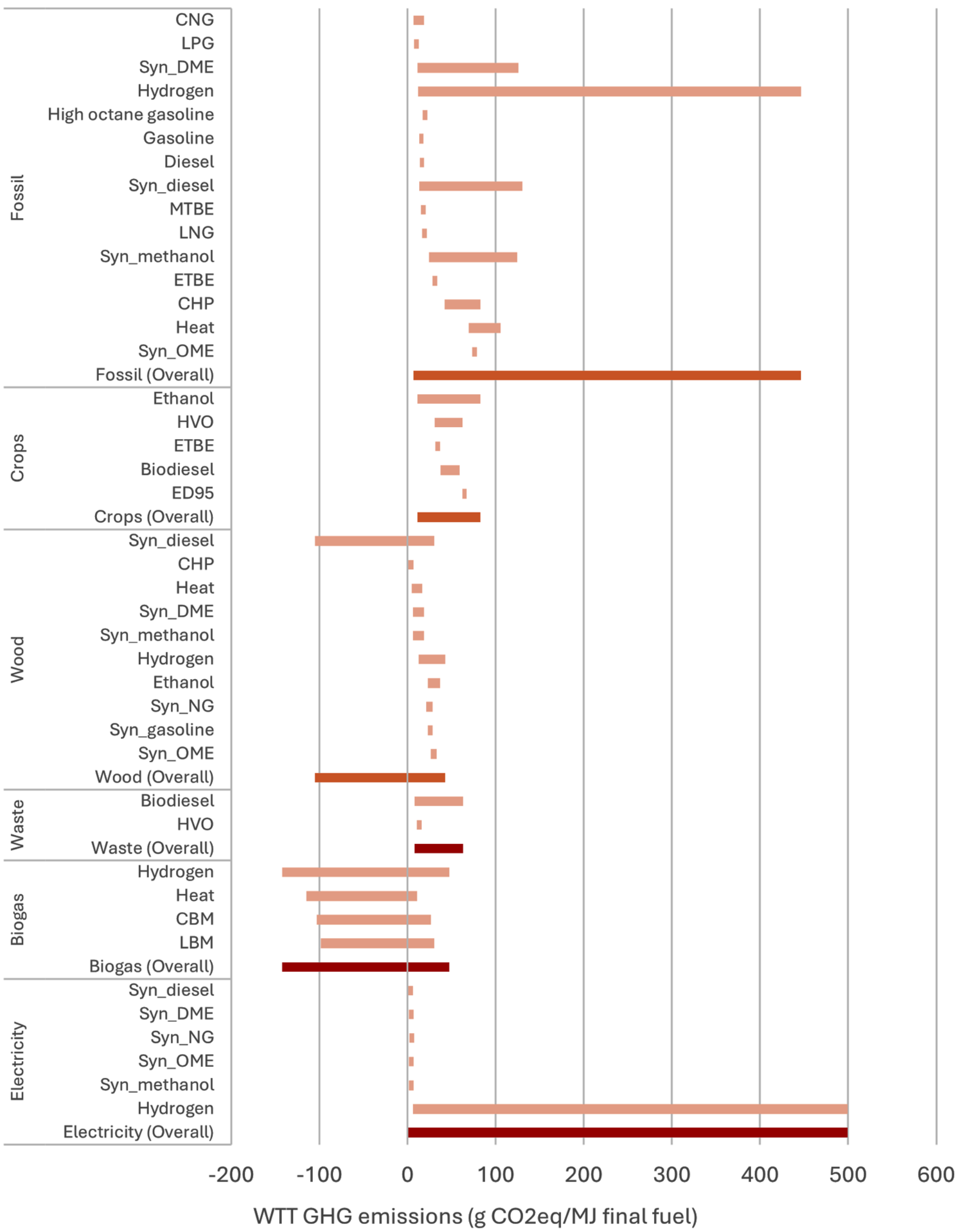
In addition, in order to assess the real footprint of using an alternative fuel onboard, it is important to consider at least the volume of the storage systems. As an example, cryogenic ammonia uses two times less volume than liquefied hydrogen for the same amount of energy.

Values from Table 1 - Fuel characteristics come from several sources: (European Commission, 2021); Stoltz et al, 2022; Prussi et al., 2020)

Table 1. Fuel characteristics

Fuel	Storage type	Storage system (L/kWh)	Fuel Temp. (T°K)	Density (kg/ m3)	LHV (kWh/ kg)	WTT CO2eq (gCO2eq/ MJ)	CO2 Cf. (gCO2/ gFuel)	CH4 Cf. (gCH4/ gFuel)	N2O Cf. (gN2O/ gFuel)
H2	Liquid	0.71-0.83	20	71	33.3	3.6-500	0	0	0
H2	700bars	1.25-2.5	288	42	33.3	3.6-500	0	0	0
MeOH	Liquid	0.25-0.27	288	796	5.52	1.8-124.3	1.375	0.00005	0.00018
NH3	Liquid	0.35-0.39	240	682	5.17	0-121	0	-	-

Figure 1. WTT GHG missions of various fuel production pathways



Note. Chart including pathways modelled in JEC v5 not representing all possible WTT pathways for each specific fuel

Table 2. Fuel production pathways and TRL (Prussi et al., 2020; Liu et al., 2020)

Fuel	Pathway	TRL	gCO2eq/ MJFuel	Note
Methanol	GPME1b	9	31.64	Piped natural gas (4000 km) to methanol, synthesis plant in EU
	GRME1	9	24.33	Remote natural gas to methanol, synthesis plant near gas field
	WWME1a (500 km)	8	10.53	Wood to methanol, waste wood, farmed wood, and waste wood via black liquor gasification/synthesis plant
	WWME1b (>500 km)	8	14.19	
	WFME1a (500 km)	8	14.98	
	WFME1b (>500 km)	8	18.64	
	BLME1a (500 km)	9	6.19	
	REME1a	9	1.80	Renewable electricity to methanol (CO2 from flue gases)
LH2	WFEL1/ LH1	8	31.72	Wood (Farmed): WFEL1 IGCC (200 MWth, WFEL3: Conventional (small-scale)
	WDEL1/ LH1	9	3.56	Electricity from wind energy
	WFLH1	8	17.81	Farmed wood, large scale gasifier and hydrogen liquefaction, liquid hydrogen road transport to retail site, hydrogen cryo- compression in to vehicle tank (35 MPa).
NH3	LT-HB	8	12.00	Electric HB with LT electrolysis
	HT-HB	5	13.00	Electric HB with HT electrolysis

As shown in Figure 1, WTT figures for fuels are largely spread, and depicts the importance of taking into account those values when considering decarbonizing shipping.

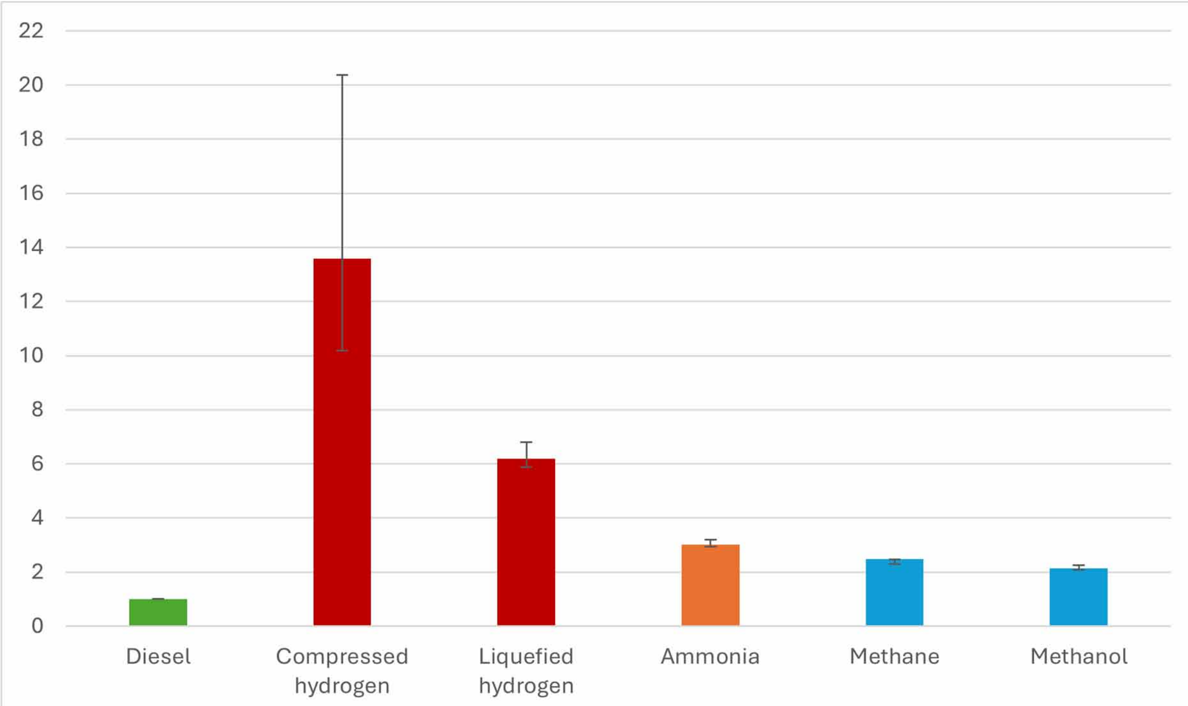
Along with the fuels emissions potential, it is important to consider the technology readiness level of the fuel production systems, as shown below, with a close-up on pathways lower than 100 gCO2eq/ MJFuel, as an example.

Fuel Tanks Considerations

Green fuels have lower emission levels; however, they tend to be less dense than regular fossil fuels (MGO, FO), and may require specific storage systems, playing an important role on the overall energy storage volumes. The following figure depicts the volume factor of alternative fuels storage tanks compared with a standard MGO tank.

It is clear that the considered fuels here have a higher volume footprint: Ammonia, for example, will take around 3 times more volume than MGO (Diesel).

Figure 2. Fuel storage volume factors (compared with MGO)



Converters Considerations

Alongside with the fuel energy densities, related tanks volume and fuels emissions, it is important to consider the converters they can be coupled with. Indeed, as converters efficiencies are different, the amount of fuel carried on-board can vary as well for the same net energy needs, minimizing the loss of cargo or autonomy.

Hence, by combining fuels and different converters, it is possible to get an order of magnitude of the overall systems performances, in terms of emissions, relative fuel storage volumes and emissions.

Table 3. Fuel cells characteristics (Stolz et al., 2022; Vanbiert et al., 2016; Percic et al., 2921; Kim et al., 2020)

FC Type	Fuel compatibility	Efficiency	TRL	Note
PEMFC	H_2 NH_3, MeOH, +++, with add. Reformer or cracker	0.5	9	Quick start-up and load following
SOFC	H_2, NH_3, MeOH, +++	0.5-0.7*	9	Long start-up time, Low power density
MCFC	H_2, NH_3, MeOH, +++ (requires CO_2 at cathode side)	0.5-0.7*	9	Long start-up time

* High temperature fuel cells can increase their efficiency by up to 20% when a waste heat recovery unit (WHRU) is used.

Fuels Comparison

Now that the main constraints (emissions, regulations, and volume) and main systems characteristics are defined, it is possible to perform a clearer comparison between sets of fuels and fuel cells.

The comparison here is based on the generation of 1 kWh of net energy by the converters. This allows comparing the required relative fuel tanks volume, emissions levels, and the Fuel EU regulatory indicator (EU GHG II).

For this comparison, the following fuel pathways are considered:

The following results are obtained when generating 1 kWh from the energy systems sets.

Figure 3 shows the Well to Wake GHG emissions (Uncertainties are related to the converters efficiencies) of each set of converter / fuel, computed according to the FuelEU Maritime regulation.

Figure 4- EU GHG Intensity Indicator for various sets of converters & fuels highlights the decarbonisation potential of various sets of converters & fuels. The red dotted lines on the figure display the FuelEU Maritime regulatory limits over time. As an example, in this scope, switching to an SOFC system fed with e-Ammonia would extend a ship's compliance until 2055. Moreover, all natural-gas-based fuels are already non-compliant and have even higher emissions levels than HFO.

Table 4. Fuel pathways

Fuel	Fuel Name	WTT Pathway / value
H_2	eh2	FuelEU Maritime
H_2	ng_h2	FuelEU Maritime
MeOH	emeoh	Pathway REME1a from JEC
MeOH	ng_meoh	FuelEU Maritime
NH_3	e_nh3	CD/HTE
NH_3	ng_nh3	FuelEU Maritime

Figure 3. WtW GHG Emissions per net KWh (Red: TtW, Blue: WtT)

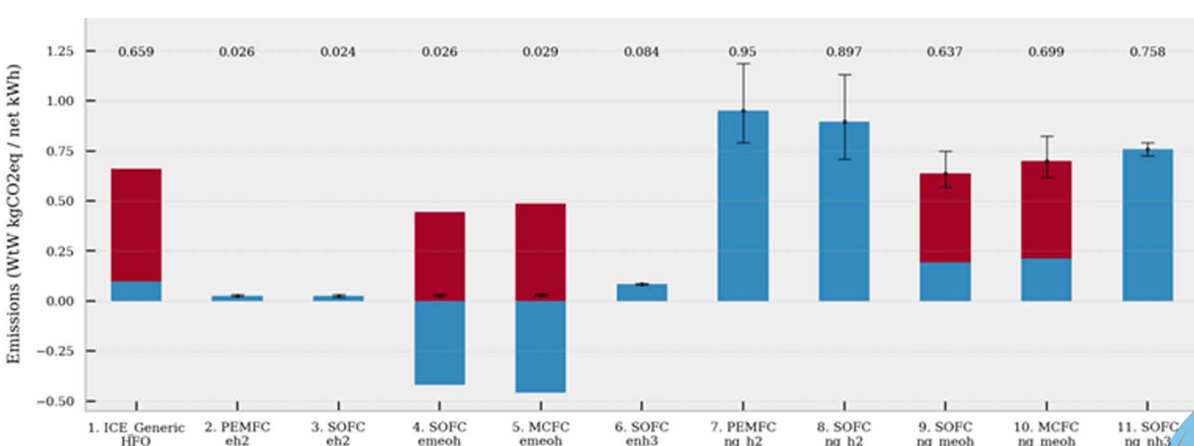


Figure 4. EU CHG Intensity Indicator for various sets of converters and fuels

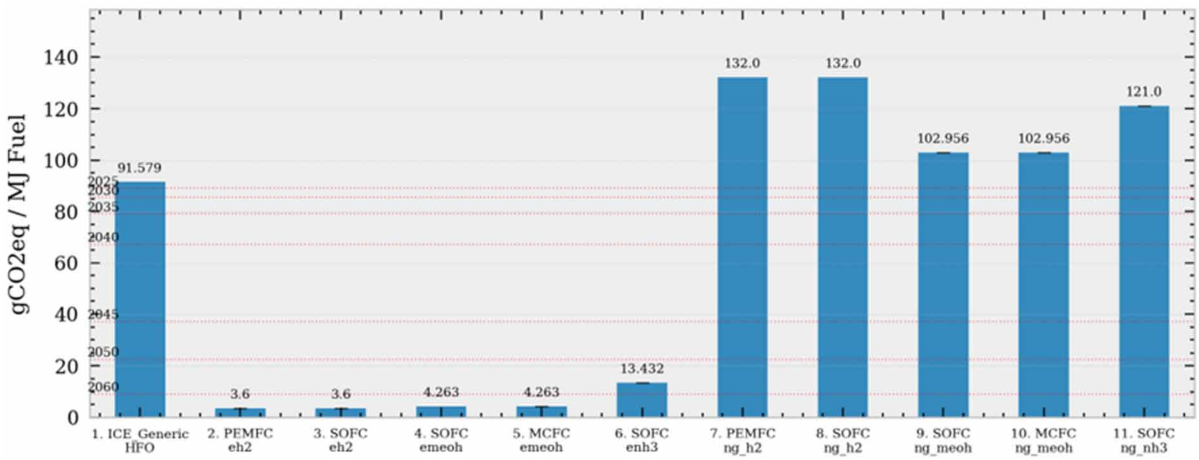


Figure 5. Normalised tank volumes to produce 1kWh net

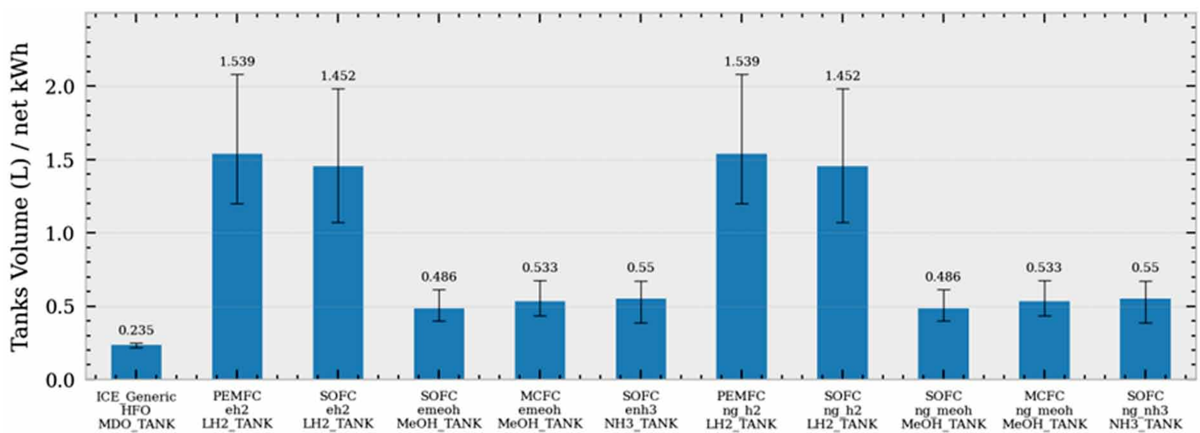


Figure 5 (uncertainties are related to the converters efficiencies) depicts the required volume of fuel tanks for each system to produce one kWh net. This indicator offers a convenient way to assess the impact on payload dedicated volume at iso-autonomy, based on a reference voyage and its associated energy requirements.

Note on Fuel Blending

As alternative fuels will be in limited supply but improving over the next years, it is worth assessing the effect of fuel blending on regulatory indicators, in order to derive the best possible fuel supply strategy. As an example, Table 5 depicts the effect on compliance of various methanol blends (from natural gas and from renewable electricity).

The orders of magnitude will be equivalent for combustion engine running with Methanol.

Table 5. Methanol blends compliance

Fuel name	% renewable in blend	Compliance year limit (as of Feb. 2023 thresholds)
ng_meoh	0	Never Compliant
meoh_25e	0.25	2035
meoh_50e	0.5	2042
meoh_75e	0.75	2047
emeoh	1	>2060

GREEN FUELS AND DIGITAL TWINS

This section discusses the potential for utilizing digital twins (DTs) for performance analysis of alternative green fuels, as well as for improvements in their manufacturing and transportation (i.e. in terms of required infrastructure), which are pre-requisites for their wider adoption by the maritime industry. In the context of fuels, digital twins can provide detailed, high-fidelity models of the fuel (e.g. its chemical composition and properties), as well as of all processes related to its production, transportation, storage, and utilization. Such models are connected to actual data captured from the fuel through chemical analyses, as well from its direct environment, via sensors. Digital twins allow high fidelity simulations and exploration of different ‘what-if; scenarios regarding the fuel, its behaviour and properties, allowing more efficient and environmentally safe scenarios and methods for its utilization.

According to (Lamanga et al., 2021), regarding carbon-neutral fuels, the aim is the development of digital twins of the power generation plant, containment system and fuel supply system. The deployment of these DTs will enable simulations of the vessel responses in actual voyages with regards to engine response, consumptions (daily rate and total), boil-off rates and power demands for the fuel supply. Based on this a systematic variation/optimization of variables including but not limited to containment system volume, pressure, boil off rate, consumptions and application/selection of handling machinery such as compressors, sub-coolers, shaft generators etc., and auxiliaries such as ventilation systems, automation systems, safety/monitoring/control systems etc. can be conducted. After the generation of an adequate number of design variants each of them can be assessed by simulation and a multi-objective decision making, and design selection can be conducted with the use of utility functions.

In addition, DTs can be used to validate the control and safety schemes, and regulatory compliance of green fuel production techniques such as electrolysis and their integration with industrial plants. (Charbonneau, 2021).

Finally, DTs can be used in research and development of advanced green fuel power conversion technologies such as fuel cells and the storage of them. Currently DTs are used in surrogate modelling methods that combine a state-of-the-art three- dimensional physical model and a data-driven model by different researchers. The result obtained in (Lamanga et al., 2021), concerning the DT of a proton exchange membrane fuel cell, can predict its outputs with a root-mean-square error from 3.88% to 24.80%. Similarly, in (Lamanga et al., 2021), a DT model was made for a solid oxide fuel cell (SOFC), starting from a 1 kW SOFC data were used to regress the parameters to scale-up the model to 25 kW. The final obtained DT was validated by steady-state data and applied to on-site operation prediction with very high accuracy.

CONCLUSION AND FUTURE OUTLOOK

State of Maturity of Green Shipping Fuels

Fossil-based fuels have been essential for industrial transportation, but in order to have a sustainable transport sector and to counteract their detrimental effects, we must move to the greener options that the alternative fuels provide. In order to offset the initial high cost of investment and the high cost of the alternative fuels right now, international organizations and states are developing legislations and rules that benefits the usage of them, but there will be comparative small progress if no market-based measures won't be taken.

One very important question cited in (Lindstad, 2022) regards the impact, to the total global GHG emissions, of decarbonizing the shipping sector, using renewable energy sources, compared to decarbonizing other sectors, namely the electricity production. As it was argued in (Lindstad, 2022 the essential for the decarbonization of shipping resources, if used for the production of electricity can offer 7 to 10 times larger GHG reductions compared to the GHG reduction achieved from decarbonizing shipping. Under this prism, we can understand there are more urgent needs of sector decarbonization than shipping. Moreover, it must be highlighted that the GHG footprint of biofuels (or e-fuels) depends largely on the raw materials that have been used in their production. For example, biogas made from waste has close to zero GHG emissions, while biodiesel made from palm oil can potentially have more than double the emissions compared to the fossil fuels (Lindstad, 2022).

An aspect worth considering is that due to the dependency of the production of energy from renewable sources on the climate, there is an inherited volatility of the production of energy, which is heavily affected by the climate change, which in our days, is more evident than ever (Lindstad, 2022). It is evident that there is a long way to go, both in the technological/research point of view and from the economic/logistics point of view to have a vial and efficient usage of the renewable energy sources in order to decarbonize not only the shipping industry in particular, but the greater issue of energy production and dependency in general, in a holistic approach.

Another consideration is with regards to the substantial investment in additional equipment and storage space that must be made to accommodate green fuels such as hydrogen and ammonia, especially in the case of hydrogen (Energy Transitions Commission, 2019)

Solutions have been proposed such as using large floating solar fields in key areas around the world close to existing shipping hubs and ports. These could provide independent energy for seasonal storage and can provide synthetic, circular fuel to existing infrastructure (shippinh.org-j)

However, the feasibility of such proposed solutions needs to be investigated further. Digital twin technology can support this, by analysing "what if" design scenarios, validate optimized control strategies, enable cost-effective regulatory compliance, validate staff operating procedures, optimize preventive maintenance practices, and upskill operations staff. (Charbonneau, 2021).

Recommendations for Fuel Selection

Based on the previously discussed factors: energy densities, safety and toxicity aspects, availability, logistic requirements, volumes footprint, GHG footprints and conversion systems, as well as taxation policies vs. incentives, it becomes clear that there might not a single solution meeting the maritime decarbonisation targets, even if some of them, namely methane, ammonia and methanol seem to be interesting options.

Indeed, different strategies might be used for different ship types and related operational requirements, taking inro account:

- Fuel characteristics (volume, production pathways, blending, ….)
- Conversion system types
- Optional technologies and systems (Wind Assistance, Cold Ironing, …)

And also, the ship's operators preferences and constraints, i.e.:

- Loss of payload space and ship operational characteristics (e.g. due to changed
- bunkering requirements, operational range, geographic location, etc.)
- GHG Regulatory limitations and related penalties,
- CAPEX, OPEX and financial performances.

Time to commercial availability of greener fuels will therefore depend largely on level of R&D efforts, and even more importantly on the level and speed of which environmental regulations/policies are implemented and incentive schemes are developed. (DNV, 2022)

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Chapter 6
Enhanced and Holistic Voyage Planning Using Digital Twins

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ABSTRACT

The chapter explains techniques and approaches to optimize a ship's voyage in terms of environmental and business parameters, utilizing the digital twin (DT) concept. It demonstrates how voyage planning and navigation management, in general, is enhanced by taking into account vessel state in real time as reflected and analyzed by the digital twin ecosystem. The theoretical backbone of voyage planning entails a multitude of state-of-the-art processes from trajectory mining and path finding algorithms to multi constraining optimization by including a variety of parameters to the initial problem, such as weather avoidance, bunkering, Just in Time (JIT) arrival, predictive maintenance, as well as inventory management and charter party compliance. In this chapter, the authors showcase pertinent literature regarding navigation management as well as how the envisaged DT platform can redesign voyage planning incorporating all the aforementioned parameters in a holistic digital replica of the en-route vessel, eventually proposing mitigation solutions to improve operational efficiency in real-time, through simulation, reasoning, and analysis.

TRADITIONAL METHODS AND CHALLENGES IN VOYAGE PLANNING

Voyage planning involves the holistic enhancement and optimization of a vessel voyage by considering various factors such as weather conditions, fuel efficiency, vessel performance, cargo considerations, and safety protocols. It encompasses a broad perspective and aims to create an overall efficient and effective voyage experience. A subset of voyage planning is route optimization that aims to determine the path that minimizes travel time, reduces fuel consumption, and enhances overall operational efficiency,

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taking into account factors like weather patterns, currents, wind conditions, traffic congestion, and other navigational challenges.

In recent years, there have been several state-of-the-art solutions for route optimization and weather routing in the maritime sector. One popular approach to routing optimization is to use dynamic programming that takes into account various parameters, such as the ship's speed, the sea conditions, and the distance to the destination. These models can be used to generate optimized routes that minimize fuel consumption while ensuring that the ship arrives at its destination on time. One example of such a model is the BunkerOpt system developed by DNV GL, which uses a mathematical model to calculate the optimal speed and route for a ship based on real-time data.

Another approach to routing optimization is to use machine learning algorithms to predict weather patterns and optimize routing accordingly. For example, the Weather Intelligence for Shipping (WIS) system developed by StormGeo uses machine learning to predict weather conditions up to ten days in advance, allowing ships to adjust their routes to avoid adverse weather conditions and reduce fuel consumption.

Pertinent literature regarding smart and efficient transportation in the industry (supply chain optimization, autonomous vehicle, logistics management, voyage planning) as well as regarding societal frameworks (traffic management, public transportation networks, suburban mobility), concerns a variety of multi-constraint optimization methods varying from Genetic Algorithms (Xing Wei and and Huang, 2021), Simulated annealing (Fermani et al.,2021) and Particle Swarm Optimization (Chondrodima et al., 2020) to AI integrated decision making using Reinforcement Learning (Kaklis et al., 2022, Kaklis et al., 2023, Bai et al., 2019) or Natural Language Processing (NLP) based approaches (Garg et al., 2021). The aforementioned practices and methodologies attempt to exploit the proliferation of IoT devices and state-of-the-art communication networks (5G) to build self-contained Information Hubs and provide a sustainable, safer and cost-effective transportation.

In the maritime sector, the optimization criteria adopted in the context of the ship routing problem deal with the minimization of voyage time, fuel consumption (or Fuel Oil Consumption, FOC) and voyage risk. The approaches, which have appeared so far in the literature, can be classified into three broader categories:

- Vessel-based optimization, which aims in optimizing a given route with respect to vessel characteristics, e.g., vessel speed, main-engine rotational speed, draft, trim and sea-keeping behavior: roll, heave and pitch motions, (Roh and Lee, 2018);
- Environmental-based optimization, which aims in optimizing a given route by taking into account environmental conditions, e.g., wind (speed, direction), wave (height, frequency, direction), currents. (Kim and Kim, 2017);
- Holistic optimization that combine the two previous approaches in a common context. (Vettor and Soares, 2015; Varelas et al., 2013).
- Analytical approaches trying to tackle the problem with the use of exact (NP-complete) and/or heuristic algorithms like label-setting algorithms, non-linear integer programming, or simulated annealing (Shin et al., 2020).

In order to incorporate more constraints, several methods split a vessel's voyage into areas of critical interest, involving for example zones of extreme weather conditions, emission control areas (ECAs, SECAs), high-risk zones (piracy), etc. Then, they seek for Pareto optimal solutions from a set of routes that are optimal in terms of Expected Time of Arrival (ETA), FOC, and safety, or they use Genetic Algorithms (Kim et al., 2017) in order to find the best route, as a composition of optimal route segments.

Methods like PSO (Particle Swarm Optimization) (Zhao et al., 2020) are also employed in order to solve the multi-constraint, non-linear optimization problem of optimal route planning.

The techniques employed in the literature for estimating FOC based on vessel characteristics and/or environmental conditions can be grouped into the following categories:

- Data-oriented approaches that combine vessel-trajectory data, gathered from sensors, satellites (AIS data), or Noon Reports, with Machine and Deep-Learning algorithms. These techniques range from simple Regression analysis like Support Vector Regression, Lasso Regression, and Polynomial Regression to ensemble non-parametric schemes like Random Forest (RF) regression, Decision Trees, or AdaBoost. Some studies have also experimented with baseline sequential Artificial Neural Networks (ANN) by tuning a number of hyperparameters (learning rate, number of neurons, number of layers, activation function). (Jeon et al., 2018, Gkerekos et al., 2019).
- Approaches where machine learning (ML) methods (also known as black-box models - BBM), are combined with theoretical models (also known as white-box models - WBM), such as the equations of motion of a freely floating body moving with constant forward speed, in order to increase the prediction accuracy. The proposed models are known as gray-box models (GBM) (Coraddu et al., 2017, Kaklis et al., 2019).

ANNs have been at the center of attention lately in many research areas. As far as vessel FOC is concerned, not many studies utilize the computational power of ANNs to approximate FOC mainly due to the problem of missing historical data. The studies found in pertinent literature dealing with FOC estimation from a deep learning perspective are presented briefly below. Some studies experiment with baseline sequential ANNs by applying a dropout in the weights in order to achieve better generalization error (Gkerekos et al., 2020) or by tuning a number of hyperparameters (learning rate, number of neurons, number of layers, activation function) utilizing brute force methods like randomized grid search (Papandreou et al., 2020, Jeon et al., 2018). In (Yongjie et al., 2020) a Recurrent NN is employed in order to estimate FOC but without further research as far as the architecture, or the generalization capabilities of the neural proposed.

The majority of the approaches found in literature regarding Operational Optimization and Navigation Management in the maritime sector, concern the implementation of standalone services in the sense that they are employing isolated information silos that lack the support mechanisms and enhancement of a centralized Information Hub that exploits the upsurge of IoT and Industry 4.0 advancements, to train, validate and update these services in real-time. Furthermore, they are usually tested on a single vessel and therefore lack the generalization capabilities of models evaluated in a variety of ships that are able to adjust and adapt to the underlying function that describes the relationship between FOC and each specific vessel, continuously, by exploiting the vast amount of data collected by IoT installations. Frameworks and technological advancements regarding the continuous monitoring of the vessel are inextricably linked with the emerging concept of the so-called Digital Twin in the shipping industry, as they employ a digital replica of the en-route vessel that is able to simulate-project and validate in real time the majority of the operational procedures.

In recent years, there has been a growing interest in using Digital Twins to optimize routing in the maritime sector. Digital twins serve as virtual replicas of physical systems, offering a dynamic platform

Table 1. Navigation management and operational optimization approaches in the literature

Category	Sub-Categories	Approach/Methodology	Input Data	Example Models or Systems
Smart & Efficient Transportation (Beyond Maritime)		Multi-constraint optimization methods: Genetic Algorithms, Simulated Annealing, Particle Swarm Optimization, AI integrated decision making, NLP.	Real-time traffic data through various sensor installments on EDGE	Xing Wei and Huang, 2021 - Fermani et al., 2021 - Chondrodima et al., 2020 - Kaklis et al., 2022, 2023 - Bai et al., 2019 - Garg et al., 2021
Ship Routing Optimization	Vessel-based optimization	Multi-constraint optimization methods	Weather data/ Operational Data/ Charter Party contracts	Roh and Lee, 2018 - Kim and Kim, 2017 - Vettor and Soares, 2015 - Varelas et al., 2013
	Environmental-based optimization	Dynamic Programming		
	Holistic optimization	RL, Dynamic Programming		

to simulate, analyze, and control real-world conditions. Unlike traditional methods that depend on historical data or pre-set conditions, digital twins make use of real-time analytics. This live data feed can include everything from a vessel's hull condition and load status to the available fuels and engine performance. The implication is a quantum leap in the level of granularity and customization that voyage planning algorithms can achieve.

By embracing this real-time, vessel-specific approach, maritime operators can leverage sophisticated algorithms designed to interpret and act upon a cascade of live data points. As a result, voyage planning becomes a dynamic process, continually updated to reflect the vessel's current actual condition. This increased level of detail not only allows for more precise route optimization but also leads to safer and more efficient voyages. Whether accounting for the wear and tear on a hull over a journey or optimizing fuel consumption based on real-time metrics, digital twins provide a holistic and up-to-the-minute view that is revolutionizing voyage planning.

In the table below we summarize the approaches found in pertinent literature regarding Navigation Management and Operational Optimization and provide the reader with a comprehensive-consolidated breakdown analysis based on the specific methodology adopted as well as input data utilized on each category.

Towards this direction, a novel approach that aims to extend a Digital Twin framework with a Voyage Planning module in the context of a multimodal-adaptive Digital Twin ecosystem will be proposed. This extension enables stakeholders to simulate diverse scenarios and optimize routes using real-time data, considering factors like weather, traffic, fuel consumption, hull conditions, and commercial considerations. Through the integration of various data sources and the application of machine learning algorithms to forecast future conditions, stakeholders can dynamically optimize routes, leading to cost reduction, enhanced safety, and improved efficiency.

Section 2 outlines the proposed perspectives to enhance voyage planning beyond route optimization and weather routing, leveraging the opportunities provided by the digital twin platform.

Section 3 provides a brief overview of the digital twin framework proposed for accommodating the voyage planning application.

Section 4, we delve into the methodologies for estimating fuel oil consumption and weather routing, both fundamental components of any voyage planning tool. We explore how these methodologies can be extended to leverage the benefits of the digital twin.

Section 5 offers considerations for potential advancements that could enhance the value of the proposed solution, as well as acknowledging certain limitations.

The chapter concludes Section 6 with a summary of voyage planning using digital twins.

INTEGRATION OF VESSEL OPERATIONAL AND COMMERCIAL ASPECTS IN VOYAGE PLANNING

In the traditional paradigm of voyage planning, strategies often rely on static data models and broad generalizations. These generalizations, while useful for general navigational purposes, fall short of accounting for the dynamic and ever-changing conditions of individual vessels. In this section, we propose specific vessel operational aspects that hold value for integration into the digital twin, aimed at enhancing voyage planning. It's notable that some aspects discussed are innovative for voyage planning, and we'll demonstrate how this innovation is further enhanced by the application of digital twins.

Trim Optimization

Trim is defined as the draft at the stern (or aft of the ship), minus the draft at the bow (or forward). Trim optimization is one of the approaches considered by the industry to improve the energy efficiency of ships, having a potential in both reducing operational costs and to decrease the emissions of the ship. Trim optimization is the selection of trim with the goal of fuel consumption reduction, by ballast water management and load distribution, which can be done without significant changes to the ship structure. The application has been investigated by Gao (2019) and Islam (2019).

The MEPC (2008) has estimated that optimizing a vessel's trim and draft can result in fuel consumption reductions ranging from 0.5% to 3% for most vessel categories. In the case of ships operating with partial loads, these savings can soar to as high as 5%. Coraddu (2017), in their research, have even demonstrated the potential for surpassing a 2% improvement in fuel consumption for handymax chemical tankers. A case study conducted by DNV-GL in 2013, which assessed the effectiveness of the commercial optimization tool known as the ECO Assistant, revealed impressive fuel savings ranging from 2% to an astonishing 14% across various draft and speed combinations for handymax bulk carriers. Furthermore, research by Yuan (2018) indicates that trim optimization for Very Large Crude Carriers (VLCCs) can lead to a notable 1.8% reduction in fuel consumption. The work of Du (2019), revealed that trim optimization has the potential to save between 5% and 6% of bunker fuel for 9000 TEU container ships. Similarly, Gao (2019) reported significant bunker fuel savings of 3% to 7% for Pure Car and Truck Carriers (PCTCs). In conclusion, it is evident that the impact of trim optimization on reducing fuel consumption can be substantial, with the extent of savings contingent upon factors such as the vessel's type, operational profile, and maneuverability in achieving the desired trim.

Typically, the optimum trim is often ascertained through reference trim tables. These tables are derived either from model-scale towing experiments or, in certain instances, from computational fluid dynamics (CFD) simulations. In the past years, alternatives to trim tables in the field of trim optimization have emerged. A range of commercial trim optimization solutions have been introduced to the market, offering diverse pricing options, levels of user-friendliness, underlying methodologies, and performance capabilities, as per MEPC (2008)

Integrating trim optimization into voyage planning with the assistance of a digital twining platform offers numerous advantages. On one hand, incorporating trim information into the fuel oil estimation process enhances the precision of voyage planning predictions, contributing to a well-informed, dynamic digital twin. On the other hand, since the primary goal of voyage planning is to minimize fuel oil consumption, integrating trim optimization aligns seamlessly with this objective.

Within the digital twin framework, calculation algorithms are continuously supplied with real-time data, including parameters essential in describing the relationship between trim and fuel oil consumption. Notably, hull condition, a critical factor often overlooked in trim optimization scenarios without access to real-time data, is meticulously addressed in digital twin applications. Furthermore, the temporal and spatial variations in weather conditions can be effectively taken into account through digital twin-powered trim optimization. Additionally, the intricacies of cargo management, particularly in cases of partial loading and unloading in port calls, can be seamlessly integrated into a digital twin application, providing trim optimization without requiring extensive crew involvement.

Route/Port Congestion and JTI

Reducing speed is the most essential method to reduce fuel oil consumption. ABS (2021) investigated the potential efficiency improvements created by just-in-time shipping by presuming an average 5 percent reduction in speed, assuming no impact on cargo-carrying capacity and no adjustment to the size of the fleet. Based on that basic analysis, the CO2 emissions savings are around 10-11 percent annually.

For a number of years, the use of data from automated identification systems (AIS) has made it possible for the industry to operationally benefit from knowing details such as the estimated time of arrival, the arrival port, draught and navigational speeds, etc.

Those data points are being used today to track vessels and to support limited adjustments to voyage planning. However, deeper analyses of the data on vessel positions and berth availability are revealing the type of information that soon could make 'just-in-time' shipping a reality.

Improving communication efficiency between vessels and ports regarding berth availability and services like tug operators holds the promise of optimizing marine traffic, delivering both commercial and environmental advantages. In the context of the discussion in this chapter about the digital twin as a dataspace actor, this concept can play a pivotal role in realizing these improvements.

Digital twins inherently exist in the digital realm, and they can offer a more seamless interface with other IT systems compared to AIS (Automatic Identification Systems). Furthermore, they can provide enriched information for a ship's voyage plan and conditions, enhancing operational effectiveness.

Conversely, data regarding shore-side infrastructure availability and readiness can be automatically accessed and factored into real-time voyage planning. This two-way flow of information, facilitated by digital twins, has the potential to significantly enhance the efficiency and sustainability of maritime operations.

Bunkering Optimization

In engines that run on oil-based fuels, different types of fuel are necessary to ensure vessels comply with regulations. These fuel types include Heavy Fuel Oil (HFO), Low Sulfur Fuel Oil (LSFO), Very

Low Sulfur Fuel Oil (VLSFO), and Marine Gas Oil (MGO). Furthermore, globally, alternative fuels are emerging as environmentally viable options to oil-based fuels. As reported by DVC GL (2019), among the fuel alternatives to marine bunker oil, LNG is the most prolific with more than 300 ships in operation. In addition to LNG, biofuels and methanol are available in certain ports. Several types of dual-fuel engines have been introduced in the market which increases fuel flexibility significantly. Beyond LNG, fuels such as methanol, ethanol, LPG (liquid petroleum gas) and soon likely also ammonia can be burned in different types of dual fuel engines, in addition to HFO/MGO. Promising steam- and gas- turbine concepts are also being considered.

The accessibility of fuels in close proximity to vessels for bunkering purposes significantly influences voyage planning. Additionally, varying fuel prices at different bunkering locations play a crucial role from a commercial standpoint. It's worth noting that storing fuels in vessel tanks contributes to increased displacement, subsequently impacting fuel oil consumption.

Integrating digital twin technology in real-time to monitor fuel type availability and prices at different locations, on one hand, and tracking fuel tanks' arrangement, capacity, and current levels, on the other, can introduce bunkering optimization as an innovative and transformative element in voyage planning. This approach enhances both operational efficiency and cost-effectiveness by making data-driven decisions about fuel sourcing and consumption during voyages.

Supplies On-Boarding Location and Frequency

In addition to applying digital twins for monitoring vessel seagoing performance and cargo operations, there is a growing focus on enhancing internal operations. One significant area of improvement is condition-based maintenance, which can be effectively facilitated through the capabilities of digital twins. In a broader perspective, the digital twin can proactively anticipate and track the spare parts required over time, streamlining maintenance processes and improving overall operational efficiency.

Integrating spare part supply into voyage planning can have a profound impact, enhancing onboard availability while concurrently reducing freight costs. By optimizing the supply location and timing, vessels can ensure that necessary spare parts are on hand when needed, minimizing downtime and maintenance delays. This proactive approach not only improves operational efficiency but also contributes to cost savings in the long run, making it a valuable component of comprehensive voyage planning strategies.

The realization of this approach is enhanced by the digital twin's predictive maintenance component that estimates in real time machinery condition and thus forecast spare parts needs

Hull Degradation and Hull Cleaning Effectiveness

Biofouling, namely the undesirable accumulation of microorganisms, algae, and animals on artificial surfaces immersed in seawater results in performance decay of hull and propellers, as discussed in XXX.

The substantial impact of biofouling on fuel oil consumption is widely acknowledged. For instance, in studies conducted by Watanabe (1969), which involved rotor and towing tank experiments, they identified a frictional resistance increase ranging from 8% to 15%. Similarly, Farkas (2020), employing Computational Fluid Dynamics (CFD) simulations, found that the total resistance increased by 50% to 120%. Moreover, Schultz's (2015) research, which included laboratory-scale drag measurements and analysis based on boundary layer similarity laws, revealed a total resistance increase of approximately 10% for a light slime film and around 20% for a heavy one. In certain cases, the total resistance increase was even more pronounced, ranging from 35% to 86%. These findings underscore the significant impact of biofouling on vessel performance and the need for effective anti-fouling measures to mitigate fuel consumption increases.

Techniques to reduce the impact of biofouling are underwater cleaning of the hull, propeller polish and application of antifouling coatings. However, effective maintenance can be responsible for up to 20% of total operational costs and, therefore, is a perfect candidate for optimisation and improvement.

Methods to mitigate the impact of biofouling include underwater cleaning of the hull, propeller polishing, and the application of antifouling coatings. However, effective maintenance practices can account for up to 20% of the total operational costs, as reported by Valchev (2022). Hence, optimizing and improving these maintenance processes present excellent opportunities for cost-saving measures in maritime operations.

Voyage planning is significantly influenced by hull degradation, and a digital twin can play a pivotal role in ensuring that the voyage planning model and its associated attributes remain updated with the actual state of the vessel. Furthermore, the digital twin can provide estimates of the benefits derived from corrective actions, such as underwater cleaning, and their impact on both operational and commercial performance. For instance, if underwater cleaning is conducted before a voyage, it may introduce operational costs and time delays into the journey. However, these factors can be offset by the improved efficiency and reduced fuel oil consumption during the voyage. Unlike dedicated systems for hull performance assessment, fuel oil consumption estimation, and voyage planning, the digital twin serves as a central system that maintains all the necessary real-time information required to assess and execute such actions effectively. This centralization of data and insights enhances decision-making in maritime operations.

AN OPEN DIGITAL TWIN FRAMEWORK FOR VOYAGE PLANNING

A Digital Twin, adapted to the needs of the maritime sector, constitutes a virtual holistic representation of the vessel that spans its life cycle and is updated from near to real-time data, utilizing simulation, machine learning and reasoning to help in decision-making, sensing and control actuation. By combining core structural properties of traditional MIS and digital twins, organizations can gain a better insight of their internal operations and pave the way for a fully automated and fault tolerant decision-making procedure, substantially improving their efficiency and effectiveness.

The framework developed within the scope of the DT4GS Horizon Europe research project, parts of it are described in the preset work, consists of a variety of SOTA tools and services that aim to vastly automate the majority of the procedures concerning the existing Voyage Planning in several ways, incorporating a variety of state-of-the-art streaming tools for real-time analysis of vessel data as well as tools for continuous integration/deployment (CI/CD) of ML/DL models regarding operational optimization, causal analysis, and event recognition. The resulting platform constitutes a prototype version of a virtual replica of a vessel that aims to assist shipowners to achieve efficiency in fleet management with tangible benefits in terms of emission reduction, environmental compliance and protection of crew safety onboard. In addition, DT4GS framework can also facilitate the refinement of the existing Voyage Planning framework by providing a platform to test different scenarios and strategies in the form of an adaptive Decision Support System. This can include simulating different routes, adjusting speeds, or optimizing the vessel's trim to reduce fuel consumption. By testing these strategies in a virtual environment, companies can identify the most efficient and cost-effective approach to the voyage and define tailor made mitigation strategy towards a carbon neutral operational blueprint.

Specification of the Digital Twin Framework

The present section discusses the specification and requirements relevant to a Digital Twin capable for voyage planning, to ensure a consistent and effective implementation, promoting seamless integration and interoperability among the various required components.

Data Acquisition and Integration

In the past years the main source of information for vessel operation resulted from the noon report, which was compiled manually by vessel crew and was sent to the Head Quarters (HQs) with the available means of communication. Increasingly, ship data used for various purposes including building the digital twin are collected automatically, from sensors. To keep track of metadata and to structure the storage and processing of sensor data, there is a need for a unique identification of sensors as well as the components and systems subject to monitoring by sensors, as suggested by LÅG (2017).

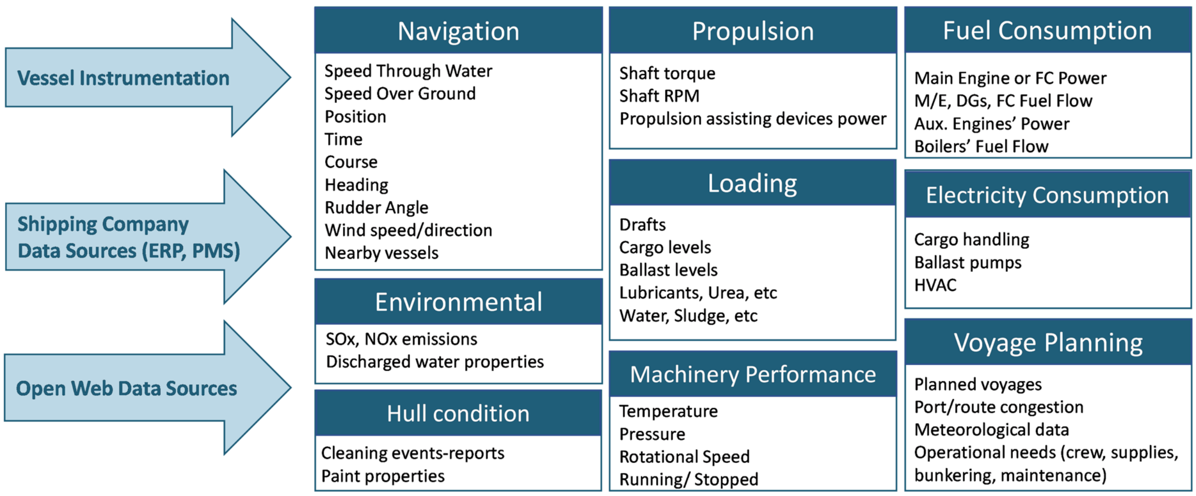
Within the context of voyage planning, data is required for the following purposes:

- To compose a digital shadow, mirroring actual vessel condition, to compare against the digital twin (simulated values) for integrity verification.
- To feed the models that reproduce vessel operation and compose the digital twin, such as training models.
- To provide the required information, such as green fuel availability and cost, port congestion, weather forecast for weather routing, etc.
- There exist three sources to acquire the required data.
- Vessel instrumentation,
- Shipping company's core systems that provide information about voyage planning, spares/stores deliver, crew on-boarding, planned maintenance, etc.
- Web data sources: weather forecast, etc

In Figure 1 are listed the most important parameters required for the deployment of a Shipping Digital Twin.

The methods for integrating vessel instrumentation depend on the available technologies, often influenced by the vessel's build year. Typically, data acquisition on ships involves various protocols such as NMEA (standard for navigational instruments), Modbus serial or TCP, HART, UDP broadcasts, analog signals (e.g., pulse, 4-20mA), SNMP, or REST APIs. Centralized sources of combined data, like the AMS, collect operational data from various subsystems of the vessel and provide it through serial communication or over LAN using protocols like NMEA, proprietary, or Modbus. Other sources of combined data include the VDR, engine control system for electronic engines, tanks level and drafts monitoring system (connected to the loading computer), power management system, and fuel conditioning system. Additionally, individual instruments like flowmeters, level sensors, torque meters, temperature, and pressure transmitters can be integrated separately.

Figure 1. Data required for the formulation of digital twin



Data Processing and Analytics

To depict a unified vessel condition, simultaneous sampling of all signals is required. A reference procedure is described in ISO 19030-2 (2016). However, in most cases, the sampling rate is not configurable, except for analog data acquisition and communication with raw sensors using request-reply protocols. To address this matter, data temporal bucketing can be applied for data synchronization in the context of a digital twin IT system. As data streams from various sources arrive at irregular intervals, temporal bucketing organizes the data into fixed time intervals, typically referred to as buckets. This process enables aligning the data to a common time scale, ensuring that all data points are associated with a specific time frame, which is crucial for generating a unified and coherent view of the vessel's condition. However in the decision of the bucketing interval length it should be taken in to account that the data sampling rate may coincide with the frequency of a natural phenomenon for the vessel in question (e.g. wave encounter frequency) and thereby influencing the accuracy of associated data point.

In addition to synchronization, data temporal bucketing allows for the creation of new variables based on existing data. By aggregating or summarizing data within each bucket, it becomes possible to compute derived quantities or perform statistical analyses. Some examples are the following:

- Fuel flows calculations such as M/E FOC = M/E INLET FOC – M/E OUTLET FOC
- Fuel mass flow estimation using volumetric flow, nominal density (at 15oC) and actual temperature
- Estimation of absolute wind speed from relative wind speed, wind direction and heading
- Unit conversions form instrument specific unit to platform standard
- Estimation of system and operational performance indicators

As the digital twin's accuracy directly relies on the data quality used in its construction, identifying data-related issues and defining specific requirements becomes critical. Poor data quality, such as missing values, outliers, or inaccuracies, can lead to erroneous simulations and unreliable predictions.

Therefore, it is essential to implement robust data validation mechanisms to identify and rectify data anomalies. Data quality checks should be performed at various stages, from data acquisition to temporal bucketing and variable creation. In cases where data discrepancies are detected, appropriate corrective actions or data cleansing processes should be applied to maintain the integrity of the digital twin system. Statistical method for outlier detection, such as Chauvenet's criterion, and rule based mechanisms can provide a means for data integrity. Custom data cleansing methods as the one described in the following paragraphs are also applicable.

Data Storage

The choice of data storage solution for the digital twin system depends on the specific implementation and requirements. There are various options available, each with its own strengths and use cases. Some common data storage solutions include:

- Relational Databases (e.g., PostgreSQL, MariaDB): Relational databases are well-established and widely used for structured data storage. They offer robust data integrity, support for complex queries, and data consistency through ACID (Atomicity, Consistency, Isolation, Durability) properties. Relational databases are suitable when data relationships and schema are well-defined and stable.
- NoSQL Databases (e.g., MongoDB): NoSQL databases are designed to handle unstructured or semi-structured data. They provide greater flexibility and scalability compared to relational databases, making them suitable for scenarios where data schemas may evolve over time or data volume is large and continuously changing.
- Time Series Databases (e.g., influxDB): Time series databases are optimized for handling time-stamped data, making them particularly suitable for storing sensor readings, historical performance data, and other time-related data. They provide efficient data retrieval based on timestamps and support data compression techniques for storage optimization.

From the perspective of the platform requirements, adherence to a strict definition of variables registry is crucial. This means that each measurement or data point should have a solid reference or metadata that precisely defines what it represents. Having a well-defined variable registry ensures consistency in data representation, avoids ambiguity, and facilitates effective data analysis and interpretation.

By adhering to a strict variable registry, it can be achieved a clear mapping between the data stored in the database and the physical or virtual variables it represents, across the different DT implementations on different applications (different ships, etc) which result in interoperability. An application would be the ability to transfer knowledge between dt instances and also reuse resources, such as simulation models.

Regardless of the specific data storage solution chosen, data retention policies, and backup strategies which may vary between implementations, ensuring a solid variable registry and well-defined metadata for each measurement is fundamental for maintaining data quality and facilitating the seamless functioning of the digital twin system. This approach promotes consistency, accuracy, and reliability in data-driven simulations and decision-making processes.

Simulation and Modelling

Indicatively, simulation is applied for the following purposes:

- Forecast future conditions: Simulation is used to predict and model the future behavior of the system or process based on current conditions and known parameters.
- Estimate parameters required for generating the digital twin but not directly available: Sometimes, certain parameters essential for building the digital twin may not be directly obtainable from data. Simulation helps estimate these parameters through modeling and analysis.
- Estimate the effect of a change in performance: Simulation allows for testing different scenarios and changes in the system to understand their potential impact on performance and outcomes.

Assist in the acquired data validation or event detection (failure) by detecting patterns that deviate from the simulation results: The digital twin can aid in data validation by identifying discrepancies between real-world data and simulated results. These deviations can indicate data quality issues or reveal anomalies that require investigation. On the other side the same approach can be utilized for the detection of deterioration events assisting in their early detection.

The modeling framework for the digital twin system must have the following main characteristics:

- Support for single moment simulation, time steps, and events based: The framework should be capable of conducting simulations at specific time points, discrete time intervals, or in response to specific events or triggers.
- Support for dockerized code, Python, Java, FMI, R: The framework should be versatile and support different programming languages and technologies, allowing flexibility in implementing and integrating simulation models.
- Integration with data-driven model instantiation and versioning systems (such as MLflow): Seamless integration with data-driven models and version control systems enhances reproducibility, transparency, and management of different model versions.
- Description of model source (e.g. binary) and versioning: The framework should provide mechanisms for storing and managing simulation models, including version control to track model changes over time.

An important aspect of modeling is its utilization for optimization purposes. Optimization is a crucial requirement for DT systems, and the following approaches are considered:

- Repetitive procedure for determining the best solution based on predefined scenarios and variable ranges: This approach involves iteratively testing different combinations of variables within specified ranges to identify the optimal solution.
- Similar approach based on Monte Carlo principles instead of using predefined scenarios: In this approach, random sampling is used to explore a wide range of possible scenarios, allowing for a more comprehensive optimization analysis.
- Utilization of genetic algorithms, such as NSGA II: Genetic algorithms mimic the process of natural selection to iteratively evolve and refine potential solutions, making them well-suited for multi-objective optimization problems.

By employing these optimization approaches, the digital twin system can identify optimal configurations, settings, or decisions that lead to improved performance, efficiency, or other desired outcomes for the modeled system or process.

System Monitoring and Diagnostics

A Digital Twin (DT) system requires robust functionality for self-monitoring and diagnostics to ensure its own health and performance. The system should continuously monitor critical metrics, such as resource utilization, response times, and event logs. Real-time performance monitoring, resource tracking, and health checks are essential for identifying anomalies and potential issues within the system. The DT system should generate alarms and alerts for abnormal conditions and include an auto-recovery mechanism to handle failures autonomously. It must offer diagnostic tools and historical performance data for troubleshooting and trend analysis. Scalability and security monitoring are crucial to ensure the system can handle increasing workloads and maintain data integrity. Integration with IT operations tools facilitates centralized management and analysis. By implementing these functionalities, the DT system can maintain its reliability, optimize performance, and provide a stable foundation for effective digital twin operations in diverse scenarios.

Compliance and Standards

According to the degree a DT interacts with the physical vessel, the corresponding shipping industry standards, elicited by the IMO, the Institute of Electrical and Electronics Engineer (IEEE) and rules of Classification Societies, should be adopted. The lowest level of interaction is observed in the case of simple data acquisition, while at the other end of the spectrum, there are aspects related to autonomy, which significantly increase the requirements related to compliance to regulations.

The Digital Twin as a Dataspace Actor

As per Nagel (2021), dataspace can be defined as “A data ecosystem, specified by a sector or application, whereby decentralized infrastructure enables trustworthy data sharing with commonly agreed capabilities”. Thus, a dataspace is produced by an ecosystem of actors that interact through the sharing of data.

A Shipping Dataspace provides the data infrastructure, specifically data connectors, for creating, managing and interacting with actors, such as weather data providers, fuel availability and pricing data providers, route and port congestion data providers, commercial brokers, and supplies availability data providers. Integration of DT in the dataspace can assist in Information exchange between them, in a uniform and secure way, providing them with collective knowledge. Another aspect cohering to the DT functionality and the dataspace is model sharing and co-simulation on an open or commercial basis. Furthermore development of applications interacting with DTs is enhanced by the standardization that the dataspace offers.

Setting up a dataspace with weather data providers, fuel availability and pricing data providers, route and port congestion data providers, commercial brokers, and supplies availability data providers provides seamless integration of these sources of information.

Dataspace components provide the appropriate infrastructure to collect, store, and analyze data from various sources in real-time. It uses a distributed architecture that enables the processing of large volumes of data while ensuring scalability and reliability. Dataspace provides a variety of processing capabilities, such as filtering, aggregation, and data augmentation, that can be used to further optimize the Routing Optimization module.

THE APPLICATION OF THE DIGITAL TWIN FRAMEWORK IN VOYAGE PLANNING

The following paragraphs focus on the realization of the specific case of FOC estimation and Routing Optimization, by consolidating the aforementioned components of the broader DT4GS frame, towards a holistic Operational Optimization Digital Twin suite that aims to improve voyage efficiency and environmental compliance.

Reference Implementation

In the present section is described a DT implementation conducted within the scope of the DT4GS research project, which is in progress at the time that this chapter is authored. In Figure 2 is provided the implementation of the framework in terms of building blocks. A messaging system is engaged to distribute data, events, and triggers to the intended peripheral components. Storage, permanent and temporary, for both configuration and data, is achieved by the combination of a time series database, a nosql database, a knowledge graph for metadata storage and a cache. The ingestion is achieved using internal connectors for data originating from the vessel, external connectors for external data sources such as CRM systems or the internet (sources not possible to be integrated into the dataspace). Data is also exchanged with the dataspace via an IDSA compliant connector. Peripheral components exist also for the following purposes:

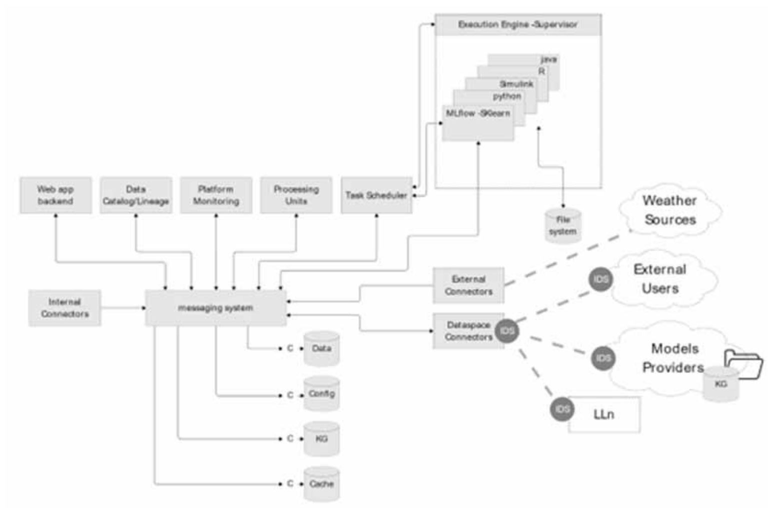
- Web app backend
- Data catalog/lineage
- Platform monitoring tools
- Processing units, assisting ingestion, producing composite variables and simple calculations Task Scheduler
- Model Execution Engine

Fuel Oil Consumption Estimation Methodology

Feature Selection

In order to unveil the relationships between the independent variables as well as their importance and role in estimating FOC, we conduct an initial exploratory analysis with Random Forest regression as the feature ranking algorithm. Then calculate the correlations between the most important features and conclude to an ideal feature set that consists of independent variables that will be utilized accordingly in the context of FOC approximation.

Figure 2. Overview of an implementation



Decision Trees (DT) is a popular classification or regression algorithm that takes into account the importance of features. More specifically, the feature importance defines the order in which features are selected for splitting the initial set of samples to subsets, from the tree root to the leaves. It is defined by the decrease in (tree) node impurity, which is weighted by the node probability. This probability is the number of samples that reach the node, divided by the total number of samples. Higher decreases in impurity denote more important features.

Assuming only two child nodes (left, right) for each node, the node importance is given by the following equation:

$$ni_j = w_j C_j - w_{left(j)} - w_{left(j)} C_{right(j)}$$

where nij is the importance of node j for feature i, wj is the weighted number of samples reaching node j and Cj is the impurity of node j. Impurity is measured using Gini Index or Entropy.

The Random Forest (RF) algorithm extends the concept of Decision Trees, for high-dimensional data, by constructing many individual decision trees during training, using each time a different random subset of the initial set of features. It then collectively examines the predictions of trees in order to make the final prediction. Respectively, RF can be used to evaluate the importance of each feature across all the trees and provide a more comprehensive ranking of feature importance.

In Table 2 we depict the experimental results from conducting regression analysis utilizing RF regression in order to rank the importance of the aforementioned features in estimating FOC.

Besides selecting the most important (i.e. informative) features, we also aim to avoid selecting highly correlated ones. For this purpose, we utilize the Spearman's Rank Correlation (SRC) coefficient. The Spearman's rank-order correlation is the non-parametric equivalent of the Pearson product-moment correlation (ρ) and assesses the strength and direction of the monotonic relationship between two ranked variables R(Xi), R(Yi) using covariance and standard deviation σ, and is calculated as follows:

$$\rho R_{(X),R(Y)=} \mathrm{cov}(R(X), R(Y)) / \sigma R(_{X)\sigma R}(Y_{)}$$

Table 2. Feature ranking using RF

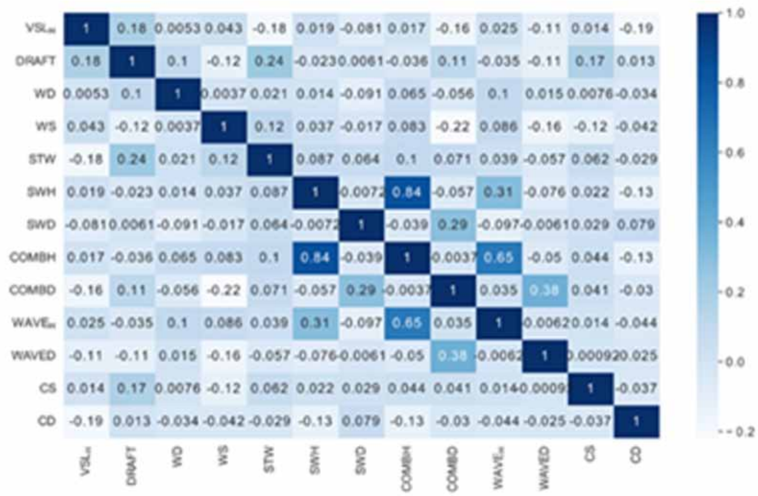
Ranking	Feature	Importance
1	STW	0.94
2	WS	0.13
3	DRAFT	0.011
4	VSL_H	0.005
5	COMBH	0.0058
6	SWH	0.0054
7	CS	0.004
8	$WAVE_H$	0.0039
9	SWP	0.0036
10	COMBD	0.0032
11	SWD	0.0028

Assembling the ranking of features depicted in Table 2 and the correlation coefficients calculated, depicted in Figure 3 using Algorithm 1, we conclude with a subset of the initial feature set that combines feature importance and independence.

Algorithm 1 Feature selection based on RF regression importance and Spearman Correlation.

Require: `featureSet` $\mathcal{F} \leftarrow$ top 10 from RF
Require: `featureSet` $\mathcal{F}_r \leftarrow$ rest of features from RF
Require: `correlations` $Corr \leftarrow$ from SRC
Require: `importances` $\mathcal{I}mp \leftarrow$ from RF
for each $f_i \in \mathcal{F}$ **do**
  set $\bar{\mathcal{F}} = \mathcal{F} \setminus \{f_i\}$
  for each $f_k \in \bar{\mathcal{F}}$ **do**
    if $Corr(f_i, f_k) > 0.5$ **then**
      if $Imp[f_i] < Imp[f_k]$ **then**
        delete f_i From $\mathcal{F}$
        set $f_{temp} = f_k$
      else
        delete f_k From $\mathcal{F}$
        set $f_{temp} = f_i$
    for each $f_r \in \mathcal{F}_r$ **do**
      if $Corr(f_{temp}, f_r) < 0.5$ **then**
        add f_r to $\mathcal{F}$ and **break**
    if $f_{temp} = f_k$ **then**
      break
Return $\mathcal{F}$

Figure 3. Spearman correlation heatmap



Data Cleaning

Raw data, collected from the sensors of the vessel, are in time-series (minutely) form and tend to be ``noisy'' (high variance, high standard deviation from the mean) and in some cases even erroneous. In order to remove noise, we employed a fit\filter technique that effectively ``cleaned'' the data but at the same time kept the bulk of information needed for training robust predictive models.

Data filtering was implemented in two stages. First, assuming that the dataset follows a normal - like distribution, we keep the data points that lie within the 99\% confidence interval around the mean.

Then we apply an appropriately designed Decision Tree based algorithm in order to further cancel the noise in FOC target distribution caused by the flowmeter sensor on the vessel. Then, we proceed to transform our dataset into 15-min rolling window averages in order to further smooth out any spikes and outliers that occur in the feature set from sensor installments.

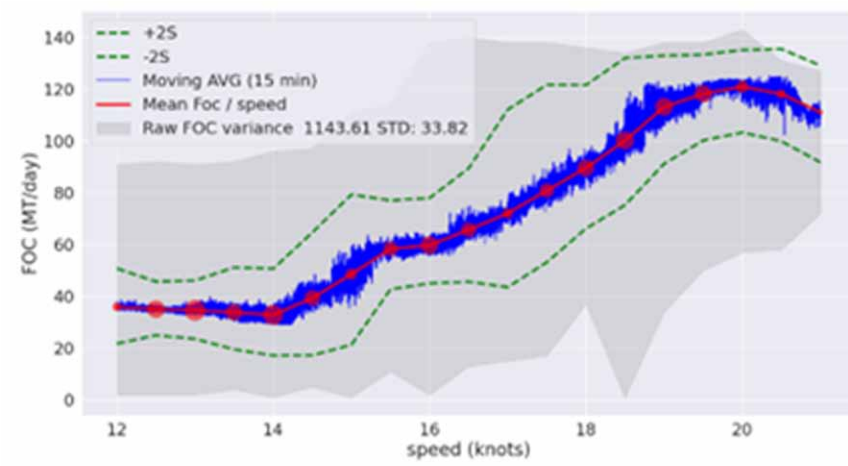
Note that the use of rolling window averages is consistent with the use of the FOC prediction model within a WR algorithm, in which decisions are based upon average values of FOC and not momentary consumption. The raw data of the vessel's speed and corresponding FOC collected from the sensors, versus the mean values per speed range (+/-0.25 V$) and the 15 min rolling window averages are depicted in Figure 4. Red circles are indicative of the number of observations found for a particular range of speed.

Model Implementation

The dynamic estimation of FOC based on vessel state and environmental conditions can be examined as a multivariate time-series prediction problem that takes into account the actual values as well as their recent history, and captures the information hidden in the values' evolution over time.

Based on the superiority of Long Short-Term Memory Neural Network (LSTM) models over traditional time-series prediction methods (e.g., ARIMA) as suggested by Siami (2014), LTSMs are chosen as the basis of our solution.

Figure 4. Raw data values vs. mean values vs. rolling window average values



The initial feature set, collected by sensor installments on-board the vessel, comprises the vessel speed through water, draft and heading and some basic weather features, mapped from external services (i.e. NOOA), such as wind speed and direction. The sampling rate of the sensor based operational data corresponds to minutely measurements.

In order to take maximum advantage of this feature set, we employ a LSTM architecture, using a pre-training step that extracts information from the original features, using spline-based regression (Friedman J. 1999). In what follows, we describe how LSTM is used for FOC estimation and detail the proposed LSTM model and its novel aspects.

LSTM is a variation of traditional Recurrent Neural Network (RNN) architecture, which has been extensively used for time-series prediction tasks.

Unlike standard feed forward neural networks, LSTM also contains feedback connections and can process single data points (e.g., images) as well as entire sequences of data (e.g., speech, video or object trajectories). Compared to RNNs, Hidden Markov Models and other sequence learning methods, LSTMs are not so sensitive to the length of gaps between important events in a time series, which makes them more preferable in numerous applications. To this end, we adopt an LSTM architecture for the prediction of FOC values from the consecutive observation, corresponding to the aforementioned features, in a time window, as described in the following paragraphs.

The input of the LSTM network at timestep t_u comprises N time-series, one for each feature of interest (speed through water, wind speed, wind angle etc) and in order to use the recent history of values in each feature, we employ a fixed-length time-window (time-lag of length m). As a consequence, the window contains the values for each time step for the weather and vessel state features that are used for the estimation of FOC at time t_u, resulting in N time-series, of length m+1, of the form $[F_{N(u-m)}, \ldots, F_{N(u-1)}, F_{N(u)}]$, for each feature F_N. Given a sequence of consecutive time-steps, and a multivariate feature set, we get the following correspondence between the input and the output of the LSTM:

$$\begin{bmatrix} \left[F_{1(u-m)} \ldots F_{j(u-m)} \ldots F_{N(u-m)} \right] \\ \vdots \\ \left[F_{1(i)} \ldots F_{j(i)} \ldots F_{N(i)} \right] \\ \vdots \\ \left[F_{1(u)} \ldots F_{j(u)} \ldots F_{N(u)} \right] \end{bmatrix} \rightarrow \begin{bmatrix} FOC_{u-m} \\ \vdots \\ FOC_{i} \\ \vdots \\ FOC_{u} \end{bmatrix}$$

Weather Routing Aspects and Integration of the Solution

In order to validate the approach in the context of a real-world application, the data driven FOC LSTM model has been coupled with a WR algorithm to support vessel routing decisions towards the reduction of FOC. The WR algorithm that has been utilized is based on the isochrone principle (Hanssen et al., 1960). It builds upon a predetermined basic route; this route can be the original route planned by the vessel's master or provided by a basic routing algorithm. In the context of this work an initial route was employed on the basis of shortest path principles. The original (initial) route is then broken into segments, with respect to a given time step (indicating the master's routing decision horizon, e.g., every 6 hours), and a graph is built around it that enables course and speed deviations, while ``following'' the direction of the vessel's original course. To this end, for each node of the original route, a set of nodes is added in a ``parallel'' fashion on both sides of the route (i.e., parallel to the direction of the original route). Edges are added between all nodes of subsequent sets. Note that nodes that are identified to be on land as well as edges that go above land segments are naturally excluded from the graph.

Once the graph is created (Figure 5), LSTM NN is used to obtain the FOC of each edge of the graph, i.e., of each corresponding sea route, given the vessel's STW, draft and corresponding weather conditions along that sea route. After scoring each sea route (i.e., graph edge), a variation of Dijkstra's algorithm for the shortest path problem is utilized to obtain the route that minimizes the total route FOC (i.e., considering the calculated FOC of each edge as its corresponding ``edge weight'' or ``distance'').

Note that since the algorithm is isochrone, the produced route also satisfies any constraints concerning the time of arrival (if any).

Note also that the decision variables for the WR algorithm are only the STW and the vessel's direction, since these are the aspects that the vessel's master can control. Obviously, any change in the vessel's speed affects FOC directly (since STW is a basic feature of the corresponding model). However, changes in speed and direction also affect FOC indirectly, since they alter the spatio-temporal state of the vessel and hence the corresponding weather conditions.

Preliminary Experimental Results

We continue by demonstrating the results of the WR optimization algorithm demonstrated briefly above. We compare the total FOC of an initial transatlantic voyage conducted by the vessel's master, with the suggested optimized route produced from the WR algorithm by utilizing the aforementioned LSTM FOC

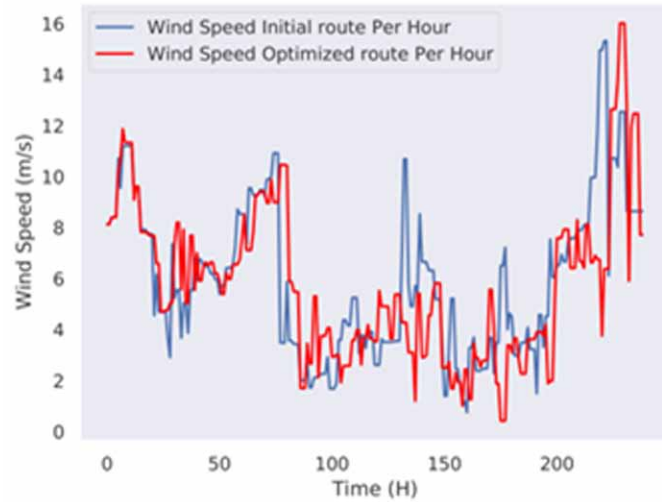
Figure 5. Graph construction comprised of alternative waypoints (red circles) for an example route

Figure 6. Initial (blue) and Optimised (red) route for one leg TAMPA (FLORIDA U.S) - TANGER MED (MOROCCO)

Table 3. Estimation based on weather service (NOAA)

Voyage	Date	Latitude	Longitude
Departure	2019-09-21	27.7°N	82.5°W
Arrival	2019-10-03	35.8°N	6°W
Basic Comparison		**Actual Route Estimation**	**Optimized Route Estimation**
Distance		4787.4	4369.36
Time (hours)		289.997	264.63
Avg. Speed (kt)		16.52	16.51
Total FOC (MT)		774.53	759.97
CO_2 (MT)		2411.88	2366.54

Figure 7. Weather comparison (wind speed) for the initial and optimised route



model. Furthermore, we calculate the total distance traveled, the estimated time of arrival, the average speed and the emissions emitted for the two alternative routes and we exhibit the results in Table 3.

Consecutively we demonstrate the weather (wind speed (m/s)) of the initial and the optimized route per hour, in Figure 7 We can clearly see that the optimized route attempted to avoid ambient weather conditions on average while at the same time complied with ETA constraints.

The accuracy of the estimations we depict in the table below rely heavily on the accuracy of the FOC model we have demonstrated in previous sections. The model showcases promising approximation capabilities, and we can therefore incorporate its prediction to the heuristic function of a path finding algorithm, being confident that the simulation results correspond to the reaction of the physical system with minimal margin of error.

FUTURE TRENDS AND IMPLICATIONS

As we look ahead, the convergence of digital twins with other cutting-edge technologies promises to revolutionize voyage planning.

Further advancements are expected in the near future in data integration. The digital twin ecosystem is extending beyond the vessel itself. Ports, fuels, and spares suppliers will increasingly become integrated into the digital dataspace. This interconnectedness will enable smoother transitions during port calls, efficient refueling, and timely maintenance. Real-time data feeds from satellites, ocean sensors, and on-board IoT devices are increasingly made available and can be exploited by the digital twin improving the on-the-fly adaption on current sea conditions, weather patterns, or other unexpected challenges, ensuring optimal navigation and safety. As standards develop, digital twins will become more interoperable across different platforms and systems. This means that a digital twin created by one shipping company could be easily used by another, leading to a more collaborative and efficient maritime industry. Additionally, the rise of blockchain and decentralized technologies can enhance the security and integrity of the data used in digital twins. This ensures that the information is tamper-proof and comes from verified sources, increasing the reliability of voyage plans.

Apart from data integration advancements in AI technologies are improving the prediction of potential risks or disruptions. By analyzing historical data, they can forecast mechanical failures, piracy hotspots, or hazardous weather long before they pose a threat, allowing for proactive route adjustments. Apart from prediction purpose AI technics are being used in combination with VR and AR technologies, allowing ship crews, planners, and stakeholders to virtually navigate routes, identify obstacles, or even conduct training exercises within a digital replica of the real-world environment.

The advent of autonomous ships will heavily rely on digital twins for navigation, decision-making, and onboard operations. Digital twins will serve as the 'brain' for these vessels, ensuring they can autonomously adapt to changing conditions, detect obstacles, and make split-second decisions. As autonomous vessels become more prevalent, the sophistication and accuracy of digital twins will be paramount in ensuring safe and efficient maritime transport.

As with any advancement in technology, digital twins will also raise ethical and regulatory questions. Who owns the data and how the dataspace is regulated? What happens in the event of a digital twin's malfunction or misinterpretation of data? How are privacy concerns addressed, especially when personal data, such as passenger preferences on cruise ships, are integrated? The maritime industry will need to work closely with regulators and ethicists to ensure that digital twins are used responsibly and that there are clear guidelines and accountability mechanisms in place.

CONCLUSION

The use case of voyage planning demonstrates how concepts and technologies that are already known can be integrated in digital Twin providing holistic and spherical solutions for domain problems.

The voyage planning can be expanded incorporating various concepts and solutions when integrated as a digital twin. Trim optimization can add a benefit of up to 5% in fuel oil consumption and the respective benefit in emissions, being enhanced by the data availability within a digital twin and on the other side the mechanism can be perfectly integrated in the digital twin. The same applies when considering detection and assessment of hull degradation due to biofouling. Interaction with ports in an automated way, facilitated by the digital from vessel side, is an important voyage planning aspect, resulting in reduced voyage cost and more efficient operation, considering that vessel speed has almost a cubic effect on fuel consumption. Further increase in efficiency within voyage planning can be achieved when considering proper position and quantity of fuel and spares supply.

Integration of these features demands an adaptable digital twin architecture with unique characteristics. We have explored these requirements and outlined specifications for a framework encompassing data, modeling, and system management. Additionally, we have proposed a specific implementation.

Finally, the application of this implementation has demonstrated a typical approach to voyage planning, which includes predicting vessel performance, determining the shortest route, and utilizing weather routing. The methodology applied is described, and the results indicate a 2% reduction in fuel oil consumption during a transoceanic -voyage.

In sum, the future of digital twins in voyage planning is one of greater accuracy, predictive capability, and dynamic responsiveness. As these systems evolve, they'll not only optimize routes for efficiency and safety but will also consider factors like passenger experience and environmental impact. The implications are vast, signaling a transformative shift in how the maritime industry approaches and executes voyage planning.

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Chapter 7
Digital Twins for Synchronized Port-Centric Optimization Enabling Shipping Emissions Reduction

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ABSTRACT

Digital twins can help ports, operators and their customers streamline processes, improve safety, and reduce emissions in transport operations that involve at least a maritime leg. This chapter discusses the necessary context for regulations, port operations, and hinterland capabilities; and frames a general methodology under this context for how port authorities, terminal operators, shipping companies, and logistics operators can implement collaborative, emission reducing practices such as slow steaming and synchro-modality. In short, a federation of digital twins that allows to move information downstream from the ship to the port, then to the hinterland infrastructure as well as upstream the opposite way can enable new levels of operational readiness and efficiency, and importantly environmental compliance. At the same time, apart from the improved general efficiency of all processes associated with transport, shipowners can minimise the need to retrofit existing ships for them to remain compliant with the emissions regulations which are bound to be stricter each passing year.

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INTRODUCTION

The decarbonisation roadmap for maritime shipping in the EU mandates that by 2050 the sector be completely free of harmful emissions. This essentially requires ships to stop using conventional fossil fuels (those which release CO2, NOx and other harmful emissions upon combustion). Other sectors, like road and railway transport, have found it relatively straightforward to engage with decarbonisation, mainly through electrification. However, although electrification has been successfully applied to smaller vessels like river barges, this is especially difficult to apply in the foreseeable future to large ocean-going vessels. Therefore, until total decarbonisation in shipping is achieved via some means such as green fuels, new propulsion technologies, or a combination thereof, considerable benefits can be reaped in the meantime by improving and streamlining shipping operations in a way that improves upon harmful emissions.

In general, there are three routes for going about vessel emission reductions in the maritime sector. First, new designs for newbuilt ships will incorporate a broad array of modern technologies for drastic emissions reduction. Second, the existing fleet can be retrofitted with emission reducing technologies (e.g., to use carbon capture or more ecological fuels among others). These concern the part which has to do with the ship's operation and performance, but there is a third route which is the focus of this chapter; to improve shipping operations outside the ship (i.e. port, hinterland) to help achieve decarbonisation goals. The efficiency of these can be improved at several levels, but a critical part is the scheduling of ship arrivals and berthing at the port. Improved scheduling can be leveraged to improve individual ship carbon emissions and help ships meet emissions requirements. Cargo arrival time to the end destination of the cargo –and not just the port of call – and total emissions can be improved by better planning of all segments of the transport chain. For example, a slower ship speed (slow steaming) can be employed resulting in lower emissions, and the resulting longer cargo arrival time at the destination port can be compensated by reducing the idle time of ships and waiting time at ports. This can be done through improved port operations consolidated with robust hinterland transport models that can better facilitate just-in-time arrivals to reduce end-to-end cargo transport times, allowing for more flexibility on the maritime transport part to reduce emissions. This relationship is described in Figure 1.

However, optimisation especially where there is uncertainty (e.g. in ship arrivals at the port or in the availability of hinterland means to further transport cargo) is predicated on information availability as well as the ability to explore alternative configurations and scenarios. Moreover, optimisation becomes more complex with an increasing number of parameters and factors affecting the problem. When we consider the whole cargo transport chain, it is reasonable to assume it is going to be significantly complex. Therefore, two key requirements in enabling synchronised optimisation for maritime emissions

Figure 1. Sailing speed decision at sea transport legs mainly depends on the port arrival time windows and the transit time between ports, affected by weather conditions, and is dictated by charter party terms and liner service schedules

reduction are (a) detailed knowledge of how the assets and processes of the transport and logistics chain operate and (b) sharing this knowledge timely across all relevant participants. 'Timely' being key here, implying in the modern era that commanding good knowledge and communications alone is not enough -this is already being done today after all- to improve the efficiency of the chain drastically, but this must be done in a computerised, automated or semi-automated manner.

Indeed, digital twins are a technology designed to address the timely information acquisition, integration, processing, and sharing. First, digital twins can contain models of assets and processes used in the transport chain with varying granularity levels i.e. from abstract to very detailed and accurate. Second, digital twins can also model the relationships among the previous. With the help of suitable infrastructure, cascade effects of events can be simulated and propagated timely across the actual (i.e. physical) infrastructures and actors in a federated fashion, so that timely action can be taken[1]. Such digital twin models are able to be used today by decision makers with real time, up-to-date data in order to explore operational scenarios. When such data are made available across the transport chain, collaboration practices such as *collective emissions reduction* and *synchromodality*[2] can become feasible. In the future, when DT systems and algorithms are more mature (mainly in terms of security and operational safety), real-time, automated decisions and actions will be facilitated using the same base digital twin system which can be extended in a modular fashion.

Returning to the challenge of applying slow steaming in a way that helps vessels remain compliant with decarbonisation regulations and emission reduction targets, this chapter will address how digital twins can support cargo transport chains with a major shipping leg. Both the shipping segment and the hinterland transport segment will be considered in this context. A port-centric approach for incorporating slow steaming in shipping operations is discussed in the next section. This assumes a Digital Twin enabled environment and aims to facilitate slow steaming by optimising port terminal scheduling and accounting for hinterland transport operations (which affect the cargo's arrival to its final destination).

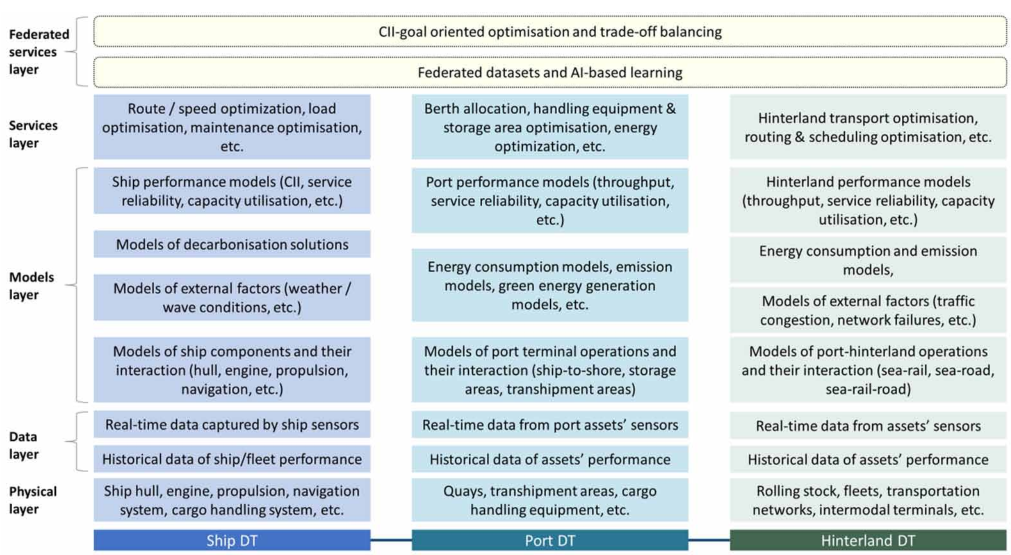
PORT-CENTRIC, DT-ENABLED OPTIMISATION METHODOLOGY FOR MARITIME SHIPPING EMISSIONS REDUCTION

In GHG emissions caused by the activity of humans, the release of CO_2 is considered pivotal and is directly correlated with the consumption of fuels (Nuchturee et al.). It is well-known that ship energy efficiency increases with a decreasing volume of fuel consumed to accomplish a particular power output (Ghimire et al., 2021). To measure ship impact on the environment, the IMO employs a rating scheme for ships, where each ship's operational environmental performance is rated annually via the operational Carbon Intensity Indicator (CII[3]) (Schroer et al., 2021). Intuitively, the CII calculates how efficient a ship is in transporting its freight (goods or passengers), by considering its CO_2 emissions weighed by the freight carried and the distance travelled. Based on the CII, the ship is given an annual rating ranging from A to E. However, each year on from 2023 until 2030, the thresholds for the rating bands will become increasingly pressing because an annual reduction factor is applied to rating bands, making the same rating more difficult to obtain each passing year. At the same time, ships rated with a D or E rating for consecutive years will be forced to take action to become compliant again (C band or better) (Hoffmann, 2022).

Slow steaming (i.e. running the ship below its rated cruise speed) has been advocated for many years as a suitable cost and emissions reduction measure, but the potential remains unclear due to the amount of parameters involved and the corresponding problem complexity. Significant parameters in that respect are related to the operations of the other stakeholders outside the ship and its operator, within the end-to-end supply chain; especially those involved in port and hinterland operations. In the past years, it has been difficult to valuate these parameters timely or at all given the limited vertical collaboration and information exchange between stakeholders, and the resulting difficulty to obtain and communicate necessary data timely enough.

To address these challenges so that slow steaming can be a viable strategy for reducing harmful maritime emissions, this section discusses a general port-centric methodology inspired and driven by modern developments in digital twin technology (see Figure 2). The primary goal is to empower shipping lines with advanced capabilities to optimize their operational strategies, using a CII goal-oriented 'slow steaming' approach. This relies on a federation of Digital Twins (DTs) at the ship, port, and hinterland level, offering a powerful approach to optimizing port operations and supply chain efficiency, while minimizing environmental impact and specifically aiding existing vessels with lower CII rating in maintaining a C CII rating which is required to sail. Each of these three key levels is described in Figure 2 across 4 layers. At the bottom is the physical layer i.e. the actual physical infrastructure. A level above is the data layer, that is all associated real-time information that is captured digitally via sensors as well as historical information that can capture the assets' performance over time. Then the models layer is responsible for processing all the data (done once, periodically, in real time or a combination thereof depending on the application) to produce useful outputs for reaching particular goals. These outputs are utilised a level above in the services layer by services built to optimise the supply chain. Across the ships, ports, and the hinterland, all these DTs are federated to reach CII-oriented optimisation goals and to balance associated trade-offs (e.g. CO_2 reduction vs. expected cost, supply capacity etc.). The following sections discuss several requirements for these aspects in more detail.

Figure 2. Federated digital twins layers and components



Port-Side Requirements

The proposed methodology aims largely to leverage the enhanced information flow due to digital twin technology so that port operations and scheduling are improved drastically. In brief, the methodology will help minimise waiting, handling and port stay times for ships, and will enable ports to better schedule arrivals, berthing, loading and unloading as well as a plethora of other critical port operations utilising real-time information. Moreover, ports are able this way to schedule considering the needs of individual ships especially regarding their expected carbon performance and the impact the journey will have on their CII rating. Last, it will enable ports to calculate and adjust real time schedules and communicate this information (e.g. suggested arrival times) to ships timely.

In order for improved scheduling to work, this need not necessarily be applied to the whole fleet of ships calling the particular port, although that would be ideal. Ships that wish to improve their performance can participate willingly on the port's scheduling and prioritisation scheme (e.g. via a subscriber scheme or via auctions), and other traffic can queue up at the port as is done today. The logic is that the port is the hub for all associated supply chain information and has three important pillars; (i) the utilisation of data pipelines to establish relevant datasets and analytics for involved actors and assets, (ii) the planning, and (iii) the communication of information to ships. These will now be discussed in more detail.

Establishing Robust Datasets and Analytics Across Actors and Assets

By federating digital twins across ports, ships, and land infrastructure, comprehensive datasets can be created and updated including both historical and real-time data on matters such as vessel movements, cargo handling, port-related weather conditions, regulatory processes and port services as well as associated local or non-local third parties. With this abundance of information, advanced analytics can be applied to gain better insights into the timing characteristics of each transport leg, which were difficult to obtain up to now timely enough. These insights, discussed further in this section, can be associated with patterns in vessel arrivals, in berth allocation, in handling cargo, and in potential transportation bottlenecks both within and outside the port among others[4]. Modern Artificial Intelligence and Machine Learning paradigms can provide robust clustering and anomaly detection algorithms and AI-powered predictive analytics can enable proactive decision-making by helping anticipate developments and events with good certainty.

Vessel Scheduling: With digital twins, improved historical information can be collected and integrated with real-time data on matters such as arrivals, departures, vessel types and their CII ratings. Statistical techniques such as time series analysis on these data can help identify patterns and trends on a daily, weekly, or seasonal basis as well as irregularities. Predictive models can help forecast future vessel arrivals based on these historical and real-time data and external factors like weather conditions and related events, and these can be leveraged by port scheduling systems to develop better schedules.

Berth Allocation: The occupancy rates of berths over time can be used to identify patterns of higher demand for berths, for particular types and sizes of berths according to the specific season and period, by particular vessels and vessel types. Optimisation algorithms can then be applied to better allocate berths based on vessel characteristics, types of cargo, and expected arrival times. Different berthing strategies e.g. on the size of berths and the service model they follow can be simulated using the ample information from the DT to better design berths and their associated processes, and to evaluate their impact on vessel turnaround times and congestion at the port.

Cargo Handling and Energy Use: The DT will collect data on cargo handling times, loading and unloading times for different types of cargo and vessels, together with the associated energy usage and CO2 footprint. Advanced data collection approaches can be used; (i) Installation of IoT sensors on containers and cargo to monitor movement and status, (ii) smart containers which can transmit data on their status, location and handling times in real time, (iii) energy meters on cargo handling equipment (cranes, conveyors, forklifts and so on), (iv) ship energy usage data with cargo handling timestamps to calculate the energy efficiency of handling specific cargo types for particular types of ships, v) emission models that estimate CO2 consumption based on the energy consumption data, the cargo data and the handling processes data. These are crucial for optimising port operations in a way that enhances sustainability and improves efficiency at the same time.

Transport Flow Analysis: Analyse the flow of cargo through the entire transport chain, from vessel unloading to final destination. Identify bottlenecks and delays within (e.g. when trans-shipping cargo to other transport inside the port) and outside the port. Simulate different scenarios, such as changes to transportation routes, the layout of port assets, or different distribution strategies to assess their impact on said bottlenecks and improve overall efficiency.

Regulatory Compliance: Ensure collected data and data collection practises align with regulations and with environmental and emissions reporting requirements and standards relevant to the maritime industry.

Simulation-Based Data-driven Planning

The integration of behavioural modelling, decision support systems and conflict resolution mechanisms can be used to assist ports in prioritising vessels with low CII rating, reduce emissions, and promote sustainability while maintaining high levels of operational efficiency. The approach allows for adaptable and transparent decision-making processes that consider both environmental and economic factors. Optimising transport and port operations can lead to reduced idling times and fuel consumption which is expected to lower collective CO2 emissions within the port as well as along the supply chain.

Port Throughput Optimisation: Maximise port throughput through appropriate application of simulation-driven planning combined with optimisation algorithms. This involves optimising the flow of ships, cargo, and resources within the port to minimise waiting and handling times, as well as increasing the efficiency of cargo handling after it has been unloaded.

Behavioural Modelling: Use agent-based modelling to capture the behaviour of individual entities. This applies to e.g. ships, port activities, trucks as well as decision-makers. Each agent can have its own behaviour and objectives. The behaviour can be established in various forms as a set of rules, as a decision tree or as a utility function that governs the behaviour of the agent based on different factors. These can be vessel type, cargo type, CII rating, contractual agreements and regulatory requirements.

Discrete Event Simulation: Complex processes at ports such as cargo handling can be modelled and solved using discrete event simulation to identify inefficiencies and bottlenecks.

Vessel Prioritisation According to CII: Collect and integrate data on the CII ratings of vessels in real-time or near real-time. The data can be obtained from vessel monitoring systems and official emissions databases. Establish criteria for giving priority to vessels with low CII in danger of losing their ‘C’ rating. This can be done via various mechanisms e.g. an auctioning mechanism where ships bid for timeslots at the port, or more port-centric scheduling which accounts for these priorities and makes suggestions to ship captains. In addition, contractual agreements can take place between the port and environmentally conscious shippers, emission reduction goals can be set, and environmental regulations should be accounted for. Decision algorithms can determine ship priority based on CII and other matters (e.g. cargo urgency, vessel size, available resources at the expected time of arrival).

Dynamic Optimisation of Port Operations: Dynamic queuing models can be developed e.g. by employing genetic or memetic algorithms to dynamically optimise port operations. These algorithms can adjust queuing priorities and allocations in real-time based on factors such as ETAs, cargo types, spatial and environmental constraints, and can dynamically optimise vessel scheduling to reduce overall emissions. This is important because not all vessels may want to participate in the prioritisation scheme offered by the port. This 'other' traffic still needs to be accounted for by port processes and optimised to the extent possible.

Conflict Resolution Mechanisms: Implement systems that can identify conflicts among vessels automatically, such as simultaneous requests and overlapping trajectories. Employ consensus-building workflows that involve relevant stakeholders including port authorities, shipping companies, and environmental agencies, to help reach agreements on prioritisation based on more transparent criteria. Auction systems where vessels bid for preferential treatment at the port based on their CII ratings can be used. These can allocate resources more efficiently and can generate additional revenue for the port. Some types of auctions make it more difficult for vessels to misreport their preferences, making the system difficult to exploit. Mechanism Design can be used to determine the exact workings of the system necessary so that the planner's objectives are reached.

Real-time Decision Support: Develop decision support systems that provide real-time recommendations to port operators and authorities. These can consider current conditions, vessel arrivals and prioritisation criteria. Use data visualisation tools to provide decision makers with clear insights into the prioritisation process, potential conflicts, and the environmental impact of decisions.

Port-Ship Interactions

In the DT-enabled maritime environment and the methodology and functionality discussed here, port-ship interactions are critical for the successful implementation of slow steaming and improved port operations. On one hand, the ship needs to provide all relevant information that will enable the port to optimise its schedule, such as ETA (this is reported today already at the start of the journey), cargo information and environmental performance among others. On the other hand, the ship must be receptive to information emerging on the port side, such as adjusted ETA window, docking information, potential port stay time, CO2 reduction and expected impact of the journey to the ship's CII rating. The ship will check the proposed conditions and an iterative process needs to be followed to finalise the plan's parameters in agreement with the port and/or participate in relevant mechanisms such as auctions.

For these interactions to be successful and fruitful, key performance indicators (KPIs) related to vessel prioritisation at the port need to be established, such as on emissions, on waiting times and on revenue generated from auctions. Furthermore, continuous monitoring and improvement of the services needs to take place, and this can be done in a way similar to CI/CD in software engineering. That is the outcomes of prioritisation decisions and interactions can be monitored and analysed, and this feedback can be used to refine algorithms, conflict resolution mechanisms and decision-making processes.Top of Form

Ship-Side Operations and Processes

In order to incorporate slow steaming to reduce emissions, several things need to be considered at the ship level. Ships must be equipped with DT-enabling technologies, and the ships must be able to communicate some of this information with ports. Today all information is collected at the operator's headquarters, and could be communicated with ports through there. In the future, information exchange could be more direct for information that is not confidential. Several DT-enabling functions have been described in the other chapters of this book. It is assumed therefore that the ship is enabled with the technology that allows it to perform speed and route optimisation according to potential conditions along the route and requirements on cargo and port arrival windows.

Therefore, the ship has a DT-based condition and performance monitoring system set up to manage potential slow steaming in collaboration with ports. The system will utilise the ship's DT to calculate the vessel's CII based on previous journeys and incorporate into that an expected CII value for the voyage ahead considering all relevant conditions such as route, speed, cargo, and weather conditions. A specific planning period for CII reduction efforts needs to be defined, and this can coincide with the IMO's timetable for re-evaluating the CII rank of the ship in question. This way the ship, will be able to calculate its expected annual CII before it actually performs the voyage, based on the proposed ETA window, and will be able to communicate this to the port. This can be updated as needed based on the actual conditions and events the ship encounters, and the port and ship can together re-evaluate the ETA window en-route, making necessary adjustments to the ship's speed and the port's schedule. On the planning side, with ample data, sensitivity analyses can be carried out to determine the potential range of CII reduction achievable by the vessel through slow steaming at various speeds. This analysis can incorporate other factors as well such as the load factor of the ship, the type of cargo and others and can be used as a reference point for the ship i.e. to have a good idea of what the ship is capable of under various circumstances.

The ship is able to request from the port preferential treatment if this is to improve the ship's CII, and as we explained in the previous section these ships that wish preferential treatment will be prioritised by the port via some criteria (e.g. help ships in danger of losing C rating first, or help ships with greatest savings in CO2 first, or according to contracts with shippers). After the ship communicates all relevant information and preferences, the port DT will inform the ship of the requested expected ETA window, the expected port stay time and CO2 reduction (or even expected CII if the port has limited access to the ship's DT) to help facilitate slow steaming for the ship and a reduced stay at the port. The ship is able through its DT to utilise multi-objective optimisation algorithms to determine the optimal route and speed for the upcoming voyage according to expected weather conditions and the schedule agreed with the port, while remaining within safety, contractual, environmental, and financial (e.g. load factor) constraints. The ship this way could e.g. apply slow steaming across the whole route if there is enough time, or selectively in parts of the route where it is most effective for emission reduction according to expected conditions. Of course, the schedule can be re-negotiated with the port en-route if it cannot be met for particular reasons, or if the ship sees a window of opportunity to further reduce costs and emissions. Data from multiple trips can be analysed to further streamline and improve the optimisation process for the particular ship over time. The decision-making algorithms and strategies can be refined based on this historical performance data and on important lessons learned by applying the process.

Land-Side Operations

The aim of the methodology is not to optimise land-side operations per se, although it can be applied in a similar manner for all aspects of land transport operations. However, the methodology aims to make the most of information becoming available through suitable DT paradigms in the land transport infrastructure. The methodology leverages various data on the landside with analysis of historical travel time data per link and mode, for particular cargo types with special requirements and so on. This can be enriched with real time data on mode availability and capacity and fed into multimodal routing algorithms to calculate stochastic hinterland transport durations and their confidence intervals. This can be done for individual vessels and their cargo, considering other cargo that needs to be carried originating either from other ships or the general transport network, and can be summed across the number of transport legs the ship's cargo needs to follow. This will produce more accurate estimates of the expected arrival time of the cargo to the destination, indicating and putting constraints on the potential time window the ship can leverage for CO2 reduction and allowing for more confidence in optimising its route and speed. At the same time, it will allow ports to make realistic propositions to ships that ships will have incentive to follow if they do not endanger their chartering agreements.

MODERN SHIPPING, PORT AND HINTERLAND OPERATIONS AND CONCEPTS IN ALIGNMENT WITH DIGITAL TWINS

To better understand how the methodology and requirements in the previous section can be implemented, this section discusses several modern operations and concepts that are in alignment with the idea of federated digital twins and can fit into the methodology in a straightforward way provided relevant data streams are established. First, we present a summary of how digital twins can benefit slow steaming as a means of decarbonisation. Then, we discuss opportunities for optimisation at the port and terminal level. Then follows a discussion on modern relevant concepts, mainly multimodal transport, synchromodality, and the Physical Internet (PI).

Slow Steaming in Perspective With Emissions, Costs, and Digital Twins

Vessel speed has a direct impact on resulting emissions because fuel consumption in vessels increases, in the least, with cubic growth for an increasing vessel speed. Therefore, a reduction of the ship's speed, thus arriving later at the port of call, is expected and has been shown to reduce fuel consumption considerably for a given journey, compared to cruising at the ship's rated cruise speed (Venturini et al., 2017; Lee et al., 2015). The counterargument against this is, of course, that the ship will arrive later at the port of call. This may seem counter-intuitive given that chartering contracts dictate arrival time windows, and in addition slow steaming will reduce a ship's load factor (i.e. the amount of cargo able to be carried within a given timeframe). Therefore, more ships will be needed to satisfy the same volume of cargo transport. This is not necessarily problematic, as it is in fact foreseen that in the future more and larger ships will be used to carry the same amount of cargo at slower speed and over shorter distances, given the need to cut emissions in combination with various geopolitical reasons (Tsai & Lin, 2023).

Today, liner vessels run mainly based on table schedules with only about 52% of them arriving within the planned arrival window (usually ± 1 day from the projected time of arrival)[5], resulting in cargo delivery delays anyway, and also in early and late vessels waiting idly to enter the port. Furthermore, these delays are unaccounted for, making it challenging for port terminals to schedule the loading/unloading of containers or other cargo. In parallel, recent research that scrutinises the recently employed emissions rating scheme of the IMO, confirms that a lower Maximum Continuous Rate (MCR) of the ship's engine, is associated with better annual CII performance for the ship. It is suggested that MCR should be set between 55% MCR and 75% MCR according to local conditions for maximum benefit in emissions reduction (Tsai & Lin, 2023).

It is straightforward to see that slow steaming, as part of an overall approach by the operator that includes additionally voyage and port selection optimisation could yield a highly cost-effective way for existing ships to comply with the increasingly demanding emission reduction targets in the near and mid-term horizon. This will minimise the need for retrofits to keep vessels operational, until they are replaced further in the future with carbon neutral vessels. Therefore, slow steaming should be considered as part of route and speed optimisation taking into account weather conditions. Furthermore, slow steaming is directly associated with port stay minimisation and we put this into perspective with the hinterland part of cargo transport. Hinterland distribution is managed by different actors than the maritime part and today the maritime and hinterland segments of the cargo's journey are treated in isolation from each other. This makes leveraging resources during the shipping leg (e.g. time) from other segments of the cargo's voyage a key area which is overlooked today. For example, although chartering contracts are strict today on the maritime leg, they often allow over-ample time in the hinterland transport part of the cargo to account for potential inefficiencies, but with better information availability and scheduling these resources can be leveraged during the shipping leg.

Now on the port side, the port is where all the above points in the discussion intersect and therefore a suitable place where they can all be considered and optimised together. A Digital Twin enabled environment at ports as well as ships, operators, and transport modes can enable the port to become significantly better at utilising its facilities (e.g. docks, cranes), increasing the availability and utilisation of resources, and decreasing waiting times and docking times. A port digital twin can be constructed by modelling port assets and their components (e.g. container cranes, containers, ship machinery, expected arrivals schedule, etc.) and their relationship with other assets (e.g. a container crane unloading a container ship). Additionally, the digital twin can maintain the real time status of the assets, for example the utilisation of a berth for visiting ships. With these, and though simulations and data analytics, the future status of the port's assets can be predicted, for example the expected time a berth will become available. A port DT can also serve the management of renewable energy sources including all the consumption points particularly cold ironing for ships (i.e. turning off the engine and plugging into the port's power grid). All these aspects are further discussed in the remaining of this section.

In short, digital twins and the associated extensive bilateral information exchange can significantly support slow steaming as a decarbonisation means in a port-centric setting in several ways:

- Slow steaming strategy integration into ship route and speed optimisation, resulting in voyage emission reduction, port stay reduction, and emission reduction during port stay.
- Enable ports to optimise ship arrivals to minimise collective emissions.
- Enable ports to prioritise ships in a way that helps them maintain their emissions (CII) rating.
- Communicate speed, ETA and docking information to ships according to the port's schedule and better monitor the schedule's implementation minimising idle and stay time at the port.

- Improved coordination with other transport processes downstream to make maximum use of potential cargo arrival time windows (hinterland transport).

Port and Terminal Optimization

Port efficiency relies on balancing demand and supply in a flexible way and integration within the entire transport system. A port is dependent of a continuous inbound and outbound flow of cargo and passengers arriving and departing from the port by different means of transport (Lind et al., 2020).

Typical port operations include incoming ships arriving at berths, the allocation of quay cranes (those which load/unload) to the docked vessels, the routing of internal transport vehicles, gantry crane deployment (those cranes which stack different items together into a single item) at the yard side, and storage space assignment. Terminal resources at the same time are limited, and potential uncertainty in vessel arrival times at the port further complicates the problem at the terminal side (Ursavas & Zhu, 2016).

To measure terminal efficiency, or rather terminal throughput, it is important to know the time each ship spends at the port. Usually, the ship's stay at the port is characterised by the ship's handling time which represents the time the ship has spent docked at the berth, and the ship's waiting time which represents other time the ship spends at the port (e.g. waiting to dock). The sum of these two characterises the terminal's service time (Buhrkal et al., 2011). A digital twin, fed by multiple data streams of real-time data and historical databases, can be a valuable tool for the coordination and synchronization of port operations, thus improving efficiency.

Berth Allocation

Prominent in literature is the matter of berth allocation to ships. In container terminals, the Berth Allocation Problem (BAP) is crucial (Buhrkal et al., 2011) as an inefficient allocation impacts all other operations connected to this (which extend beyond the port itself), increasing processing times and costs considerably (Ursavas & Zhu, 2016). The BAP in short refers to the problem of assigning quay space and service time to incoming ships that need to be loaded or unloaded, with the goal of minimising service time and maximising quay occupancy (Bacalhau et al., 2021). In general, it is a difficult problem to solve with most variations being computationally intractable. In its general form the BAP assumes there is a given berth layout at the terminal, and a set of vessels that must be served within the planning horizon. A number of parameters associated with each vessel are needed to properly capture the necessary information into the planning, such as draft, length, clearance needed from other ships, expected handling time, and Expected Time of Arrival (ETA) (Bierwirth & Meisel, 2010).

From there, the BAP may have a several constraints. For example, spatial constraints may affect berthing positions, there may be different draft restrictions for different positions, and the fact that usually it is inefficient to relocate large container ships once moored. With regard to ship arrivals these can be static i.e., vessels are assumed to be already waiting at the port and are capable, at extra cost, to moor earlier if needed, or dynamic where ships cannot moor earlier than their ETA (Imai et al., 2008) and arrive during container operations (Bierwirth & Meisel, 2010; Buhrkal et al., 2011). Then regarding the terminal's layout, this can be discrete, dynamic, or hybrid. A discrete layout is when the quay is divided into berths (sections), with each berth being able to serve only one ship, and this is a relatively straightforward problem to solve. A continuous layout imposes no such restrictions meaning berthing positions are arbitrary within the quay, which improves space utilisation at the cost of increased problem complexity. A hybrid layout attempts to draw upon the best of both worlds, by partitioning the quay into small berths, allowing larger ships to occupy more than one berth, and small ships to share the same berth. Last, it is an issue how one represents vessel handling time. Different quays, or even berths may offer different handling time, and vessels may have different expectations i.e., the cost of waiting for each ship may be different for the same unit of time (Ursavas & Zhu, 2016). Stochasticity in vessel handling times is often difficult to handle, and therefore the larger portion of proposed solutions consider deterministic time i.e., where the handling time is fixed and known for each ship, given the berthing position, the number of cranes serving it and the work schedules of those cranes. Most BAP problems aim to minimise service time, and the performance of a berthing plan is measured usually in terms of cost (Bierwirth & Meisel, 2010). However, this does not account for vessel emissions reduction which the methodology in Section 2 aims to address.

Related with berth allocation is the prediction of ship arrivals at the port. Data mining approaches on the prediction of early and late arrivals have been employed and it has been determined that knowing the ETA of ships, as well as ship length, is critical for terminal operations to work smoothly and efficiently (Pani et al., 2015; Yu et al., 2018). Our work takes this a step further by allowing ports to make suggestions to ships, enabling them to compute optimised slow steaming speeds based on plans they calculate with multiple criteria. These plans not only include service time minimisation on the terminal side, but also consider the environmental footprint of ships and aim to help ships maintain their CII ranking while at the same time improving operations.

Transshipment

Transshipment today is very common and refers to changing transport modes often consolidating small shipments (or deconsolidating large ones) (Kumar et al., 2020). This is deeply related to synchro-modality which is discussed in more detail in Section 3.3. Properly synchronising transshipment operations to be efficient and sustainable means in practice that less storage and cross-docking is needed (fewer intermediate hubs need to be used). Important problem parameters can include demand at the nodes, supply available at each node, storage capacities, time, cost, budgets and so on [Kumar et al, 2020]. The problem of transshipment is relatively straightforward in deterministic settings (i.e. where arrival times, quantities and other problem variables are known), but this is rarely the case in reality where several uncertainties exist, for example due to weather conditions, lack of exact information or even unobtainable information, and the stochastic setting complicates the problem dramatically (Crainic et al., 2021).

Transshipment occurs often within port terminals as well, where the goods have to be unloaded from vessels, then be trans-shipped within the terminal itself to other facilities for e.g., rail or truck transport, where they need to be loaded again. This is especially the case in multi-terminal transshipment ports, where minimizing the distance between the quay and the yard (where containers are stored) upon the berthing of a vessel is found key to increasing throughput (Heilig et al., 2019).

Crane Assignment and Scheduling

Related to the BAP is terminal crane assignment and scheduling, whose operation is critical for the transshipment of containers within the terminal. Assignment and scheduling are often treated separately formulating the Quay Crane Assignment Problem (QCAP), and the Quay Crane Scheduling Problem

(QCSP). These need to adhere to certain constraints such as berth layout, workforce planning and crane specifications, and newer solutions often integrate them with each other.

The QCAP attempts to assign quay cranes to ships so that all transshipments in the plan can be satisfied. it is often a straightforward problem to solve using simple rules of thumb. Therefore, the QCAP has not sparked extensive research interest, although it can have a significant effect on the handling time for vessels (Bierwirth & Meisel, 2010)

The QCSP is involved with determining the QC schedule given a set of transshipment tasks to be performed, and a set of assigned quay cranes. The QCSP is generally difficult to solve and has been shown to be NP-hard for more than two cranes where processing times are not uniform and tasks cannot be skipped (Pani et al., 2015).

Collaborative Terminal Clusters

Collaboration among stakeholders involved in maritime shipping and cargo transport is often emphasised highly in the literature as one of the driving forces to make transportation more efficient. This includes collaboration at various levels. For example, collaboration between terminals and shipping lines – often when the terminal and shipping operator are within the same group of companies, allows ships to have berthing priority in their terminals and can lead to better service times and control over shipments due to the easy exchange of information (Venturini et al., 2017). Collaboration of the port with the port users in general has been shown to lead to a reduction of operational costs, increased transparency and therefore trust, better planning, improved compliance with regulations for collaborating supply chain members (Ambra et al., 2018).

Of particular interest is the concept of ports collaborating with each other. More specifically, although research is focused on vertical collaboration along the supply chain, horizontal collaboration (i.e. between ports) is often neglected. At the same time, vessel scale and size are constantly increasing but expanding ports further is difficult for a variety of reasons such as regulations, local opposition, and stakeholder opposition to name just a few (Corman et al., 2017). Additionally, intra-port competition today is often considered unproductive because competitive advantages are lost as ports become more and more congested and a framework for determining cooperation policies is often sought after (Christiansen et al., 2017; Corman et al., 2017).

It is believed that collaboration between ports could expand the service network of ports despite the global competition and could reduce transshipment costs as well as improve service times. Furthermore, the digital evolution of services offers an opportunity to collaborate in a more meaningful way for the improved environmental performance of the shipping sector (Ambra et al., 2018). For large trade hubs, such as Singapore, the port is an important asset facilitating entry and exit routes for the regional business and services sector. This kind of gateway port has a regional port cluster for regional distribution, which includes freight generators and receivers, industrial areas, distribution centres, processing firms, administrative bodies and so on (Giusti et al., 2019). Especially in the Mediterranean, ports are considered advantageous because they are close to the Middle East and Asia through the Suez Canal. However, the widening of the Panama Canal has stimulated more severe competition for traffic between Mediterranean ports, for fear growth will be restrained. Competition, though, in the Mediterranean may be pointless because shipping companies often treat the region as a single transit area, with large ocean-goers making only one or two port calls. The collaboration of ports, therefore, may be able to help boost the region because competitiveness does not only depend on internal port characteristics, but also includes characteristics and activities outside the port (Christiansen et al., 2017).

A cluster where ports collaborate more closely may help build a network of excellence among different businesses and transportation modes. Such clusters could be based on regional characteristics as different regions pose different objective differences (Dong et al., 2018), or even across regions closer together, where the flow of currency, information, workers, and commodities is increased and there are linked economic relations (Giusti et al., 2019). Clustering can consider several other factors apart from geographic proximity, such as hinterland connections, quay depth and length, the type of cranes at each port, the feeder distribution network and so on (Christiansen et al., 2017). This will help leverage resources from a larger pool, and combinations of resources which were not available before (Corman et al., 2017). In the proposed methodology, port clustering can be leveraged to provide vessels with more flexibility in choosing their port(s) of call and route, and the ports to better optimising their schedules. Given the goal is to minimise ship service times along with emissions, the cluster can draw upon its resources to ensure ports do not get congested.

Hinterland and Multi-Modal Transport

Digital twins can be an essential foundation for simulating or predicting arrival processes for the hinterland transport part, or where multiple modes of transport are involved in a single leg. The improved exchange of information will better facilitate slow steaming by providing more accurate information on the availability of hinterland modes such as trucks, trains, and infrastructure for diverse needs, making their use by cargo shippers more efficient.

Performance of freight transportation is one of the crucial elements for the sustainability of logistics and supply chain. The costs for the freight transportation can reach up to 60% of the total logistics costs for shippers and inefficiencies in transportation costs can be characterized by economic, social and environmental inefficiencies and unsustainability. Despite efforts by transport companies, the percentage of empty trips remains high and average truck fill-rate is low. At total transport level, most trucks in Europe fell in the range between 15% and 30% empty journeys. Moreover, freight transportation (in developed countries) is responsible for nearly 15% of greenhouse gas emissions. This ratio has been increasing despite ambitious reduction targets.

The utilization of multiple transport modes for delivery of cargo is a widely adopted concept in supply chain logistics. Multi-modal transport is defined by the UN (UNECE, 2001) as “the carriage of goods by two or more modes of transport” with intermodal and combined transport arising as subcategories. Intermodal transport arises when goods are stored in a single loading unit that utilises multiple modes, and combined when initial and final legs by road are included. The motivation for the utilization of multiple modes in transporting goods lies in the unique characteristics and advantages associated to each transport mode, the unique characteristics of the goods being transported and the geography between every origin and destination. The fundamental advantage that arises with utilizing multiple modes is that the benefits associated to using a specific combination of modes for a transport leg are higher than the cost that arises from transferring (transhipping) the goods from one mode to another.

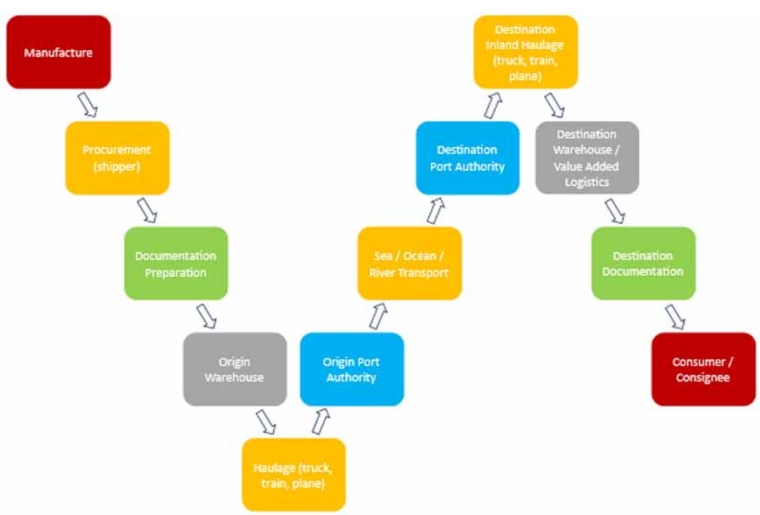
Multi-modal transport can either be a requirement as in the case of intercontinental trips, or an option when more than one transport modes are available which is typical in hinterland transport. The utilisation of multiple modes for the delivery of goods often makes consolidation of cargoes difficult to achieve, which is further driven by increasing performance requirements on the demand side such as just-in-time delivery. To address this challenge the co-ordination of the transport system and the supply chain it serves is required in an integrated approach. Improved collaboration and information sharing across the entire transport chain can improve performance in hinterland transport operations. This is further explored in the following section.

Synchromodality: Transport Chain Collaboration

The modern cargo transport logistics chain from manufacturer to the consumer (see Figure 3) is already fairly complex and typically involves at least a sea or river transport operator, a terminal operator and an intermodal operator (Kapkaeva et al., 2021). At the same time, the fragmentation of export information and the multiple information exchanges with high handover frequency necessary negatively affect efficiency (Aloini et al., 2020). Digital twins can lay a foundation for new interactions and collaborative approaches amongst organisations (Reim et al., 2023) and can facilitate collaboration in a more meaningful way, especially with regard to green energy and improved environmental performance (Ambra et al., 2018).

Today, the bulk of international cargo is transported through containarized intermodal transport, where vessels handle the intercontinental leg and vans handle last mile delivery. Research as well as recent experience (e.g. with the COVID pandemic, the Suez Canal obstruction in 2021, as well as the recent Red Sea attacks on cargo ships) have shown that port and route disruptions can trigger cascade effects which can propagate quickly with impact on the whole supply chain. Ship rerouting is proposed by many as a mitigation measure (Wendler-Bosco & Nicholson, 2020). Even so, intermodal supply chain resilience modeling is still in its infancy. Indeed, vertical collaboration through the supply chain for better real-time exchange of information, such as collaboration of shippers with ports, and ports with road/rail haulers is believed to be one of the key areas for reducing congestion at ports and ship turnaround times (Ambra et al., 2018). Deep integration of information technology in 'intelligent ports' is expected to improve resource utilization efficiency drastically, and the collaboration among stakeholders cannot be stressed enough for port efficiency increase (Dong et al., 2018; Aloini et al., 2020).

Figure 3. A modern cargo transport logistics chain



Therefore, to enable information sharing and flexibility in supply chains, a certain level of stakeholder collaboration and coordination is required. One approach to collaboration, synchromodality is an evolution of multimodal, intermodal and combined transport and it involves different and strongly integrated transportation modes. The aim is to provide an efficient, sustainable supply chain with low environmental impact while optimizing resource utilization. Synchromodality builds on the vision of flexible, high-level management of corridors proposed by intermodal transport to meet the wider interests of the whole supply chain and not only for a specific shipment or company (Giusti et al., 2019).

From a stakeholder perspective, cooperation can be perceived as an integration of networks to improve consolidation of flows and increase overall delivery efficiency. Network integration can be vertical as in intermodal transport. Vertical integration is paramount but challenging. In synchromodal logistics horizontal network integration is also essential as it contributes to routing flexibility (Tavasszy et al., 2017). Horizontal network integration directly impacts the availability of rerouting options, which in practice might convey to the use of a different vessel which alters the shipment's schedule, the use of a rail-leg instead of a sea-leg to expedite delivery, bypass port congestion, or the use of a different intermediate multimodal terminal for short term storage.

Stakeholder collaboration is also a fundamental enabler for network information completeness and availability. Information sharing benefits all stakeholders involved, and especially logistics service providers (LSPs) who deal with route planning and real-time route adjustment decisions that are significantly benefitted by improved quality and visibility of the supply chain. Cargo consolidation can be implemented, as dynamic information about spare capacity becomes available (Schulte et al., 2017). Integration of data sharing though has proven to be a tricky issue, because several transport operators perceive data as valuable assets and as a result prefer to operate within organizational silos.

Another essential enabler for synchromodal logistics is shipment flexibility that allows for some slack in managing and consolidating cargos. Shipments are typically loaded on scheduled rail and sea services, although there is more robustness in road transport as road vehicles carry less capacity. In synchromodal bookings, transport is typically amodal, allowing LSPs to optimize the available capacities provided there is information availability to effectively respond to any uncertainty and delays that might arise. To achieve that, LSPs might consider the change of modes or prioritization of shipments, and this may require the development of new business models and strategies among different LSPs. The value of flexibility is particularly important in the transport of perishable goods, where upon a potential delay LSPs might assign a shipment to a faster mode or choose to prioritize the shipment over other, less critical cargoes. The dynamic actions LSPs can utilize to exploit the flexibility available in the system include rescheduling of shipments and if possible, transport legs, rerouting, prioritization and modal shift. Flexible synchromodal operations can improve delivery reliability in case of disruptions while enabling dynamic adjustments also has significant cost and emissions savings benefits (Ambra et al., 2018).

Synchromodality can also be a driver for the efficient operational management of assets extending beyond transport, to inventory management and production scheduling (Dong et al., 2018). Information sharing and synchronized decision making between various stakeholders can yield improved consolidation of cargo and improved utilization rate of assets.

To achieve synchromodal transport, the provision of real-time information is essential. In an environment of continuous monitoring and information availability of both the network and the cargo, all stakeholders involved have the capacity to track their assets and make appropriate adjustments when necessary. The added value of information availability has been illustrated in the dynamic control and re-scheduling of railway traffic (Corman et al., 2017) or the re-assignment of tasks of fuel supply vessels inside and outside major hub ports (Christiansen et al., 2017). A digital twin can therefore provide transportation chain actors opportunities to optimize the choice of transport mode and route for serving their clients. This should strengthen their strategic relationship to logistics service providers, such as carriers and transshipment hubs.

The Physical Internet

The Physical Internet (PI) aspires to build upon the concepts of synchromodality and integrate operational concepts from the Internet that has successfully developed into a global data transfer system across heterogenous networks exploiting standard protocols.

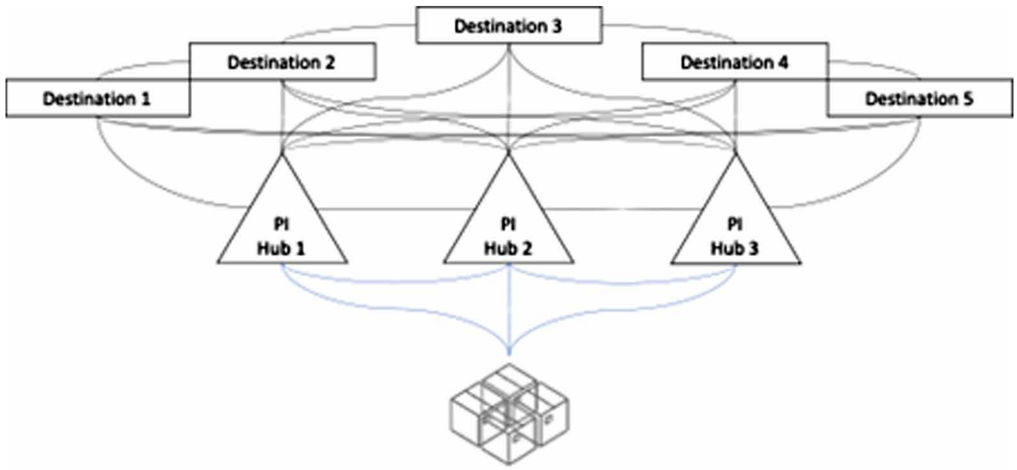
In the Internet, data packets are transmitted from a source host through different networks to a destination host. Routers decide over which link (pathway) the data packet is sent to the next router closer to the destination. If the physical medium must be changed, for example from Ethernet cable to Wireless Local Area Network (WLAN), modems are used. To enable the flow of data packets over the networks, two protocols are particularly important: the Transmission Control Protocol (TCP) and the Internet Protocol (IP). The TCP dictates how data and/or messages can be broken down into transmittable packets, manages the flow of these packets across the Internet, and ensures that the data that was transmitted reaches its destination. The IP provides routing and addressing rules for packets so that routers can send the packets to the appropriate destination host.

Based on the concept of the Internet, the PI aims to implement a network of independent physical distribution networks in which operations are performed by the existing network operators (logistics service providers (LSPs)) or new players that emerge out of the PI. This physical network-of-networks is envisioned as enabling the efficient flow of goods between senders and end-customers through distribution, consolidation and intermodal centres/hubs (equivalent to routers in the Internet) in a manner similar to that employed in the movement of data packets over the Internet (Dong & Franklin, 2021).

Improved transportation efficiency is therefore an important objective of the Physical Internet. More specifically, it aims to reduce logistics costs by revolutionizing how transport and logistics is practiced, and to improve on critical variables such as cost, utilisation rates, and emissions through improved multimodal and synchromodal integration and open accessibility to both static and mobile infrastructure. The core constraints, objectives and business processes involved in planning, coordinating, and executing the transport of goods from origin to destination remain largely unaltered in a PI approach. What changes under the PI are the standardisation and interoperability of transport, logistics systems and processes. For these features of the PI to materialise, several information and decision support systems as well as standardisation and integration services require to be introduced, that can be broken down into the following core-protocols[6]:

- *Encapsulation*: Standardises the packaging process of cargo and goods that are consolidated/deconsolidated into π-containers for transportation via the PI. It is also responsible for the consolidation/ deconsolidation of π-containers into π-movers.
- *Shipping*: Specifies what has to be transported as well as the transportation process conditions and constraints. It is responsible to make appropriate adjustments to the shipping instructions to ensure compliance.
- *Networking*: Networking defines the interconnected infrastructure of available processing, storage and transporting facilities (transport services, terminals, distribution centres, warehouses) through

Figure 4. A physical internet enabled network of ports which operate as PI hubs to several inland destinations for cargo



which the goods will be transported from their origins (manufacturing, distribution and other locations) towards their customer(s) locations.

- *Routing*: Routing is a process that creates a plan that describes the stage by stage detailed visiting and usage of networking nodes and links from origin to destination.

It is self-evident that the PI and DTs are concepts which complement each other well, and the improved information flow and real-time processing DTs can provide can significantly benefit the adoption of the PI.

A case study has been developed[7] aiming to illustrate the impact of introducing flexibility in vessel operations. The case study assumes a Physical Internet enabled network (see Figure 4) of ports that operate as Physical Internet Hubs and a vessel loaded with cargo that require to be delivered to multiple hinterland destinations. The network assumes multimodal hinterland links between all ports and destinations as well as road links between the ports and between the destinations being available. The aim of the case study is to quantitatively assess the performance of a fixed schedule and compare it against a flexible port calling approach where the vessel skips one or more ports (hubs) depending on the availability and efficiency of hinterland connections. The scenarios analysed include low and high port congestion cases, low and high frequencies of hinterland services, as well as prioritization of vessels at specific ports to account for port ownership schemes.

An integer program is used for assigning ports of call to the vessel in the flexible scenario, and simultaneously determining the unloading port for each cargo as well as the route that will be followed to its destination. The case study (see Figure 5) considers twenty-one vessels of various operators and cargo loading levels over the course of a week. It is observed that one of the three PI Hubs is frequently omitted from vessel schedules, with company 0 and company 1 vessels omitting PI Hub 3 and company 2 vessels omitting PI Hub 2. This behaviour is associated to the company-specific port entry costs. This is far more efficient in comparison to the inflexible scenario, where vessels are forced to call all ports, consistently showing slower turnaround times for discharging the cargo towards the hinterland destination, also at higher cost.

Table 1. Containers discharged per PI hub by each vessel over the course of a week

PI Hub 1	PI Hub 2	PI Hub 3	day	company	vessel
68	16	0	0	0	0
132	47	0	0	1	1
226	0	7	0	2	2
69	17	0	1	0	3
160	52	0	1	1	4
189	0	15	1	2	5
69	26	0	2	0	6
159	38	0	2	1	7
176	0	19	2	2	8
79	23	0	3	0	9
151	46	0	3	1	10
165	0	14	3	2	11
66	20	0	4	0	12
154	69	0	4	1	13
196	0	11	4	2	14
62	13	0	5	0	15
150	52	0	5	1	16
204	0	22	5	2	17
49	16	0	6	0	18
166	67	0	6	1	19
207	0	13	6	2	20

CONCLUSION AND FUTURE OUTLOOK

In this section we summarise the main capabilities and features of digital twins at the port, ship and hinterland. On the port side digital twins can be used to schedule ship arrivals to ports, aiming to minimise the overall emissions cost. The port-side digital twin receives information about the voyage plan, expected arrival time (ETA) and other ship characteristics (such as its CII) from the digital twins of arriving ships. Then the digital twin calculates the availability of its resources (e.g. cranes, berths) and creates arrival schedules that serve ships under specific priority, aiming to minimise total emissions caused by the ships' idling time, and to help ships apply slow steaming. The digital twin can communicate the new schedules to the ships' digital twins suggesting an optimal ETA. Such scheduling will need to be carried out periodically as both the ship situation (e.g. disruptions due to bad weather), and the port's own assets (e.g. breakdowns in cranes) can change. In more advanced scenarios, digital twins of collaborating ports could share information and agree between them the allocation of ship arrivals, thus achieving further reductions in ship idling times and emissions.

Apart from short-term planning, a DT environment can significantly improve long term planning. A port and its partners can capture historical, ongoing, and predicted future trade data in a digital twin. Digital twin models could then be exercised with different parameters and relationships that port decision-makers should include in their strategic decisions, such as investment in infrastructure, port design, and terminal capacity. Therefore, the importance of collaboration among stakeholders for port efficiency cannot be overemphasized, and the contribution of digital twins is expected to be pivotal. In short, a port Digital Twin can provide an array of advantages: (i) knowledge aggregation (both models and data) for the port transportation network; (ii) a global decision support and optimization platform; (iii) immersive visualisation based on real time intelligence; and (iv) innovative customer support services.

On the ship side, using the digital twin as well as data available from the digital twins of collaborating ports, and the cargo's inland destination, the digital twin should be able to identify the general port area (cluster) that can serve the destination. The digital twin should then be able to select a destination port constrained by cargo expected arrival is on time. Using the digital twin, a routing options matrix can be created, considering all ports in the sub-cluster and considering both the hinterland and the sea-side routes. Using historical data from the port digital twin, port delays and transport mode associated emissions could be calculated. Based on that, an updated routing options matrix based on a consolidation function that integrates time, cost and emissions can be created. For each port/hinterland route combination, a speed which optimises the CII should be straightforward to calculate. Combinations which have high impact on CO2 and/or are likely to delay inland cargo arrival should be eliminated. From the viable set of routes, the one with the lowest fuel/emissions can then be selected, or this can be balanced together with other criteria. The ship digital twin should then inform the selected port so an ETA can be agreed upon if the ship wishes preferential treatment according to the port's scheme, or at least inform the port of its ETA as well other associated information.

The hinterland side is the set of digital twins belonging to organisations such as logistics service providers, distribution centres, land-based carriers and customers. Their task is to calculate internal demand and availability schedules which they will pass on to digital twins upstream. Based on such (demand) schedules, the upstream digital twins of ports and ships can then calculate optimised schedules that minimise emissions, as explained previously. When the upstream digital twins commit to transportation schedules, they update the hinterland digital twins which in turn can make updated calculations and predictions and optimise their internal processes and resources according to new real-time information.

Standardized digital models of all components in the shipping industry is the next wave of standardization if the industry is to achieve higher levels of capital productivity driven by improved analytics, operational and strategic decision making. Large players have started moving towards this already, and those who will remain behind will have a competitive disadvantage especially with the new emissions regulations. The physical instances of all components need to have embedded sensors that generate standardised data stream to maintain the fidelity of their associated digital models. Business and emission reduction objectives can both be guided by digital twins, provided the maritime industry cooperates to standardize digital data and models of digital components (Lind et al., 2020).

Those groups with deep knowledge of each asset, such as crane manufacturers, port infrastructure designers, and ship designers, need to develop or advise the creation of standard models of such assets and components. Furthermore, process models need to be developed, for example related to ship docking or crane operations. Such models need to be validated using historical data that are collected and stored in the digital twin. Then, digital twin-based simulations can answer a plethora of questions and what if scenarios related to future projected demand, capacity and availability. Therefore, the transportation chain can become more agile and data driven, allowing for better utilisation of assets, reduced wastage of resources (both material and immaterial such as time), and consequently improved energy consumption, and resulting emissions.

Nevertheless, all these are predicated on the willingness of the participating parties to collaborate and share data. Synchromodality and the Physical Internet are significant concepts which can act upon this improved information flow, however, trade industries have traditionally been secretive and this needs to change to the extent that it improves collective interests without compromising individual competitive advantages. Therefore, in conclusion, we argue that despite the obvious benefits of digital twins, the solutions to the problem are not purely technical, but require new legislation, incentives, and business models which will bring about the change in perspective necessary to reach unprecedented heights of efficiency and business acumen.

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ENDNOTES

1. e.g. see the recently concluded EU Horizon 2020 project PRECINCT (Grant Agreement No. 101021668) https://www.precinct.info
2. i.e. the combined use of different transport modes to improve the operational efficiency, sustainability, and the general flexibility of the supply chain.
3. See EEXI and CII - ship carbon intensity and rating system (imo.org)
4. We discuss here operations which are considered critical for the efficiency of the maritime supply chain, otherwise the discussion can be endless. Nevertheless, the digital twin technology and our discussion can really apply to any aspect of operations where there is a time/efficiency element which can benefit from improved information flow and optimisation, where the planner finds it beneficial to fund its improvement.
5. According to our work with COSCO in EU Horizon 2020 project PLANET https://www.planet-project.eu

Chapter 8
Application of Digital Twins in the Design of New Green Transport Vessels

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ABSTRACT

The growing complexity of green transport vessels results in a gap between current ship design methods and new green transport vessel design. Innovative technologies such as digital twins (DTs) show the potential in supporting future complex designs when combined with suitable current ship design methods. The current state-of-the-art in DT-enabled design processes is still in its early research phases, both in the maritime world, and general engineering community. The most recent literature is presented, as well the role of optimization in the early design phases. Two complimentary design approaches are proposed, aimed at the concept design phases of green ships, where most of the design requirements are set (via design requirements) and locked-in (via initial design decisions). First, a DT-based green transport vessel design method is proposed which is then evaluated through a case study on an LNG-powered handysize bulk carrier. Four design scenarios are presented to show the ability of the design approach to simulate vessel behaviour, providing a feasible design space, and supporting early design decision-making. Second, an optimization-based DT design approach is proposed also covering the early concept design phase. Combined, the two complimentary DT design approaches help address the gap in enabling DTs in the design of green transport vessels.

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INTRODUCTION

The shipping industry is facing great challenges concerning emissions and sustainability. The IMO has adopted a strategy to achieve net-zero greenhouse gas (GHG) emissions from international shipping close to 2050, and commit to ensure an uptake of alternative zero and near-zero GHG fuels by 2030 (IMO, 2023). This is in addition to the European Commission aiming to implement a price on the amount CO_2 emission per year in the shipping industry by 2024 (European Commission, 2023). It is, thus, necessary for the shipping industry to reduce GHG emissions of ships not only during operation but within each stage of the ship life cycle including design, manufacturing, operation, maintenance and decommissioning. This creates a need for introducing new green technologies (Hirdaris and Cheng, 2012) and a revised design strategy that supports this goal and also handles the ever increasing complexity of ships and transport vessels.

Digital Twins in Ship Design

Digital Twins (DTs) are currently one of the most promising tools that can radically improve each stage of the ship life cycle from early design to decommissioning and help meet the climate goals (DT4GS, 2023). In order to improve every stage of the green ship life cycle it is necessary to establish a DT-enabled ship design framework. This chapter follows the definition of a digital twin (DT) used by Grieves (2015), DT4GS (2023), and Mauro and Kana (2023), and in which a DT is defined as having 3 components: (1) the physical entity, (2) the virtual entity and (3) the connection between the physical and virtual entity flowing in both directions. To date, DT literature has mainly focused on monitoring and predictive algorithms, functional during the operation phase, and generally lacks a framework for implementation and design (Medina et al, 2021; Psarommatis and May, 2022; Mauro and Kana, 2023).

DT based design is not a topic commonly researched in the literature. Especially not in the shipping industry where the concept of DT alone is underrepresented compared to other transport industries (Mauro and Kana, 2023). Even in other industries such as aerospace, civil, and automotive, research into methods for DT based design is still in the early phases and as a result is inconsistent and does not have a standardized framework (Psarommatis and May, 2022).

There are multiple reasons why it is so challenging to create a detailed framework for DT based design. Firstly and most importantly the definition of DT has been used inconsistently intertwining the concept of DT with other versions of digital entities. Secondly, the concept of DT based design with the synchronised DT from Grieves (2015) is relatively new and in a very early stage of development globally. Thirdly, as stated, the developments have mainly focused on the operation and maintenance stage and not specifically on the design process.

Existing Applications of DT Based Design in the Maritime Sector

According to Mauro and Kana (2023), there is a delay in the research progress related to the design phase within DT research in the maritime field. It is therefore critical to evaluate the state of the art and limitations of DT based ship design in more detail. Based on the review by Mauro and Kana (2023), and supplementing additional recent research, 16 papers within the maritime industry focusing on the design phase and digital twins are identified and summarized in Table 1.

Table 1. Categorization of research on DT-based maritime design

Reference	Content	Field
Hu et al (2023)	Application	Ship design
Mouzakitis et al (2023)	Technology	Ship design
Wang et al (2022)	Framework	Power, propulsion, and energy systems
Xiao et al (2022)	Paradigm	Ship design
Fernandez (2021)	Concept	CAD modelling
Sapkota et al (2021)	Framework	Structures
Arrichiello and Gualeni (2020)	Concept	Ship Design
Fonseca and Gaspar (2020)	Technology	Ship Design
Nikolopoulos and Boulougouris (2020)	Paradigm	Ship Design
Mondoro and Grisso (2019)	Paradigm	Structures
Munoz and Ramirez (2019)	Concept	CAD modelling
Dimopoulos et al (2018)	Technology	Power, propulsion, and energy systems
Erikstad (2019)	Concept	Ship design
Erikstad (2018)	Concept	Ship design
Ferguson (2017)	Concept	Ship design
Stachowski and Kjeilen (2017)	Concept	Ship design

Adopted from Mauro and Kana (2023): **Concept**: the work prioritises the concepts, definitions and capabilities of DT in the maritime industry; **Technology**: the paper describes or details DT's enabling technologies; **Paradigm**: the study provides a general description of the DT application in the marine field, with no in-depth analysis or case study**; Framework**: the study starts with a general description of the DT, providing a framework implementation and a rather-detailed case study; **Application**: after a detailed description of DT application in the maritime field, the paper also provides technical details and a detailed case study.

All the papers related to ship design occur since 2017. Mauro and Kana (2023) argue that maritime industry research is more focused on building the digital models to support DTs, and thus the design phase is still in an early research stage. In addition, there are some obvious problems that can be drawn from this brief review. First, it is evident that there is a very low amount of papers that elaborate on the design phase and how to implement the DT. Additionally, very little papers include essential information such as specific methods, input data, output data or reliability of the design. Accordance to Mauro and Kana (2023) the current literature on DT based ship design is in the "formation stage" where, "very few papers are published as the technological foundations are not mature enough to support effective applications". Second, there is no consistency on the definition of the DT, nor has the DT been defined sufficiently. The structure of the digital twin is also not defined and therefore there is an abundance of papers trying to define the virtual representation of the DT. Third, the assigned methods have been applied only once allowing no iterative improvement on the methods in different case scenarios. From the overview, a distinction can be made between the design of a physical entity while consequently designing a DT specifically tailored to the physical entity or developing a virtual space in which digital twins can be developed for different types of ships.

Ship Design Optimization and Digital Twins

Early ship design provides significant opportunities to gain high efficiency at a relatively low cost. According to some estimates (Zhang et al, 2020), more than 50% of the product efficiency, e.g., its sustainability, is based on the decisions made in the early design phases. Historically the conventional early ship design was non-flexible and relied on the strict prescriptive requirements for specific parameters of a ship from a technical task defined by a customer (e.g., ship length, breadth, service speed, equipment) and empirical design rules defined by classification society (e.g., minimum freeboard and double bottom height). As demonstrated by Andrews and Erikstad (2015), straightforward application of the conventional ship design approach narrows the available design space and often results in a single-point design focus.

Acknowledging the existing issues, IMO has adopted new goal-based design (GBD) regulations for bulk carriers and oil tankers (IMO, 2010), which entered into force in 2016, marking a significant shift towards more well-informed decision-making in ship design. The GBD approach aims to quantify various performance indicators of a ship, avoiding predetermined rules whenever possible. This approach significantly expands the design possibilities and fosters more innovative solutions by optimizing the parameters of a ship for specific key performance indicators (KPIs). Although GBD is a powerful ship design paradigm that allows for avoiding disadvantages associated with prescripted regulations, its capabilities are greatly constrained by prescribed requirements from a technical task.

Expanding the design considerations beyond the existing boundaries (e.g., by including more parameters into design variables and modeling ship operations and lifecycle) would result in more innovative and efficient ships enabled by a systemic outlook and designing for the customer goals instead of requirements. To do so, in practice, the prescriptive design requirements can be replaced with quantifiable goal-based KPIs defined considering the purpose, operation conditions, and lifecycle of a ship. The importance of systemic outlook in ship design and its significant impact on ship lifecycle efficiency is noted in many studies (Papanikolou, 2010; Gaspar et al, 2013; van Lynden, 2022).

Moreover, the green transition in shipping requires a responsible design approach where one actor transparently accounts for the future GHG emissions during the entire lifecycle of a ship. The decarbonizing objectives adopted by IMO are quantified and clear, and compliance with them is needed to be demonstrated in practice. The existing practices result in a diffusion of responsibility for the environmental efficiency of a ship between the creators of a technical task and a conceptual design. In contrast, a more responsible approach can simultaneously account for the optimal design solutions (i.e., by providing the detailed requirements for a ship, including major technical decisions, serving as inputs for the conceptual design stage) and corresponding operational guidelines for achieving the declared environmental performance in practice.

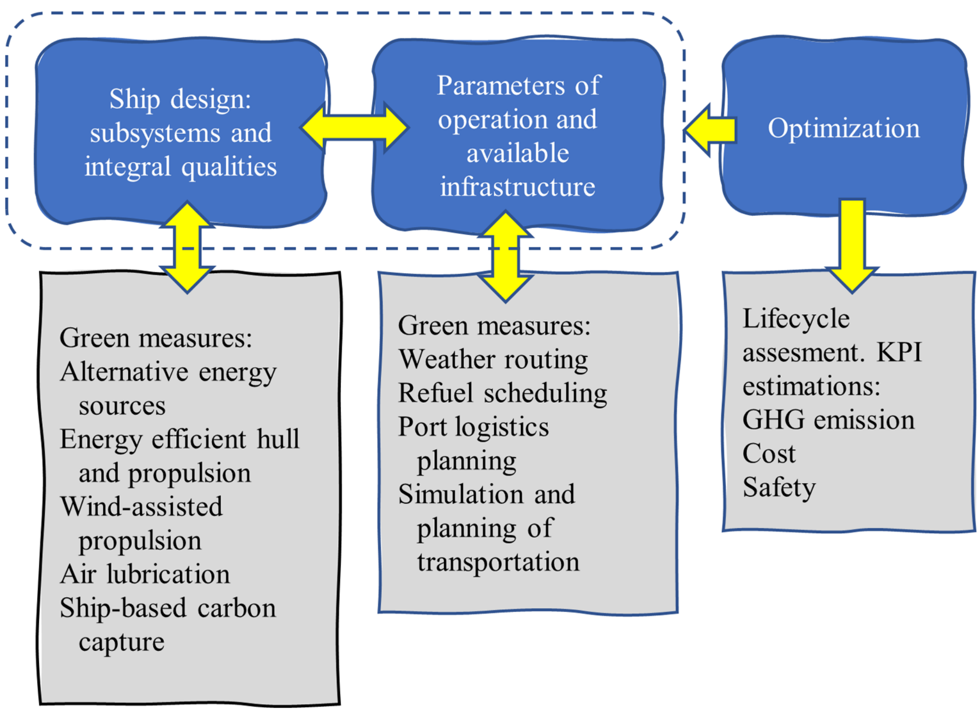
The lack of such considerations results in many ships operating far from their optimal operational profile, e.g., slow-steaming containerships, bulkers, and tankers, initially designed for higher speeds (Rutherford et al, 2020), and ships with energy efficiency devices operating out of their design conditions (Tran, et al, 2021). Separate consideration of logistics and operation overlooks ship design features and limitations, while isolated ship design overlooks lifecycle features. Sustainable early conceptual ship design optimization allows for utilizing a significant decarbonizing potential by bridging fleet composition planning and conceptual ship design. Alternative technologies for decarbonizing shipping may be included in optimization as ship design variables, significantly affecting a ship's design qualities and operation profile.

Sustainable early conceptual ship design optimization requires a framework that includes an algorithm for mathematical optimization and a flexible surrogate-based digital twin of a ship. Ship design qualities and the operational context to-be-considered are case-specific and can be divided into general and task-related. Figure 1 shows the essential factors to be considered for sustainable early conceptual ship design optimization. Optimization aims to search the design space for favorable solutions to minimize the GHG lifecycle emissions of a ship, estimating other KPIs like safety and cost-efficiency.

A DT may vary from a highly detailed replica of an existing ship run in parallel with a real ship to less detailed information models for future vessels. As a rule, the higher fidelity of a digital twin, the less part of a design space (i.e., alternative ship designs) we can evaluate with it. The main difference between the "classic" DT of a ship for the conceptual design and the DT for the early conceptual ship design optimization is the range of their applicability and the absence of big data for innovative design alternatives.

The many potential candidate solutions in the design space require developing reliable but simple methods to estimate their design qualities (i.e., subsystems performance) and system-level performance in a limited time. A combination of analytical white box models (e.g., classic ship theory with numerical integration), grey box semi-empirical surrogate models, and empirical black box models can meet these requirements and are often employed in ship design optimization to replace complex and time-consuming methods, e.g., FEM and CFD (Tavakoli, et al, 2021; Kondratenko, et al, 2023). The typical examples of surrogate models for the early conceptual ship design optimization are the Holtrop and Mennen (1982) method for estimating ship resistance and energy consumption, Townsin and Kwon's (1983) method for

Figure 1. Factors to be considered in sustainable early conceptual ship design optimization



estimating the speed loss due to added resistance in wind and waves, and Lindqvist method (1989) for estimating of ship resistance in level ice.

There is no need to study all the internal and external factors of a specific vessel operation – that would make the model too complex with a high probability of errors. Accordingly, the development of the early conceptual design optimization approach for a specific vessel type starts from the preliminary study of the potentially most influential factors to be considered.

The critical quality of the DT for the early conceptual ship design optimization is integrity. If the DT has integrity, changes in the performance of subsystems result in a shift in system-level performance, and vice versa, if relevant. As a chain is no stronger than its weakest link (Reid, 2011), having an equal level of fidelity of surrogate models of subsystems is beneficial. Developing an in-depth surrogate model requires more effort and pays off only if surrogate models of other subsystems are in-depth too.

This chapter subsequently presents two complementary ship design approaches under development. First, a DT-based green ship design process being developed at TU Delft is presented (Section 2) with a case study on an LNG-powered handysized bulk carrier (Section 3). Second, an approach for DTs in early ship design optimization under development at Aalto University is presented (Section 4). Conclusions related to both the state-of-the-art and the two design approaches are discussed in Section 5.

A DT-BASED GREEN SHIP DESIGN PROCESS[1]

Requirements for the DT-Based Green Ship Design Process

A design process capable of enabling DTs for green transport ship design is needed. The following requirements have been established for such a new design process:

1. The design process should calculate the vessel's resistance, stability, and safety indicators, and compare them to up-to-date IMO and the International Organization of Standardization (ISO) standards.
2. The design process should provide robust estimation of vessel's financial performance and emission performance (such as EEDI and EEOI) with simulation models. The calculation error in the concept design phase should be limited to <15% (general engineering acceptable error).
3. The digital models for financial and emission behaviours should be built to assist the design and decision process. The models should be applicable to the full lifecycle, including design, production, operation, and deconstruction/ retrofitting.
4. The design process should provide feasible plans for the general layout and cargo space to assess potential conflicts.
5. The design process should support expansibility within the service life (about 20 years), which is the ability to integrate, add, or replace functional systems of the designed vessel.
6. The design process should incorporate efficient information integration (in every design iteration) between multi-discipline design specialties and overall performance simulation.

Design Framework

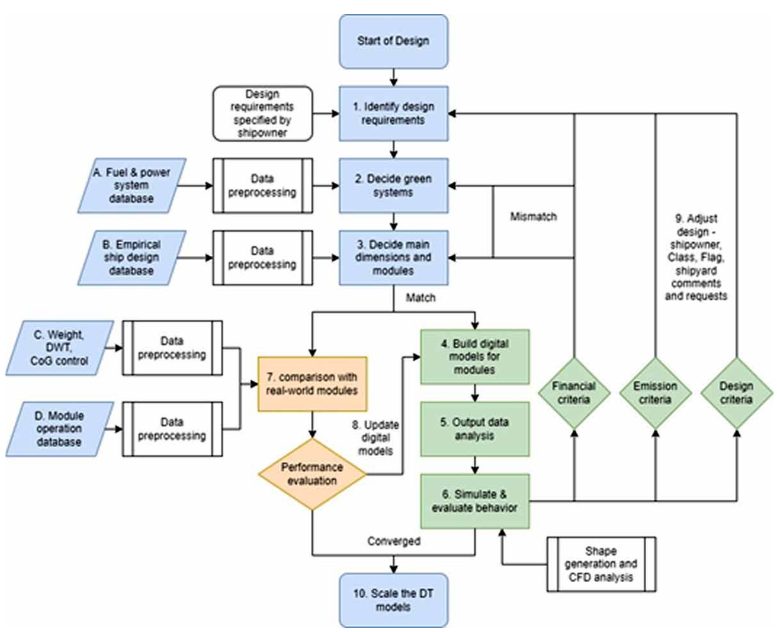
To satisfy the design requirements and bridge the gap between global green targets and transport ship design, a DT-based green ship design process is proposed in Figure 2. In the design process, the colored blocks indicate the general design steps (blue), the virtual part of DT steps (green), and the physical part (orange) of DT steps. The details of each step are described below.

Step 1-Identify design requirements. In Step 1, the ship type and mission is decided, followed by the general design requirements such as emission level, deadweight, and speed. The targets for the requirements are based on the calculation models, such as EEDI, or the cost model. Many times shipowners provide initial requirements for the main dimensions of the vessel, such as maximum draft or breadth, which may depend on harbor or canal limitations.

Step 2-Decide green systems. In Step 2, the green power systems are chosen based on route distance, technical limitations, and fuel consideration. If the vessel can't reach required EEDI, additional green power systems are considered, typically requiring a design office to prepare a Feasibility Study. In detail, fuel type, propulsion system, and power plant configuration should be determined in this step, which provides the input variables for the emission models and other calculation models. A database of alternative fuels, engines, power systems, and propulsion systems after preprocessing is provided as input for emission estimation models. Comparison between the emission outputs of different green power systems is thus provided as references for designers when making the decision in this step. Given the interplay between the choice of green systems, and the ship layout, this step is done in close coordination with Step 3.

Step 3-Decide main dimensions and modules. After determining the green power systems, in combination with the commercial design requirements and the system functional study, the main dimensions of the vessel and the system modules are determined. The empirical ship design database after preprocess-

Figure 2. Proposed DT-based design process



ing is provided as the initial design template in this step. In addition, weight, deadweight tonnage and centers of gravity have also great impact on design process and should be taken into account.

Step 4-Build digital models for modules. Based on the dimensions and modules decided in Steps 1-3, the digital models of the system modules can be built. The digital model of the whole vessel is not built in the early design stages, as the main objective in this stage is to enhance the design of modules.

Step 5-Output data analysis. The output data and model calculation results are collected, integrated, and analyzed in Step 5. The data analysis results are further used in the following steps.

Step 6-Simulate and evaluate behavior. The data patterns are used in Step 6 to simulate system behaviors via relevant machine learning and data regression and analysis techniques. At this step, it should also be possible to generate a hull shape and perform CFD analyses.

Step 7-Comparison with real-world modules. Based on the main dimension and module parameters, similar real-world functional modules are selected as comparison objects. The changes in dimensions and other vessel characteristics are reflected in the different real-world module data. As a result, the operation database of various working modules on transport vessels is provided as a substitute for the physical entity. This step should be simultaneously conducted with Step 4.

Step 8-Update digital models. The real-world operational results from Step 7 are evaluated in Step 9. The performance data is compared with the financial, emission, and general vessel (resistance, stability) criteria. According to this, the digital models are updated.

Step 9-Adjust design. In Step 9, the design of the vessel and modules are iteratively adjusted based on the behavior simulation and resulting performance evaluation results. According to the design requirements identified in Step 1, financial and emission criteria are determined, to which the performance of the DT modules are compared and instruct the adjustment of ship modules and dimensions, as well as the green system designs. If the financial and emission requirements are in conflict, or not realistic after DT simulations, the design requirements decided in the first step should also be iteratively adjusted.

Step 10-Scale the DT models. When the performance evaluation results of the DT models satisfy the overall design requirements, the DT model could be transferred into a full-scaled vessel supporting the following lifecycle phases.

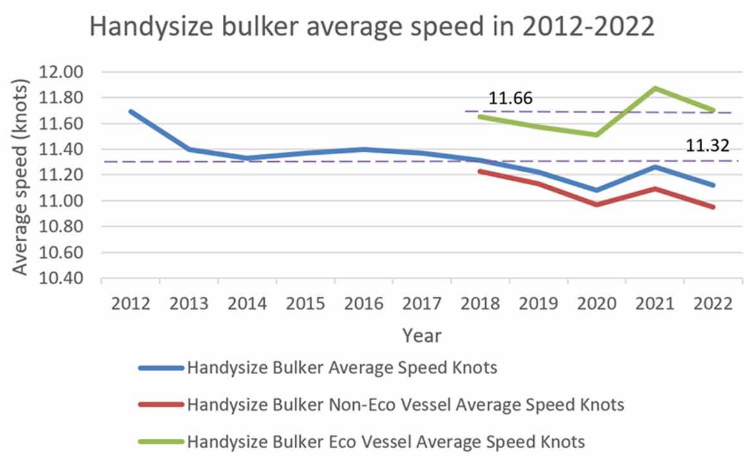
CASE STUDY: HANDYSIZE BULK CARRIER

To test the feasibility of the proposed DT-based design process, a case study on a handysize bulk carrier is presented. As the design method is aimed at green transport vessel design, the case study vessel should be typical in terms of the energy transition, cargo space conflict, and data support for DT models. The reason for choosing a handysize bulk carrier is that bulk carriers have the second-largest HFO-equivalent fuel consumption (IMO, 2020) and the largest available data on Clarksons (Clarksons, 2023). In this section, the proposed design framework is run from Step 1 to Step 10, after which the output results and layout plans are discussed.

Design Process

Step 1–Identify design requirements. The vessel's capacity and design speed are chosen based on reference vessels from Clarksons. The average capacity of new-built handysize bulk carriers is 37,500 DWT,

Figure 3. Average speed of handysize bulk carriers
From Clarksons (2023)



and the average design speed of Eco handysize bulk carriers is 12 knots (see Figure 3). The full list of requirements is:

- Vessel type: handysize bulk carrier
- Vessel capacity: 37,500 DWT.
- Design service speed: 12 knots with a 15% sea margin allowance
- The vessel should satisfy the IMO 2025 EEDI target.
- Single hull, double bottom, with hatch covers.
- The vessel should satisfy up-to-date applicable regulations and standards.
- Crew accommodation ability of 14 persons, the accommodation structure should be placed aft or fore.
- Cargo type: normal bulk and steel.
- Good maneuverability and stability characteristics at service.
- Self-load and discharge ability with 4 cranes on board.

Step 2–Decide green systems. All of the handysize bulk carriers in service from Clarksons database are powered by diesel fuel oil. To ensure the case study provides a reference for new-build transport vessels in the near future, fuels that have high availability, relatively low prices, and power existing engine products are considered. Batteries are not considered since transport vessels usually have large capacities and long travel distances, requiring large power storage onboard. MAN offers commercial engine products powered by alternative fuels that comply with IMO Tier II and Tier III (MAN, 2023). As the DT-based design process requires real-world data for the physical entity part at the early design stage, available operational data from real vessels are important for the case study. Compared to other alternative fuels, LNG has a longer history of powering bulk carriers (the first LNG fuelled bulk carrier was delivered in Feb 2018 (Lloyd's Register, 2018)). Thus, the operational data of LNG-fuelled bulk carriers are more advanced than the other alternative fuels. Based on this consideration, LNG is chosen as the power source for this case study.

From a design perspective, LNG fuel tanks differ from diesel fuel tanks in terms of shape and volume, which needs to be considered as they will influence the vessel's cargo space. IMO has defined three types of LNG tanks: type A, type B, and type C. For now, type A tanks have been mainly used for large amounts of LNG storage and flat-surface LNG carriers (Liquified Gas Carrier, 2023), whereas type C are already applied in the fuel tanks for LNG-powered engine sets. In this case study, the type C tank is chosen as the fuel storage tank. This decision further influences the layout and cargo space calculation models in the following steps.

After deciding the fuel type of the vessel, the selection of the main engine and the auxiliary engines is done by analyzing reference bulk carriers with similar displacement. The reference vessels are selected from the full handysize bulk carrier set in Step 1, and have a displacement between 37,475 DWT and

Figure 4. Main engine power of reference vessels
From Clarksons (2023)

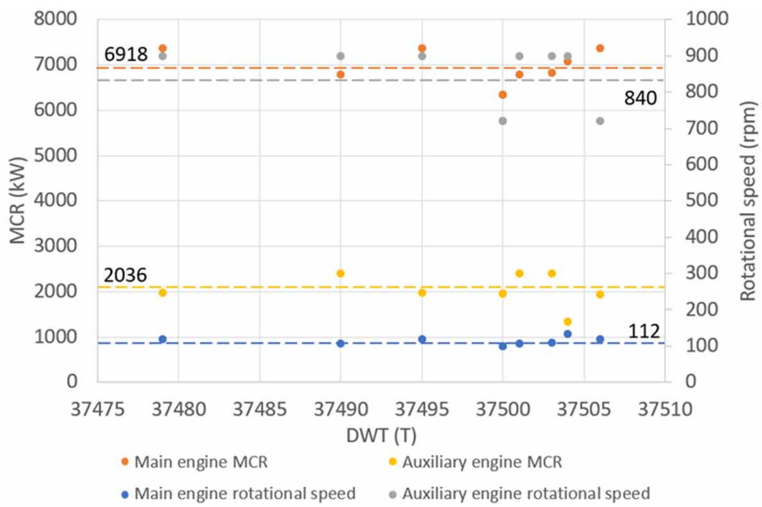
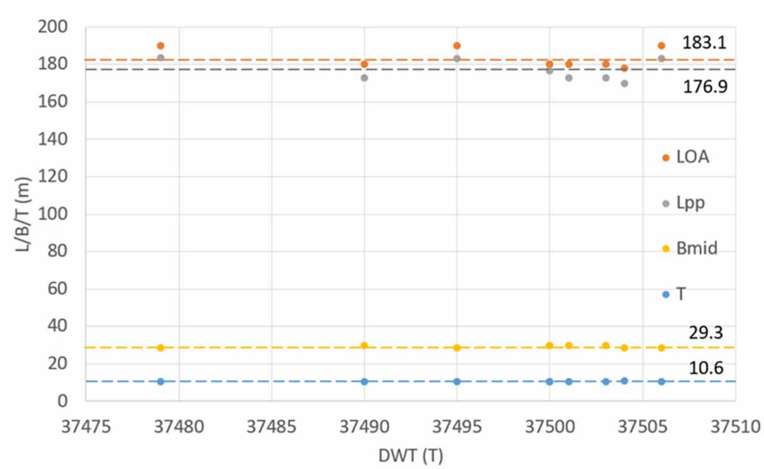


Figure 5. Main dimensions of reference vessels
From Clarksons (2023)



37,510 DWT. All are equipped with eco-electronic engines. As shown in Figure 4, the average MCRs of the main engine and auxiliary engine are 6918 kW and 2036 kW. These decisions can be adjusted according to model results after the first round of the case study.

Step 3-Decide main dimensions and modules. The ship's overall length is decided based on the length of bulk carriers with similar displacement. Figure 5 shows the main dimensions of the 9 reference bulk carriers, where two vessels have the same main dimensions. It can be seen that the average overall length is 183.1 m, and thus, the overall length of the first design is chosen to be 183 m. The molded breadth, draught, and length between perpendicular can be calculated using the equations developed by fitting results from the bulk carrier database (Equations 1-3). The fitting functions draw on the form of Papanikolaou's equation of breadth (Papanikolaou, 2014).

$$B = 0.09845 * L^{1.0202} \tag{1}$$

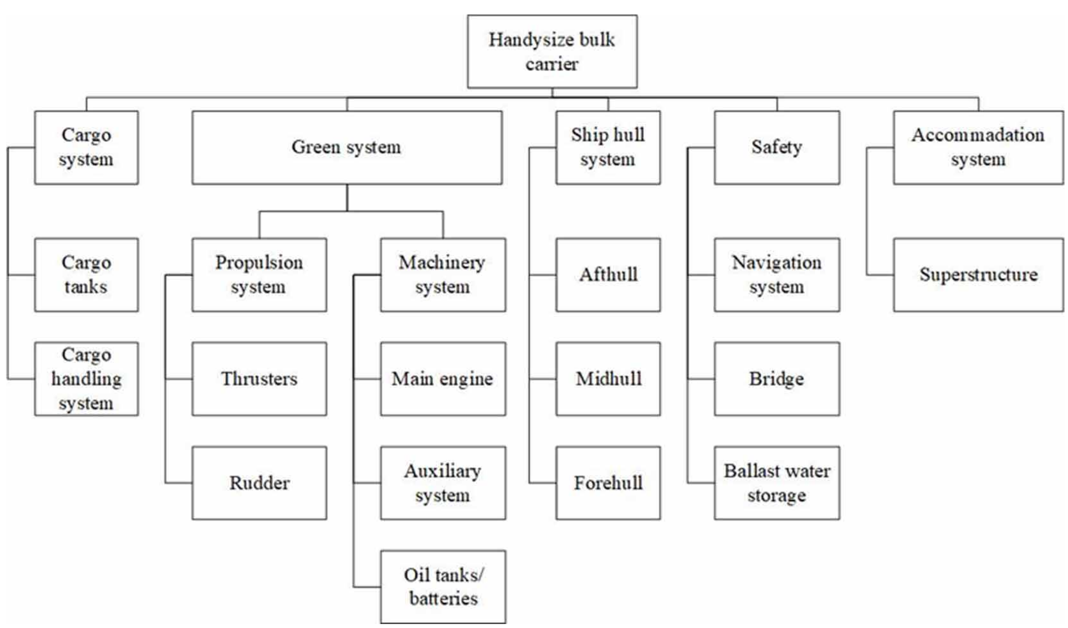
$$T = 0.01492 * L^{1.2586} \tag{2}$$

$$L_{PP} = 0.8712 * L^{1.0202} \tag{3}$$

The modules of the vessel and the DT models are based on the system blocks of the handysize bulk carrier. The system breakdown of the bulk carrier is shown in Figure 6. For each subsystem block, corresponding DT models should be built in the following steps to assist the design process.

Step 4–Build digital models for modules

Figure 6. System breakdown of LNG-powered handysize bulkcarrier



Main Variables

The main variables for the digital models, including those from Step 3, are:

- The overall length: LOA (m)
- The design speed: V (knots)
- The fuel type: in this case study the fuel types analyzed are very low sulfur fuel oil (VLSFO) and LNG.

Besides the main variables, other constant factors are used as input for the models and can be adjusted in every design round. By evaluating the model results under certain financial and emission criteria, designers can change the interval of the variables and inputs based on the evaluation to optimize the design. Specific constant inputs used in this case study will be introduced in the subsection of each digital model.

Resistance Model

The resistance digital model is based on the Holtrop & Mennen method (Holtrop and Mennen, 1982).

Required Power and Bunker Size Model

Having the total resistance, the brake power can be calculated by Equations 4-6.

$$P_E = R_{total} * V \tag{4}$$

$$P_B = \frac{P_E}{\eta_H * \eta_O * \eta_R * \eta_S} \tag{5}$$

$$P_{engine} = (1+0.15+0.1)*P_B \tag{6}$$

Where P_E (kW) is the effective towing power, P_B (kW) is the brake power, P_{engine} (kW) is the engine power considering a sea margin of 15% and an engine margin of 10%. The rotation efficiency ηR and hull efficiency ηH $_a$re calculated based on the Holtrop & Mennen method. The open water efficiency ηO i_s estimated using an in-house TU Delft program called PropCalc (PropCalc, no date).

The required energy and corresponding required bunker size are calculated based on Suy (2022) and Terun et al (2020). The estimated cargo capacity (Equation 7) is calculated by the fitting equation from handysize bulk carrier database of Clarksons.

$$\mathrm{M}c_{argo=} (2149.72+0.56*\mathrm{D}WT)*\theta \tag{7}$$

Where θ is the fullness of the vessel The required energy for one trip is calculated based on the average fuel consumption and voyage time (Equation 8) (Suy, 2022):

$$E_{req} = C_{avg} * cEDV_{V\ LSFO} * t_{voyage} * \frac{\eta_{ICE}}{\eta_{conv} * \eta_{reformer}} * (1 + margin) \tag{8}$$

where E_{req} (GJ/trip) is the required energy, C_{avg} (m^3/day) is the average VLSFO consumption based on engine power and specific fuel oil consumption values, $cEDV_{V\ LSFO}$ (GJ/m^3) is the contained volumetric energy density for the alternative energy source of the design vessel, ηI_{CE} is the converter efficiency of the internal combusted engine, $\eta re_{former\ i}$s the reformer efficiency for alternative fuel. Energy storage of 4 single trips is applied in this case study so that the vessel can find the lowest bunker price within four trips. So the required bunker size of the vessel can be calculated via Equation 9-10 (Suy, 2022):

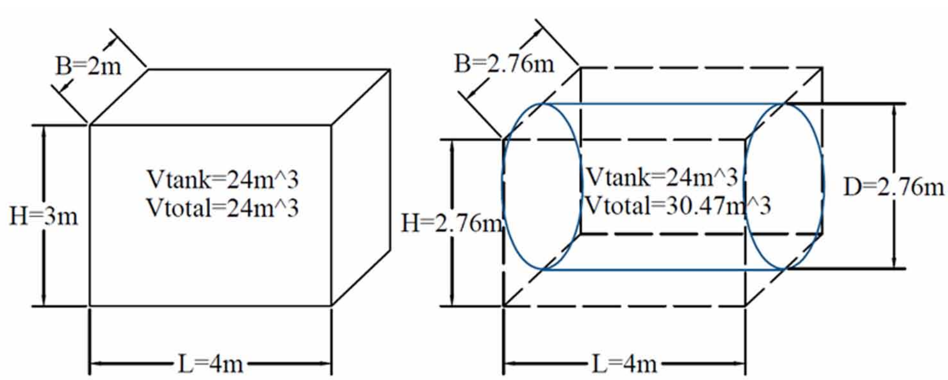
$$V_{trip} = \frac{E_{req}}{cEDV_{alter}} \tag{9}$$

$$V_{req} = V_{trip} * 4 \tag{10}$$

Where V_{trip} (m^3/trip) is the alternative fuel volume consumption on one trip, $cEDV_{alter}$ (GJ/m^3) is the contained volumetric energy density of alternative energy sources, and V_{req} (m^3) is the required volume of energy carrier (required bunker size). As mentioned in Step 2, the digital model calculations consider type C tanks in this case study. Assuming the volume and length of the fuel tanks are the same, Figure 7 illustrates that the LNG type C tanks take up larger rectangular space than diesel fuel tanks as they are in cylinder shapes. As a result, the required bunker size of LNG should add a term of the volume difference caused by the cylinder shape as shown in Equation 11.

$$V_{add} = L_{tank} * D_{tank} * \left(1 - \frac{\pi}{4}\right) = 0.215 * L_{tank} * D_{tank} \tag{11}$$

Figure 7. Tank comparison between diesel and LNG



$$V_{tripdiesel} = \frac{E_{req}}{cEDV_{diesel}} \tag{12}$$

$$V_{reqdiesel} = V_{tripdiesel}*4 \tag{13}$$

$$V_{diff} = V_{req} + V_{add} + V_{reqdiesel} \tag{14}$$

Similarly, the diesel fuel consumption for one trip and the required volume of diesel can be calculated via Equations 12-14. By evaluating the difference between the required volume of diesel and alternative energy sources, designers can estimate to what extent the choice of energy sources influences bunker size, which in turn affects the cargo space. This cargo space difference also influences the revenue potential of the vessel.

Financial Model

In the financial model, the profits of the vessel are estimated. The variables are property factors of the energy sources, which in this case study is LNG. The financial property of the designed vessel in this case study is the overall profit of the vessel in its whole service life. The profits can be calculated by Equation 15-17 (van der Molen, 2021).

$$Profits = Revenue*n - Costs \tag{15}$$

$$Revenue = M_{cargotrue}*F*\eta t_{rip} \tag{16}$$

$$M_{cargotrue} = (2.149.72+0.56*(DWT - V_{diff}))*\theta \tag{17}$$

Where F (USD/ton) is the average freight rate of bulk carriers under 80,000 DWT from Clarksons, ηt_{rip} is the average number of times the cargo is delivered in one year for handysize bulk carriers, $Mc_{argotrue}$ (t) is the cargo loaded on one trip taking into account of the cargo space change from the application of alternative energy sources, Vd_{iff}(m3$^{)}$ is the required bunker size difference between vessels using alternative energy sources and diesel. In this case, the cargo space decreases as the required bunker size of LNG is larger than the most widely used diesel. This change in the cargo space is directly reflected in the decrease in revenue and therefore the overall profits.

The CAPEX, decided by the building cost, depreciation, scrap price and interest rate, is based on the work of van der Molen (2021). To estimate the capital cost of green bulk carriers using alternative energy sources, the costs of diesel fuel should be substituted by that of alternative energy sources. The costs of diesel fuel and alternative energy source systems consider the capital costs of engine, exhaust gas cleaning, and storage (Baldi, et al, 2019; de Vries, 2019; van der Molen 2021).

The carbon tax and fuel cost calculations are based on the low scenario carbon tax value in 2020 (USD/ton CO_2) (van der Molen, 2021), emission factor, number of cargo delivered in one year, and fuel price P_{fuel} (USD) (Baldi et al, 2019).

Emission Model

The emission model consists of calculating the EEDI value and the EEDI reference lines. The calculation methods are based on IMO regulations (MEPC, 2013, 2018). In this case study, the innovative emission reduction technologies are assumed to be auxiliary system optimization and hull optimization, with power reduction potential of up to 60% (Dere and Deniz, 2019) and 15% (Singh and Pedersen, 2016). The effective factors f_{eff} corresponding to these emission reduction technologies are set as 1 according to the IMO regulation (MEPC, 2021).

Step 5–Output data analysis. With the original design variables input, the first-round digital model results are collected and analyzed in Step 5. Table 2 and 3 provide the output IMO EEDI target values and the behavior output results of the vessel. The required engine power is lower than the chosen engine in Step 2, which is caused by the lower design speed than the reference vessels. The digital models calculate the bunker size in both LNG and VLSIFO-powered scenarios, and thus the volume difference

Table 2. IMO EEDI targets

EEDI 2019	EEDI 2024	EEDI 2025
5.69	5.06	4.43

Table 3. Output results of digital models

Components	Value
LOA (m)	183
B (m)	29.2
T (m)	10.5
Design speed (knots)	12
Total resistance (kN)	348.1
Travel distance (nm)	1575.2
Required engine power (kW)	5100.6
Bunker size LNG (m^3)	1747.9
Bunker size diesel (m^3)	1030.0
Bunker size difference (m^3)	717.9
Estimated cargo load (t)	20473
Profits (m$)	112.2
EEDI	5.08

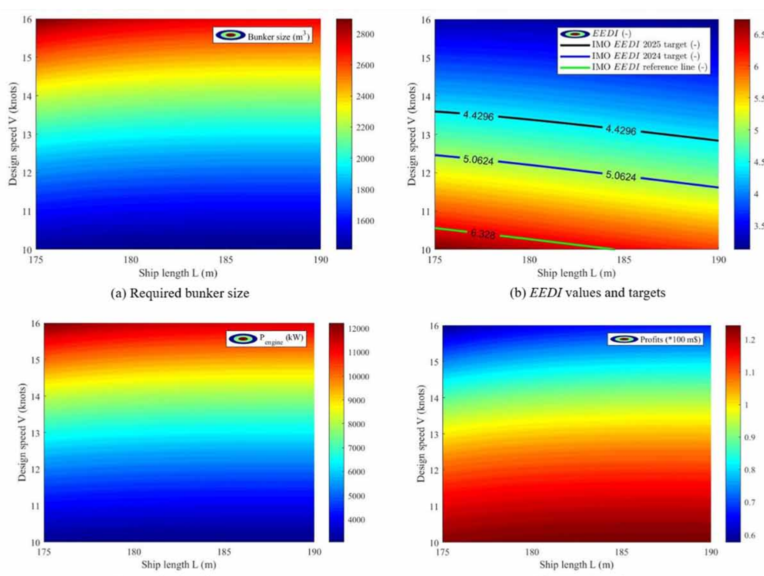
between LNG and diesel can be illustrated. The first-round EEDI value 5.08 does not satisfy the IMO 2024 and 2025 targets, which indicates possible modifications in the design variables in the next round.

The digital models and results are verified by properties of the reference vessels from Clarksons. The average property values of the 9 reference vessels are calculated in Table 4. The deviation values show that the main dimensions have very low deviations (<1%), while other properties have relatively large deviations. The main engine MCR and the EEDI model results have 14.1% and 5.64% deviation from the reference average, which are larger than that of the main dimension models, but still within the error benchmark set in the design requirements (15%). However, the bunker capacity model has a higher deviation (-19.3%) and an opposite trend from the engine power. This may be caused by the estimation method used in the digital model. It is assumed that the bunker capacity should provide a bunker space for 4 trips of the vessel, while in practical operations the required bunker capacity might differ from this

Table 4. Reference vessel verification

Component	Reference average	Model results	Deviation (%)
DWT	37497 T	37500	0.008
LOA	183 m	183 m	0
B	29.3 m	29.2 m	-0.34
T	10.6 m	10.5 m	-0.94
Speed	14 kn	14 kn	0
Main engine MCR	6918 kW	7893 kW	14.1
Bunker capacity	1612 m^3	1300 m^3	-19.3
EEXI / EEDI	4.61 (EEXI)	4.87 (EEDI)	5.64

Figure 8. Heat map plots of LNG-powered handysize bulk carrier

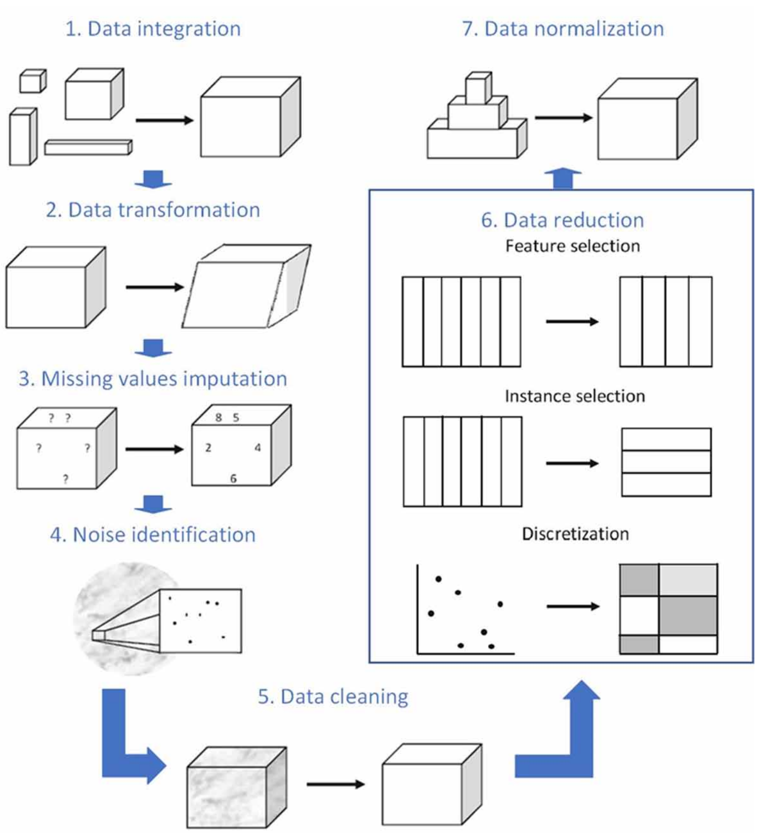


assumption. As detailed bunker designs are not provided on Clarksons, the individual bunker designs of different vessels sail in various sea areas cannot be estimated. Overall, the digital models have been verified to give acceptable results except for the bunker capacity. It is still up to the user to decide how many trips the bunker capacity should be able to support, so the digital models will maintain the settings in the following steps in this case study.

Step 6–Simulate and evaluate behaviour. After the first-stage verification of the built digital models, the vessel's behavior across a range of main variables (different design decisions) can be simulated. For a fixed vessel capacity (37,500 DWT), the financial and emission performances are simulated. The LOA and design service speed intervals are taken around the design decisions in Step 1 and Step 3, respectively LOA = [175m, 190m] and V = [10knots, 16knots]. For each combination of overall length and design service speed, the vessel's required engine power, bunker size, profits, and EEDI values are calculated using the digital models built in Step 4, resulting in the heat maps in Figure 8.

It can be seen that engine power, bunker size, and overall profits are relatively less sensitive to ship length, and mostly depend on design speed. From the design speed of 10 to 16 knots, the required engine power increases from ~3000 kW to ~12000 kW, the bunker size increases from over 1500 m^3 to 2800 m^3, while the overall profits decrease from around 125 m$ to 60 m$. The EEDI value is heavily influenced by both the ship length and the design speed. It is clear that the first-round design speed of

Figure 9. proposed data pre-processing framework
Adapted from García et al. (2016)



12 knots and ship length of 183 meters cannot satisfy the design requirement, and should be modified in the next design round.

When considering both the financial and emission benefit of the vessel, a good design should aim for higher profits and a lower EEDI value. As the ship length does not influence the profits significantly, the design speed will be the most important decision. The designer should choose the lowest acceptable design speed within the EEDI feasible design space in order to reach the highest overall profits.

Step 7-Comparison with real-world modules. Assuming the vessel's engine logbook and the cargo record book are available, Figure 9 shows the proposed data preprocessing framework, based on García, et al (2016), and described below.

Data Integration

The available data sources may include the vessel's engine logbook, ship logbook, and cargo record book, from which the engine operational data (fuel consumption, SFOC, main engine load, auxiliary engine load, energy reduction from innovative technologies), trip information (trip distance, time at berth), and cargo-related properties (mass of cargo, freight rate, crane productivity, fuel price, vessel fullness) may be recorded. Digital data sources can be downloaded from online reports, while hand-written logbooks and record books should be sorted and added to the dataset. The digital models for this case study are built in Matlab, so the dataset can be directly read by the calculation codes later on.

Data Transformation

The dataset needs to be transformed into variables and units that are related to the digital models. For example, the vessel fullness might be represented by the mass of cargo in the original data entry, which needs to be divided by the cargo capacity to give a non-dimensional percentage. Also, some of the required data such as the auxiliary engine load is calculated based on the original data entry of the power load of different load groups. These calculations should follow the IMO instructions (MEPC, 2018) and be done in the data transformation step.

Missing Values Imputation

Missing values caused by recording interruption and mistakes should be filled in in the imputation step. For example, if one day of the engine logbook is missing, the engine load and fuel consumption on this working day should be estimated based on the operational profile, vessel tasks, previous data, and experiences. The discontinuity of data sources can cause under/overestimation of certain properties (engine load, etc) and lead to deviated comparisons and calculation results of digital models.

Noise Identification

The noise in the data can be described as unrealistic or abnormal values in the dataset. Designers can define constraints for every required data component. Values beyond these constraints in the dataset are considered noise and can be deleted. Some of the possible constraints are shown in Table 5. Also, theoretical calculations can be taken as a reference for the data. For example, the shaft power is estimated based on Holtrop & Mennen method in the digital model, the result value can provide a first-step

Table 5. Potential data constraints for noise identification

Components	Constraints
Fuel consumption	More than 40 tons per day
SFOC	Lower than ±10% difference from the value provided by the producer
Shaft power	More than ±15% difference from the estimated value
Auxiliary engine load	More than 20% of the main engine MCR
Trip distance	More than 384 nm a day (at 16 knots all day)
Mass of cargo	More than 95% of gross tonnage
Vessel fullness	Greater than 1

comparison for the dataset. If the shaft power recorded in the engine logbook varies from the reference value more than tolerance, the data is defined as an unrealistic value.

Data Cleaning

The data cleaning process is done by filtering the identified noise from the dataset. This way, the abnormal data will not influence the comparison between real-world data and digital model results. The dataset should be within the constraints completely after this process.

Data Reduction

The data reduction process aims to reduce the dimension of the dataset without reducing its quality. Data reduction can be done in three ways: feature selection, instance selection, and discretization. The reduction goals of these three processes are removing irrelevant redundancy, reducing dataset size, and dividing numerical features into a limited number of intervals (García et al, 2016). In this case assumption, only the engine logbook, trip logbook, and cargo record book are available. So the size of the data may be manageable. As a result, only feature selection is applied in this case.

Data Normalization

Data normalization was not required in this DT case. However, in general, care should be taken to normalize data to ensure that proper trends are evaluated.

Input Data Comparison

The pre-processed input data is used as validation for the settings in the digital models. The input values should be changed to real-world data in order to increase the authenticity of the digital models.

Vessel Performance Comparison

The vessel performance dataset is compared to the model results. Both the digital models and the real-world data collection can be adjusted in this process. If the difference between the calculation results and real-world data is relatively large, then the designer can check either from the model construction and factor assumptions or from the sensor and recording accuracy of real-world data sources.

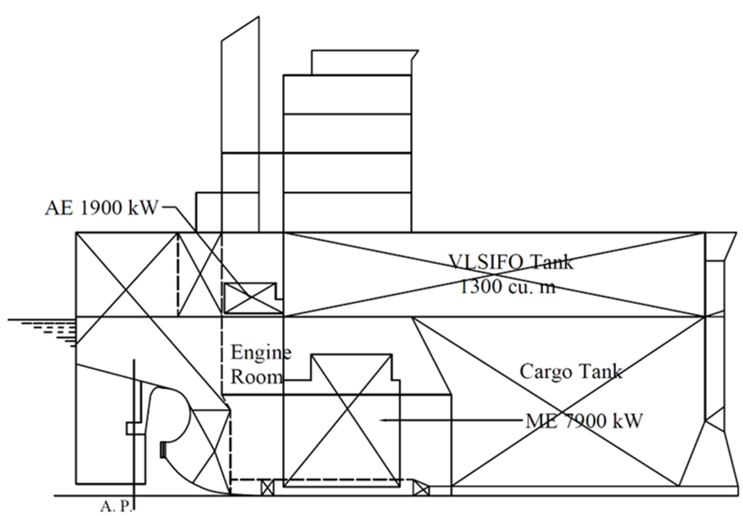
Step 8-Update digital models. The settings and results of the digital model built in Step 4 are compared with real-world data in Step 7. In this Step, the digital models are updated according to the comparison results, for example, specifically by modifying the input value of engine power reduction by innovative technologies and adding additional cost to the profits calculation model.

Step 9-Adjust design. After updating the digital models based on comparison results from Step 7, the design is adjusted according to the financial and emission criteria in Step 9. The adjustment of the design can be taken in the vessel's green system, main dimensions, and operational profile. In the second round of the design process, the design speed increases to 14 knots within the feasible speed area simulated in Step 6.

There are four ways to solve this problem of the increase in bunker size due to LNG,: (1) maintaining the vessel size while decreasing the cargo space; (2) maintaining the cargo space while increasing the vessel size; (3) maintaining the vessel size and cargo space while reducing the travel distance, and (4) placing the additional bunker on the tank deck. The option of reducing the design speed is not considered because the lower design speed (12 knots) does not satisfy the IMO EEDI target.

In this subsection, these four design scenarios are simulated, and the resulting influence is determined based on the overall reference aft layout of the handysize bulk carrier when powered by diesel. This layout is based on the calculation example given by IMO (MEPC, 2018) (see Figure 10). The main engine is located in the engine room, the auxiliary engine is located above the engine room, and the fuel tank is located under the deck near the engine room. This layout will be modified based on different design scenarios. Based on this the four design scenarios are:

Figure 10. Reference layout of a diesel powered bulk carrier
Adapted from MEPC (2018)



Scenario 1-Decrease the Cargo Space

In this design scenario, part of the cargo space is replaced by the LNG tank, indicated by the green area in Figure 11(a). The main dimensions of the vessel are not changed.

Scenario 2-Increase the Ship Length

In this design scenario, the overall ship length is increased, leading to an increase in the fuel tank and the cargo tank, which are indicated by the blue and orange areas in Figure 11(b).

Scenario 3-Reduce the Travel Distance

In this design scenario, the main dimensions and the layout of the vessel do not change (Figure 11(c)). There are two operational plans to reduce the travel distance: (1) reducing the total voyage distance and (2) adding bunker stops along the original route. The former means the ship owner should find a new contract with a shorter distance. So the feasibility of this plan highly depends on the market and sailing area. The latter means the ship stops and refuels in the middle of the trip, and then continues the original route. This plan will cause additional berth and bunker time, thus increasing fuel consumption, travel time, and cost.

Scenario 4-Move the LNG Tank to the Deck

In this design scenario, the LNG tank is moved to the deck, and the original fuel tank is modified to a cargo tank (Figure 11(d)). This design is based on the IMO calculation example (MEPC, 2018) and the world's first LNG-fuelled 50,000 DWT bulk carrier approved by Lloyd's Register (Lloyd's Register, 2018). The main dimensions of the vessel are not changed.

The overall performance of the design scenarios is simulated by the digital models, and the results are listed in Table 6. The green and red values are the optimal and worst objective values in the 4 LNG scenarios and 1 diesel scenario. Each design scenario has its benefit: Scenario 1 (decreasing the cargo space) can keep the existing displacement and contracts; Scenario 2 (increasing the ship length) makes the largest cargo space and lowest EEDI, which allows a lower operational speed; Scenario 3 (reducing the travel distance) enables the highest profit when reducing the entire contract voyage and almost does not change the vessel's layout; and Scenario 4 (moving the LNG tank to the deck) increases the cargo space while keeping the main dimensions and operational profile. From the model result comparison in Figure 12, it can be seen from the red and green dots that design scenario 2 (increasing the ship length) is the overall optimal choice as it has the second highest profit, the highest estimated cargo load, and the lowest EEDI value.

Increasing the ship length reduces the EEDI value most significantly. The design speed is mostly limited by the EEDI targets: within the acceptable EEDI range, the lower the design speed is set, the higher the overall profit will be. The chosen design speed at 14 knots is based on the vessel behavior simulation results from Step 6, at which the 183-meter-long vessel can satisfy the IMO 2025 EEDI target. The estimated cargo space is the largest when increasing the ship length, and the second largest when moving the LNG tank to the deck.

Figure 11. Design scenario layouts
Adapted from the reference design in MEPC (2018)

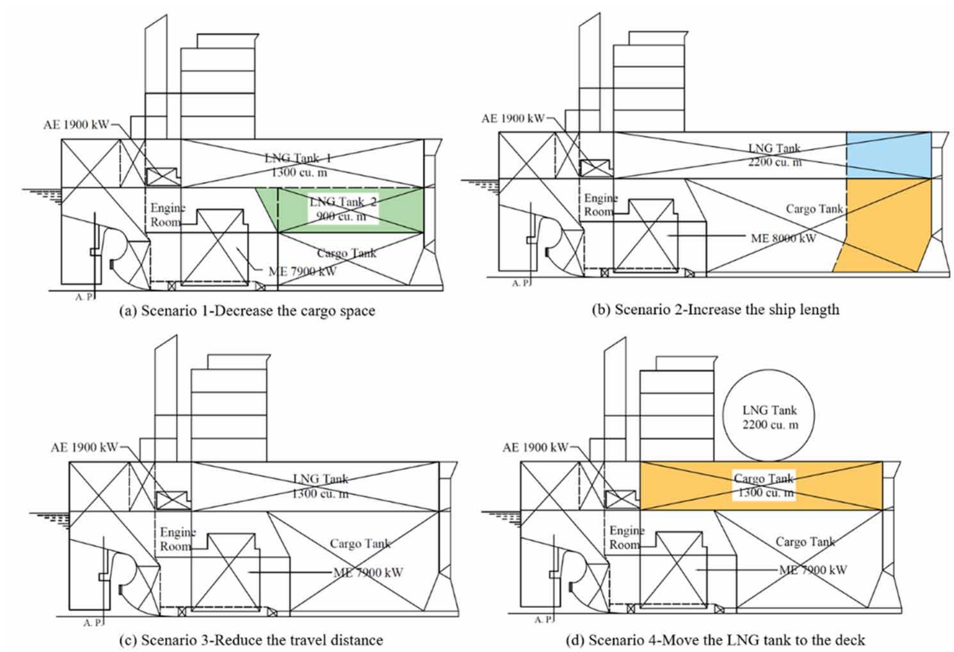
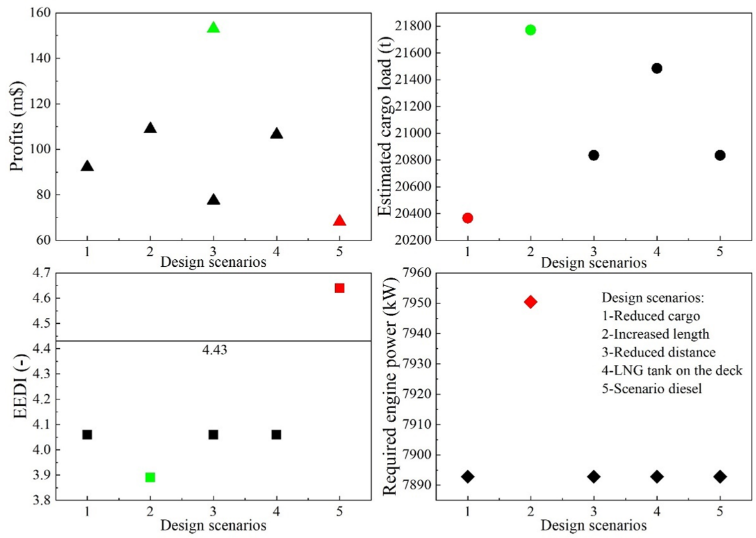


Table 6. Output of digital models from the 4 design scenarios and the diesel scenario

Components	Reduce Cargo	Increase Length	Reduce Distance	LNG tank on deck	Diesel	Original design
LOA (m)	183	190	183	183	183	183
B (m)	29.2	29.2	29.2	29.2	29.2	29.2
T (m)	10.5	10.5	10.5	10.5	10.5	10.5
Design speed (knots)	14	14	14	14	14	12
Total resistance (kN)	461.7	464.8	461.7	461.7	461.7	348.1
Travel distance (nm)	1575.2	1575.2	595	1575.2	1575.2	1575.2
Required engine power (kW)	7892.8	7950.4	7892.8	7892.8	7892.8	5100.6
Bunker size LNG (m^3)	2193.5	2212.1	1292.4	2193.5	-	1747.9
Bunker size diesel (m^3)	1292.6	1303.5	761.6	1292.6	1292.6	1030.0
Bunker size difference (m^3)	929.5	929.5	559.4	900.9	-	717.9
Estimated cargo load (t)	20366	21772	20835	21486	20835	20473
Profits (m$)	92.2	108.9	153.0/77.5	106.6	68.2	112.2
EEDI	4.06	3.89	4.06	4.06	4.64	5.08

Figure 12. Results comparison of the design scenarios



The four LNG-design scenarios all satisfy the IMO 2025 EEDI target, while the diesel scenario does not. It is still up to the ship owner and experts to decide which design scenario is the best considering their financial goals, emission goals, and facilitation.

Step 10-Scale and Evaluate the DT Models. Once the vessel's behavior from the digital model simulations and real-world data converge and satisfy the financial and emission goals, the DT models can be transferred and combined with visualization methods. Along with the design decisions and design process recorded in the DT framework, this information can be used in the detailed design, manufacture, and operation of the vessel. Some of the digital models and settings, like the profit estimation and cargo-related settings, may have deviations from practical trips, these values and magnitudes can be altered and scaled according to the needs of the user. Finally, the accuracy and efficiency of the DT-based design framework can be evaluated and improved when applied to more and more design tasks.

Application in Retrofit

The case study is focused on the design of a new LNG-powered handysize bulk carrier. However, the proposed design method and the design scenario assumptions in Step 7 can also be applied to the retrofit of diesel vessels, as described below:

Step 1-Identify design requirements. The capacity, design speed, and overall performance requirements of the vessel can be the same as the original vessel. The main changes will happen in the EEDI target and financial target.

Step 2-Decide green systems. In this step, the alternative power source and the power system will be decided based on the emission target and the vessel's original layout and structure. Designers should consider mainly the bunker size difference and engine room layout difference. Design scenarios 1, 2, and 4 can be taken as possible design plans for designers: decreasing the cargo space, increasing the ship length, and moving the alternative fuel tank to the deck. It should be mentioned that not all the alternative fuel tanks can be placed on the deck like LNG in the case study, so a careful check of related regulations is essential in this step.

Step 3-Decide main dimensions and modules. Most of the main dimensions and modules of the target vessel will remain, except for the green system. The reference design data used in this step in the new design process will be replaced by the target vessel's own properties.

Step 4-Build digital models for modules. Digital models built for the new builds can still be applied to the retrofitting. However, the financial model should be modified as the building cost is now the cost of retrofitting instead of the new-building cost. Also, the fitting equations to calculate the vessel's main dimensions, as well as the cargo space, can be replaced by the target vessel's own values.

Step 5-Output data analysis. This step has no difference from the new design cases.

Step 6-Simulate and evaluate behavior. This step has no difference from the new design cases.

Step 7-Comparison with real-world modules. Because of the retrofitting task, the fuel data, engine data, and operational data of the vessel itself, as well as its peer vessels, can be provided. Along with the alternative fuel database, the real-world comparison is more credible for retrofitting tasks.

Step 8-Update digital models. This step has no difference from the new design cases.

Step 9-Adjust design. The optimal combination of the main variables can be identified in the behavior simulation step, and one of the design scenarios is already chosen as the retrofit plan in Step 2. In this step, designers can evaluate the vessel performance of other design scenarios, and the difficulty of modification in terms of cost, time, and technical issues. The retrofit design plan can be adjusted after these evaluations.

Step 10-Scale and evaluate the DT models. This step has no difference from the new design cases.

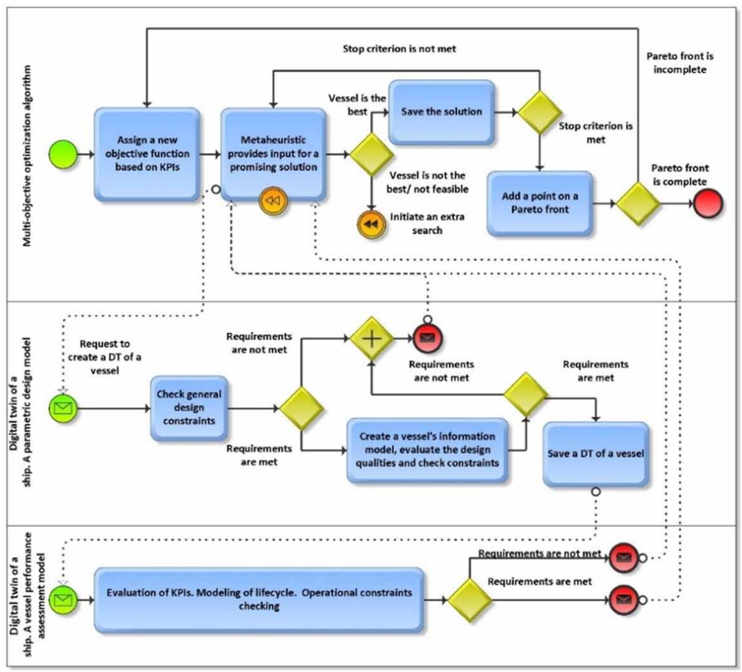
DTS IN EARLY SHIP DESIGN OPTIMIZATION[2]

Early conceptual ship design optimization is a complex problem with strict requirements for a mathematical optimization algorithm. The digital twin combines many nonlinear, discontinuous, and non-differentiable submodels with constraints, so the optimization algorithm must work with any objective function. Moreover, the algorithm must provide global optimization due to many local optima and do it fast due to many potential candidate solutions. This can generally be formulated as a multi-objective mixed-integer nonlinear programming (MINLP) problem with constraints.

Metaheuristic optimization algorithms are well suited for complex real-world scenarios and meet all the above requirements (Torres-Jumenez and Pavon, 2014). The strength of metaheuristics lies in their flexibility, robustness, and ability to handle diverse problems. They are widely used in various fields, such as engineering, operations research, finance, computer science, and artificial intelligence. Unlike deterministic global optimization methods, which are usually unsuitable for real-world scenarios, metaheuristic optimization algorithms do not necessarily guarantee finding the absolute optimal solution but provide near-optimal solutions within a reasonable time. Metaheuristic optimization algorithms are typically stochastic, inspired by natural or physical processes, and use heuristics to guide the search process.

They maintain a population of candidate solutions and iteratively improve them through various exploration and exploitation strategies. Examples of popular metaheuristic algorithms include Genetic Algorithms (GA), Particle Swarm Optimization (PSO), Artificial Bee Colony algorithm (ABC), Ant Colony Optimization (ACO), and Tabu Search (TS). Some mathematicians see promising combining the

Figure 13. The principal flowchart of the early conceptual ship design optimization
Adapted from Kondratenko and Kujala (2021) in BPMN 2.0 process flow notation



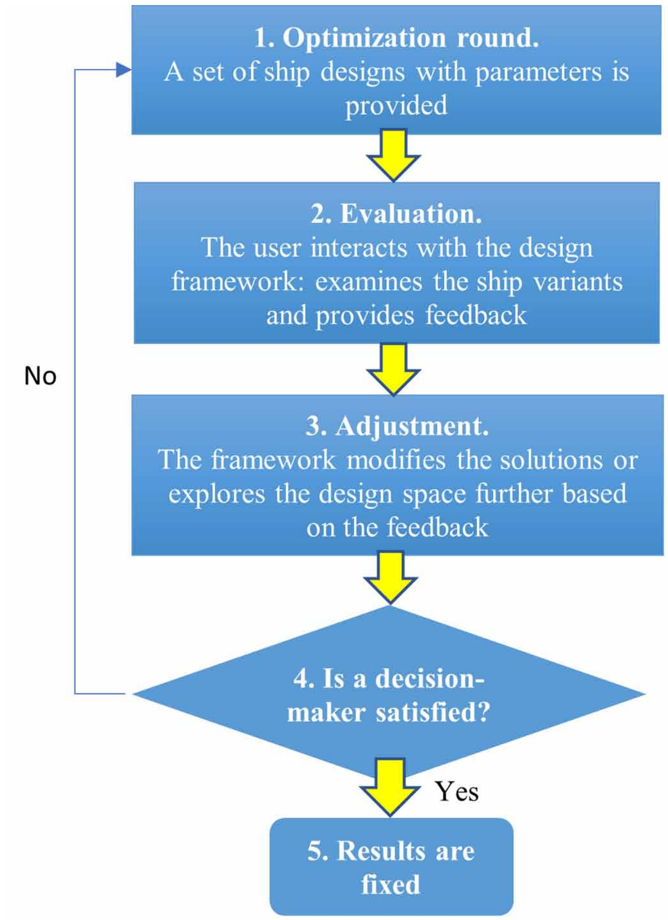
methods from different groups, e.g., making the initial screening using a metaheuristic and then using a deterministic global optimization method to find the end solution (Talbi, 2015).

Multi-objective optimization is usually required as ships are often optimized for several KPIs. Any multi-objective optimization approach is an adaptation of a single-objective optimization algorithm. Usually, the result of multi-objective optimization is a set of Pareto-optimal solutions: for each of them, the improvement of one objective results in the deterioration of another objective.

Figure 13 presents the principal flowchart of the early conceptual ship design optimization and shows the roles and interaction principles of the digital twin and the optimization algorithm. Adaptation of a single-objective optimization algorithm for a multi-objective problem usually uses some adaptive weighted sum methods, which reassign the objective function based on the KPIs for every optimization cycle.

Significant prospects can be attributed to interactive multi-objective optimization in the early conceptual ship design, which is currently underrepresented in research and mainly limited to ship layout optimization (le Poole, et al, 2022; Wang, et al, 2023; Igrec et al, 2019). Unlike traditional optimization techniques, interactive optimization involves direct user interaction in the optimization process by contributing additional insights step-wise, which is especially beneficial for complex real-world problems (Kania et al, 2023; Shavazipou et al, 2022). Although Pareto optimization is flexible and provides informative results with many alternative ship design options to the user (i.e., the tradeoffs between KPIs satisfying the constraints), an expert judgment may be used for considering factors that are difficult to include in the formal optimization problem. Figure 14 presents a general flowchart for interactive multi-objective optimization in the early conceptual ship design. The user may guide the optimization to faster convergence and more realistic or personalized solutions using human intelligence, experience,

Figure 14. Interactive multi-objective optimization in the early conceptual ship design



and heuristic thinking, e.g., by prioritizing some regions of the design space, modifying some parameters of the optimal solution, or even activating or deactivating constraints and KPIs.

CONCLUSION

This chapter first showed the research gap related to the immature status of the state-of-the-art in DT-enabled design processes, both in the maritime world, and greater engineering community. In short, there is no industry or academic consensus yet of how to implement DTs into the design process, let alone from the early design phases. To address this, this chapter proposes two complimentary design approaches independently developed by TU Delft and Aalto University.

The first approach by TU Delft consists of 10 steps and can iteratively simulate and optimize vessel performance. A case study on a handysize bulk carrier was presented and showed the feasibility of the proposed design method. Four design scenarios based on the four possible solutions to handle the increase in volume caused by alternative fuel are presented, and compared.

Results showed that the proposed design method provides acceptable output results, simulates behavior of different design scenarios, and supports early design decision-making. In the case study, increasing the ship length is the optimal layout plan with the best EEDI value, highest cargo capacity, and second-highest overall profits. The approach by Aalto university showed the applicability of optimization during the earliest design phases and how it can help with enabling DTs in green transport vessel design.

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ENDNOTES

[1] This ship design process is proposed by TU Delft, and complements the optimization based approach proposed by Aalto University in Section 4.

[2] This section presents an optimization based approach to DT-enabled ship design proposed by Aalto University and is designed to complement the design process presented in Section 2.

Chapter 9
A Ship Digital Twin for Safe and Sustainable Ship Operations

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ABSTRACT

Shipping is responsible for over 90% of global trade. Although it is generally considered a safe and clean mode of transportation, it still has a significant impact on the environment. Thus, state-of-the-art models that may contribute to the sustainable management of the life cycle of shipping operations without compromising safety standards are urgently needed. This chapter discusses the potential of artificial intelligence (AI) based digital twin models to monitor ship safety and efficiency. A paradigm shift is introduced in the form of a model that can predict ship motions and fuel consumption under real operational conditions using deep learning models. A bi-directional long short-term memory (LSTM) network with attention mechanisms is used to predict ship fuel consumption and a transformer neural network is employed to capture ship motions in realistic hydrometeorological conditions. By comparing the predicted results with available full scale measurement data, it is suggested that following further testing and validation, these models could perform satisfactorily in real conditions. Accordingly, they could be integrated into a framework for safe and sustainable ship operations.

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INTRODUCTION

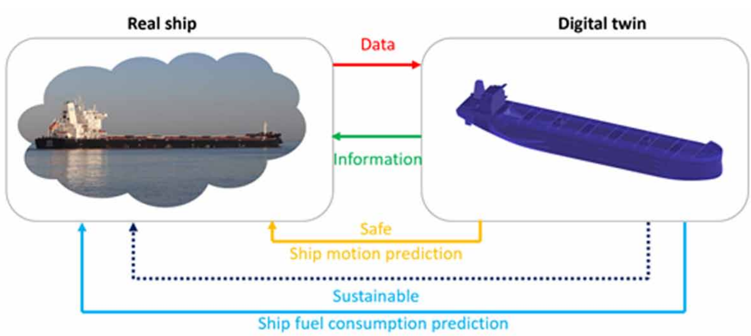
Shipping plays a crucial role in global trade, accounting for over 90% of the transportation of goods worldwide (UNCTAD, 2022). While it is generally considered a safe and environmentally friendly mode of transport, it still has a significant impact on the environment (UNFCCC, 2022). As a result, there is a growing need to ensure the safety and sustainability of ship operations by embracing modern technology.

Originally developed by NASA, digital twins involve creating a virtual replica of a physical object or system to simulate and analyse its performance in real-time (Allen, 2021; Zhang, Hirdaris, & Tsoulakos, 2023). They can be described as machines or computer-based models that simulate, emulate, mirror, or "twin" the existence of a physical entity. For example, a ship digital twin refers to a virtual replica or representation of a real ship. This digital replica can be created by combining real-time data, simulation models, and advanced analytics, allowing for visualization, analysis, and optimization that aims to assure safe and sustainable operations in real operations (see Figure 1).

It is important to acknowledge that the accuracy of physics-based models may be limited to "as build" design or when it comes to dealing with complex operational conditions and extreme events (Kaur et al., 2020). Through deep learning algorithms offer the potential to improve the predictive capabilities of digital twin models (Huang et al., 2021; Lee et al., 2022; Nielsen et al., 2022). To address the challenges associated with predictive analytics and visualisation hybrid methods should be employed. For example, digital twin optimal deep learning models are designed to accurately predict ship motions (Nielsen et al., 2022; Zhang, Taimuri, Zhang et al, 2023) and fuel consumption (Chen, Lam, & Xiao, 2023; Uyanık et al., 2020; Zhang, Tsoulakos, Kujala et al, 2023). They may be combined by utilizing advanced AI methods training physics-based idealisations using comprehensive big data sets. Such predictions may enable ship operators to make informed decisions and minimize the ecological footprint of fuel-efficient shipping operations.

This chapter introduces an AI-based digital twin designed for enhancing the safety and sustainability of ship operations. In Section 2, an overview of digital twin models applicable to maritime operations is presented. The AI-based digital twin comprises of two layers, with the primary objectives to estimate ship fuel consumption and predict ship motions (Section 2 for further details). To evaluate and demonstrate the practical application of this approach, full scale measurement data is utilized, focusing specifically on a bulk carrier and a RoRo/Passenger ship (RoPax) (see Sections 4 and 5). Section 6, highlights the promising prospects of AI-based digital twins in the realm of developing intelligent decision support systems and for effectively monitoring ship safety and efficiency.

Figure 1. The ship digital twin for proactive optimization of ship operations



AN OVERVIEW OF DIGITAL TWIN MODELS FOR USE IN MARITIME OPERATIONS

Ship operations relate to seakeeping and ship performance in adverse conditions (Hirdaris & Mikkola, 2021). Models that may be used for the estimation of ship fuel consumption or seakeeping can be broadly classified into two categories namely (a) physics-based models and (b) Artificial Intelligence (AI) models.

In the area of ship efficiency, physics-based models can approximately estimate ship fuel consumption based on key assumptions that utilize the relationship between ship resistance and engine power (Kim et al., 2023; Tillig & Ringsberg, 2019). The estimation of fuel consumption is achieved via ship - propeller - engine performance models (Vitali et al., 2020). To accurately assess the total resistance experienced by a ship, both calm water and added resistance are considered (Kim et al., 2023; Lang, 2023). The physics-based models entail accounting for various components, including frictional resistance, the resistance of appendages, wave resistance of the bare hull and bulbous bow, as well as additional resistance arising from the immersed transom and model-ship correlation (Molland et al., 2017). In most cases, physics-based models have been employed to estimate ship resistance in still water. Empirical methods proposed by the International Towing Tank Conference (ITTC) have been widely utilized (ITTC, 2002). The Holtrop-Mennen model-based methods have also been used at the preliminary design stage (Holtrop & Mennen, 1982). In recent years, Computational Fluid Dynamics (CFD) has been utilized in detailed design (Campbell et al., 2022). Empirical methods can be utilized to estimate the added wave resistance (Hasselmann et al., 1973; Luo et al., 2016). To account for the effects of wave-induced added resistance and ship motions, semi-empirical models have been proposed. These models are based on experimental data and incorporate empirical equations to estimate added resistance in waves (Liu & Papanikolaou, 2020; Liu et al., 2016) and added resistance attributed to ship motions (ITTC, 2014; ITTC, 2017). Ship propulsion systems are often analysed using ship-propeller-engine performance models or simplified models based on the law of resistance transfer (Wang, 2020). However, their accuracy may be limited when dealing with complex operational conditions (Fan et al., 2022; Yan et al., 2021).

Artificial Intelligence (AI) methods offer a potential solution to overcome the challenges associated with physics-based models by leveraging big data to elucidate the intricate relationship between measured ship fuel consumption and a multitude of influential parameters (e.g., ship mechanical data and dynamics, main engine characteristics, weather conditions, and other relevant factors) (Chen, Lam, & Xiao, 2023). Review papers that discussed the potential application of AI methods in predicting ship fuel consumption (Fan et al., 2022; Yan et al., 2021), identify three main clusters of commonly utilized methods namely: (i) supervised machine learning (Coraddu et al., 2017), (ii) unsupervised machine learning (Hu et al., 2019), and (iii) deep learning (Kim et al., 2021). These methods may utilize diverse data sources and their combinations, such as voyage reports, Automatic Identification System (AIS), meteorological, and sensor data (Du et al., 2022). Diverse data sources enable accurate predictions. These algorithms can be used to predict ship fuel consumption based on well-defined scenarios for a specific ship. However, they often struggle to accurately predict real-time ship fuel consumption for an entire ship voyage under complex operational conditions. This is because traditional machine learning/deep learning methods may not effectively deal with complex influencing factors and make informed predictions of ship fuel consumption.

A digital twin may be utilized to closely monitor seakeeping and maneuvering, especially during challenging operational conditions (Lee et al., 2022; Major et al., 2021; Schirmann et al., 2018). For example, research in big data science has the potential to predict hydrodynamic derivatives by utilizing results from model tests or full scale measurements data. To date parametric estimation methods have been employed to quantify ship motions, relying on available ship mathematical models to train large data streams. For example, Wang et al. (2019) utilized the nu-support vector machine to identify hydrodynamic derivatives of the 3-DoF Abkowtiz model. Zeng et al. (2021) employed the Extended Kalman Filter (EKF) method to determine the hydrodynamic derivatives of an MMG model (Zeng et al., 2021). Non-parametric estimation models, such as Artificial Neural Networks (ANN) (Silva & Maki, 2022), Long Short-Term Memory (LSTM) 43, Gaussian process regression (Ouyang & Zou, 2021), and locally weighted learning methods (Woo et al., 2019), utilize simulated free-running tests to predict ship motion dynamics. Notably, Lou et al. (2022) developed neural network models to predict the motions of unmanned surface vehicles based on results from open seas manoeuvrability tests in 3-DoF.

The critical review of methods for the ship digital twins in ship operations indicates that existing digital twin models have their limitations. A common challenge is the accuracy of the digital twin representation. While digital twins aim to replicate physical objects or systems, there may still be discrepancies due to limitations in data collection, model accuracy, or real-time updates. For example, accuracy in terms of visualisation can be compromised because of the limited ability of parametric or non-parametric statistical regression models to consider medium to long-term environmental conditions. A high-fidelity digital twin requires careful calibration, validation, and continuous improvement to ensure reliability and accuracy.

MULTI-OBJECTIVE AI-BASED DIGITAL TWIN MODELS FOR SAFE AND SUSTAINABLE SHIP OPERATIONS

The digital twin presented in this chapter encompasses two essential deep learning layers, each serving a distinct purpose in enhancing ship operations. Figure 2 represents the architecture of the digital twin models, illustrating the integration of bi-directional Long Short-Term Memory (Bi-LSTM) with an attention mechanism layer for the prediction of ship efficiency and a transformer layer for the identification of ship motions.

Layer 1 focuses on idealizing the ship energy systems and predicting fuel consumption [12]. This layer can accurately estimate the ship fuel consumption in various operating scenarios. It considers ship operational characteristics (ship speed, draft, trim, etc.), and the influence of environmental conditions (wind, wave, and current, etc.). Predictive analytics may be crucial for ship operators who seek to optimize fuel usage, reduce costs, and decarbonise fleet operations.

Layer 2 can be used to understand and optimise seakeeping behaviour in real conditions [9]. Ship motions may influence ship stability, safety, and cargo integrity. Hence, the transformer integrated into this layer is trained using collected datasets that capture the complex relationships between various ship systems and operational factors (e.g., rudder angle, propeller rpm, speed, heading, weather condition) that may impact ship motions in 6 Degrees of Freedom (DoF) and in real-time. In this case, predictive analytics can enable ship operators to proactively respond to potentially hazardous conditions (e.g., ship–ship collision and ship grounding), adjust navigation strategies, and ensure ship safety.

Layer One: A Digital Twin Model for Fuel Efficiency Estimation

This section introduces the deep learning model based on Bi-LSTM with attention mechanisms [12], depicted in Figure 3. The model combines the strengths of Bi-LSTM, which can capture both past and

Figure 2. The overall procedure of AI-based ship digital twin

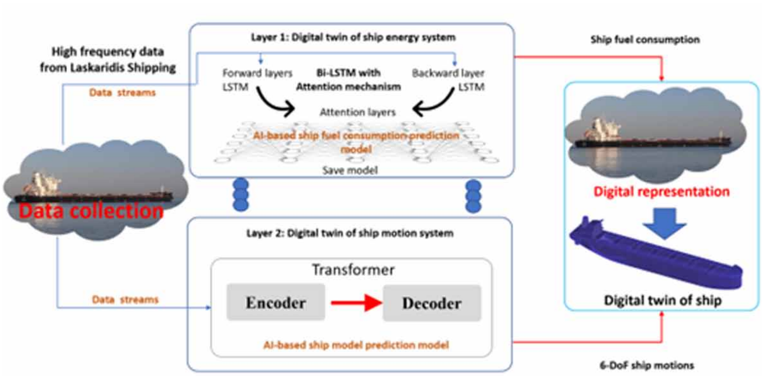


Figure 3. The schematic of AI based digital twin of ship energy system

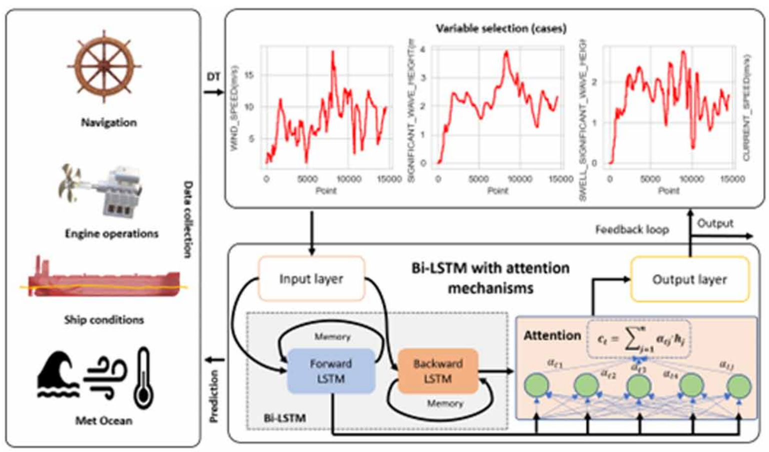


Table 1. Algorithm one: Bi-LSTM with attention mechanism for ship fuel consumption prediction

1 Input: Data collection SFC(n), see more in Section 2.1
2 Output: AI-based ship fuel consumption surrogate model
3 Select key variables X(n) and ship fuel consumption SFC (n) in the time domain
4 Split the training data set $data_{train}$ and $data_{test}$ from X(n) using k folds cross-validation method.
5 For batch $data_{batch\ size}$ in $data_{train}$
6 For L-length data $data_{l}$ in $data_{batch\ size}$
7 For $\boldsymbol{i}$ = 1 to L
8 Using forward LSTM to an encoder $\overrightarrow{h_t}$
9 Using backward LSTM to an encoder $\overleftarrow{h_t}$
10 End For
11 Compute Attention score αi and ct
12 Compute ship fuel consumption SFCt from ct
13 End For
14 Training the model to identify ship energy system in real operational conditions
15 End For
16 Save the prediction model: AI-based ship fuel consumption prediction model

future dependencies, with attention mechanisms that enable the model to focus on relevant parts of the input data streams. Table 1 provides a summary of the algorithm, outlining the step-by-step procedure followed, including data pre-processing, model architecture setup, training process, and prediction generation. The architecture of the system, as illustrated in Figure 4, comprises four main components namely: (i) input layers, (ii) Bi-LSTM layers, (iii) attention layers, and (iv) the output layer.

The layers of the deep learning model are summarized as follows:

The **input layers** accept key variables obtained from navigation data, engine operation data, ship condition data, and hydrometeorological conditions from full scale measurements. Then these selected variables are pre-processed and fed into the subsequent layers.

Each **bi-LSTM layer** consists of two LSTM sublayers. Each LSTM unit comprises 4 interconnected elements, including the input and control signals for the input, forgotten, and output gates [45]. These components work together to regulate memory storage, retention, and output. Figure 4 depicts the internal structure of the LSTM unit (see red box). The input x_t at a time increment t and the output h_{t-1} of the hidden layer neuron at a time increment t-1 represent the joint inputs to the hidden layer. These inputs are then multiplied by distinct weight vectors, and upon application of the activation function, the control signals f_t, i_t, o_t, of the forgotten gate, input gate, and output gate are generated. This process is represented by Eqs. (1-3), where the weight vector is denoted by w and the activation amount by b. The biases for different connection weights are represented by b_f, b_i, and b_o, and σ(•)is the sigmoid activation function.

$$f_t = \sigma(\mathrm{w}f_{[}\mathrm{h}t_{-1,}\ \mathrm{x}t_{]} + \mathrm{b}f_{)} \tag{1}$$

$$i_t = \sigma(\mathrm{w}i_{[}\mathrm{h}t_{-1,}\ \mathrm{x}t_{]} + \mathrm{b}i_{)} \tag{2}$$

$$o_t = \sigma(\mathrm{w}o_{[}\mathrm{h}t_{-1,}\ \mathrm{x}t_{]} + \mathrm{b}o_{)}\ o_t = \sigma(w_o[h_{t-1}, x_t] + b_o) \tag{3}$$

The state of a cell $\tilde{C}_t$ is presented as per Equation (4). The value of the memory unit C_t is updated as per Equation (5). Accordingly, the output of hidden layer neurons h_t can be presented as per Equation (6)

$$\tilde{C}_t = \tanh(w_C[h_{t-1}, x_t] + b_C) \tag{4}$$

$$C_t = f_t C_{t-1} + i_t \tilde{C}_t) \tag{5}$$

$$h_t = o_t \tanh(C_t) \tag{6}$$

where tanh(•)represents a hyperbolic tangent activation function.

Ships are systems of systems that navigate through complex operational conditions (Zhang et al., 2021). To effectively capture the complexity of ship systems using real operational data for ship fuel

Figure 4. The architecture of Bi-LSTM with attention mechanisms

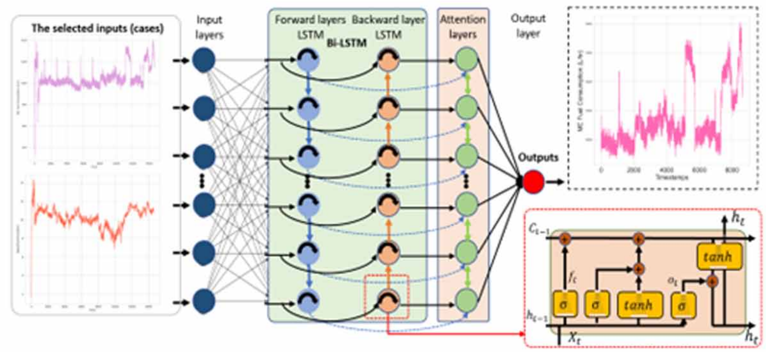
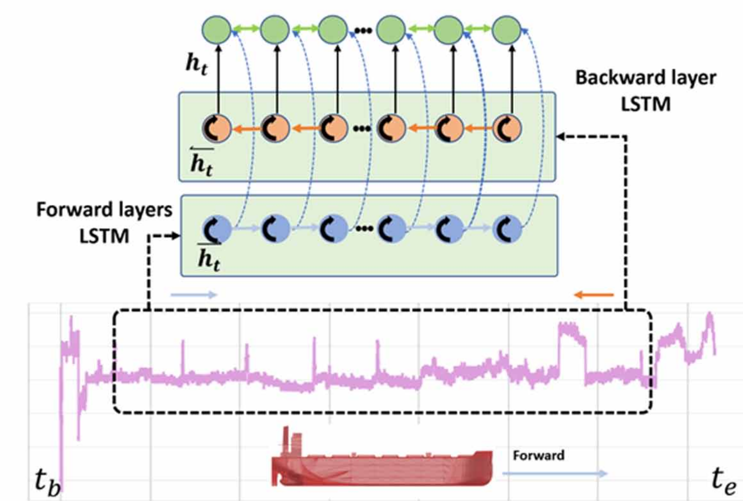


Figure 5. Capturing and utilizing information from both forward and backward directions



consumption prediction, it is essential for the model to learn from both past and future information in the data streams. While a standard LSTM model only considers information from past time frames in the data stream, the bi-LSTM layer overcomes this limitation by addressing the problem of disregarding relevant past information (Ma et al., 2022). This is because it comprises both forward and backward LSTM sublayers, see Figure 4. Forward sublayers process the input stream in a forward direction i.e., from the beginning t_b to the end t_e. In a backward direction the sublayers operate from the end t_e to the beginning t_b, see more in Figure 5.

A bidirectional LSTM processes input data stream in both forward and backward directions. By concatenating the outputs of the forward and backward LSTMs, the model could obtain a representation that incorporates both past and future information, as shown in Figure 5. Given an input data stream $X = [x_1, x_2, \ldots, x_n]$, a bidirectional LSTM generates hidden states in both forward and backward directions as shown in Eqs. (7-8). The hidden states from both directions are concatenated to obtain a comprehensive representation at each time step as Equation (9).

$$\overrightarrow{h}_t = \mathrm{LSTM}\left(x_t, \overrightarrow{h_{t-1}}\right) \tag{7}$$

$$\overleftarrow{h}_t = \mathrm{LSTM}\left(x_t, \overleftarrow{h}_{t-1}\right) \tag{8}$$

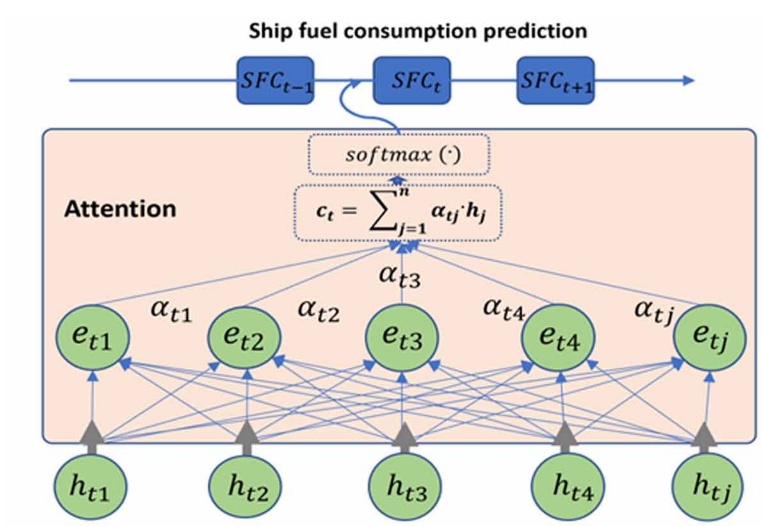
$$h_t = \left[\overrightarrow{h}_t, \overleftarrow{h}_t\right] \tag{9}$$

where t represents the time step, and $\overrightarrow{h}_t$ is the hidden state in the forward direction. $\overleftarrow{h}_t$ is the hidden state in the backward direction, [;]denotes the concatenation.

The **attention mechanism** allows the model to dynamically focus on different parts of the input data streams, thus assigning varying levels of importance to different time steps [9]. This enhances the ability to emphasize critical information from data streams, which is useful to capture extreme scenarios of ship operations in real complex operational conditions. The attention layers calculate attention scores and weights for each time step based on the hidden representations from the Bi-LSTM layers, as shown in Figure 6.

Given a specific time step t, the attention weight αt_j of other hidden layers for the current input for xt is calculated as Equation (10). The alignment score et_j computed using a trainable alignment model is defined as Equation (11). The context vector ct is the weighted sum of the hidden states, which reflects the attended information at time step t as Equation (12). The final output SFCt at time step t is generated by passing the context vector ct through a linear transformation and an activation function as Equation (13).

Figure 6. Attention mechanism for the prediction of ship fuel consumption



$$\alpha_{tj} = \frac{\exp\left(e_{tj}\right)}{\sum_{j=1}^{n} \exp\left(e_{tj}\right)} \tag{10}$$

$$e_{tj} = w_{\mu}{}^{T} * tanh(w_w h_t + b_w) \tag{11}$$

$$c_t = \sum_{j=1}^{n} \alpha_{tj} h_j \tag{12}$$

$$SFC_t = softmax(W_c \cdot c_t + b_c) \tag{13}$$

where, W_c, and b_c are parameters (weight matrices or vectors) that are typically trained and determined during the process of model training.

(iv) The **output layer** receives the context vector, which is the weighted combination of the hidden representations obtained from the attention layers. The context vector captures the most relevant information from the input data stream. The output layer processes the context vectors and predicts the ship fuel consumption for the given time step, see Figure 6.

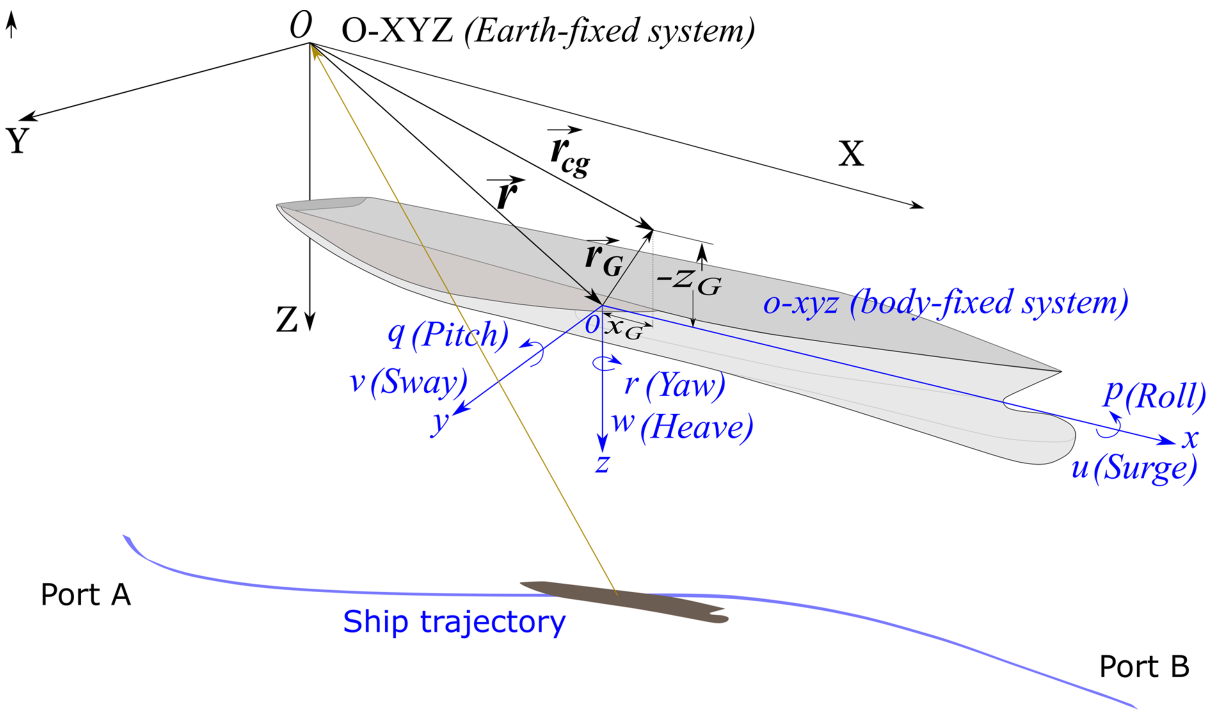
Layer Two: A Digital Twin for the Prediction of Ship Motions

The transformer is an advanced deep learning architecture that utilizes self- and multi-head attention mechanisms [9]. It enables the differential weighting of input features to determine their importance. This section introduces a transformer-based digital twin of the ship motion system. A transformer-based deep learning method is employed to train ship trajectory data streams and make long-term ship motion predictions in the time domain. Figure 7 illustrates a ship trajectory with time series of ship motions influenced by environmental conditions that are used to train the model. Each point on the trajectory includes ship control actions, desired inputs, environmental conditions, and 6-DoF ship motions. The model can identify and forecast 6-DoF ship motions as shown in Figure 8. The transformer architecture, illustrated in Figure 9, consists of encoder and decoder modules, each containing multiple blocks represented by grey areas (Han et al., 2021).

The encoder module incorporates multi-head attention and a feed-forward neural network, enabling the mapping of time series data related to operational conditions, control devices, and desired inputs (see $\boldsymbol{X}$ in Equation (14)) to a new continuous series ($\boldsymbol{Z}$ in Equation (15)), see Figure 8. This mapping is achieved via an "attention mechanism" defined by the *SoftMax* function in Equation (19). The objective is to predict the time series of ship motions ($\boldsymbol{Y}$ in Equation (16)) using an autoregressive method. The attention mechanism employed in the digital twin model facilitates the retention of crucial information during the training and prediction of significant data streams [49].

$$\boldsymbol{X} = \{x_1, x_2, x_3, \ldots, x_n\} \tag{14}$$

Figure 7. 6-DoF ship motion dynamics along ship trajectory



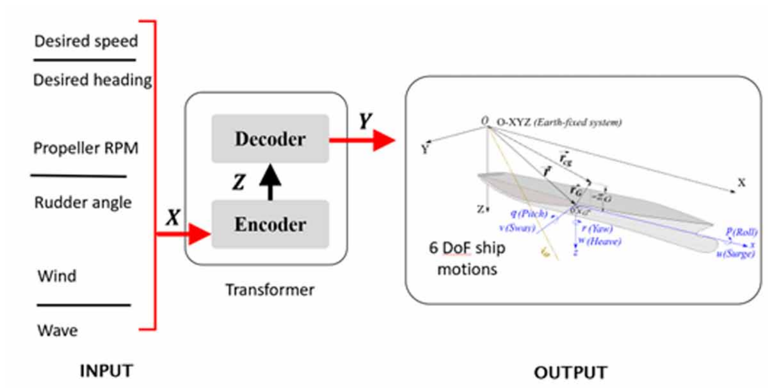
$$\boldsymbol{Z} = \{z_1, z_2, z_3, \ldots, z_n\} \tag{15}$$

$$\boldsymbol{Y} = \{y_1, y_2, y_3, \ldots, y_n\} \tag{16}$$

where, $\boldsymbol{X}$ denotes the matrix of control devices, conditions, and desired inputs in the time domain; $\boldsymbol{Y}$ denotes the matrix of the 6-DoF ship motion in the time domain; $\boldsymbol{Z}$ denotes a matrix after encoding; x_n denotes the inputs of control devices, conditions, and desired inputs at point n; y_n denotes the outputs of 6-DoF at point n.

Figure 9 presents a deep learning network consisting of an encoder and decoder, both composed of multiple layers of attention. The network aims to process and analyse training data streams of ship motions. Initially, the ship motion data is fed into an "Input Embedding layer", which treats the data as a lookup table to generate a learned vector representation of ship motions. A feed-forward neural network layer then learns the number of lookup tables from the training database, allowing the ship motion data streams from different ship trajectories to be organized into vectors. To account for variations over sea depth and across a trajectory, a smart positional encoding scheme is employed to incorporate positional information of data streams into the vectors from the Input Embedding layer [48,49]. This encoding process is defined mathematically by Eqs. (17)-(18) (Vaswani et al., 2017). The input vectors, resulting from the embedding and positional encoding of ship motion data, are combined and used to train the encoder and decoder modules of the model [9].

Figure 8. Transformer architecture for ship motion prediction

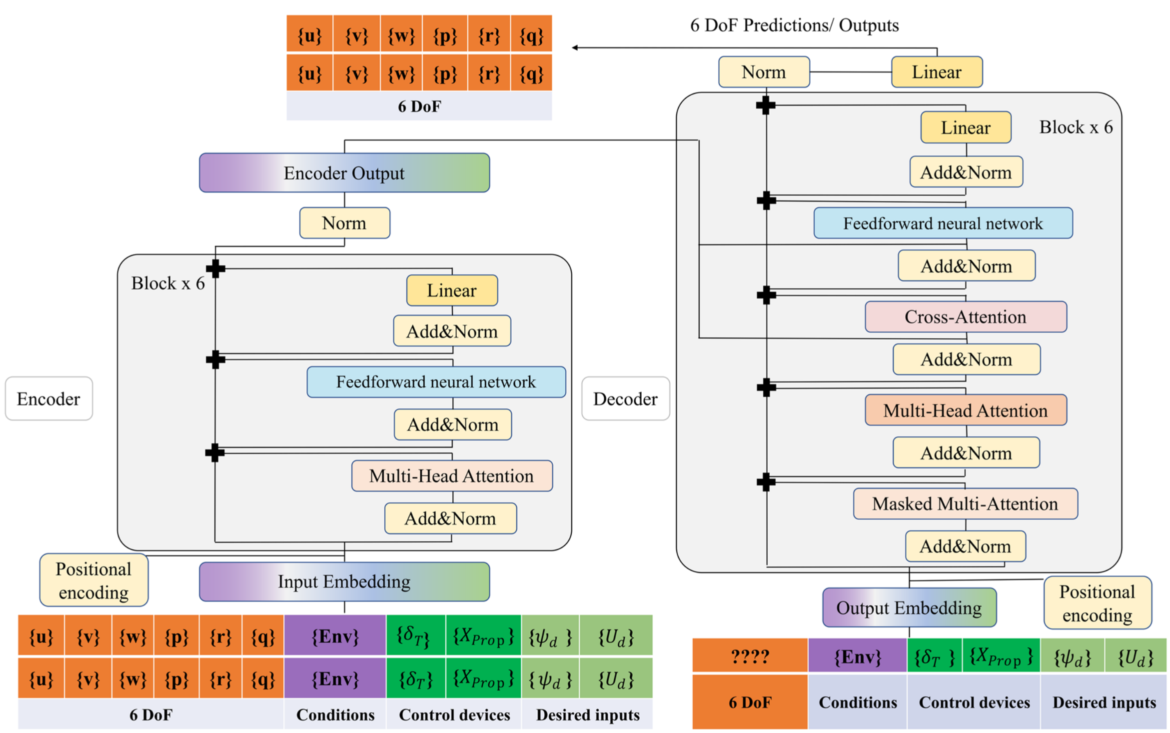


$$PE_{(pos,2i)} = \sin\left(pos / 10000^{2i/d_{\text{model}}}\right) \quad (17)$$

$$PE_{(pos,2i+1)} = \cos\left(pos / 10000^{2i/d_{\text{model}}}\right) \quad (18)$$

where, *pos* denotes the location of the time series of ship motions, and *i* presents the dimensionality of d_{model}.

Figure 9. Transformer architecture for 6-DoF ship motion prediction



Once the vector with positional encoding is passed to the encoder and decoder modules (Figure 9), the encoder module is employed to map the input time series to a set of new continuous series. The decoder module utilizes an auto-regressive technique to generate the output time series for ship motion prediction, see Eqs. (14)-(16). Both the encoder and decoder consist of similar sub-layers. As illustrated in Figure 9, the encoder and decoder modules encompass the following components: (1) Attention mechanism/multi-head attention/marked multi-head attention layer; (2) Add & Norm function layer; (3) Feed-forward networks (FFN) layer; and (4) Linear layer [9].

(1) Attention mechanism / multi-head attention layer

The attention mechanism in the deep learning model provides exceptional long-term memory for ship motion time series, allowing the model to attend to and focus on the ship motion information during the entire voyage. The attention layer and SoftMax functions are defined based on Equation (19) in the transformer architecture, as described in Vaswani et al. (2017).

$$z = Attention(Q,K,V) = SoftMax\left(\frac{QK^T}{\sqrt{d_k}}\right)V \tag{19}$$

where Q, K, and V are query, key and information value vectors,

$$Q \in R^{n\times d_k}, K \in R^{m\times d_k}, V \in R^{m\times d_v}$$

are the matrixes, including query, key, and value of attention; d_k denotes the dimensions in blocks. $Q=X\times QW$, $K=X\times KW$, $V=X\times VW$. QW, KW, and VW are weight matrices; z denotes an element of the matrix Z which is calculated using *SoftMax* functions.

Each attention process in this model functions as a learning mechanism for ship motions. Multiple attention heads can predict output vectors, which are then concatenated into a single output vector. This multi-head attention approach enables the learning of more comprehensive information about ship motions compared to a single attention layer. The multi-head attention layer consists of individual attention layers as denoted in Eqs. (20)-(21). The marked multi-head attention layer represents a hidden layer within the multi-head attention. The use of a mask indicates a matrix that scales the attention scores of the multi-head attention layer, as further detailed in Bhattacharya et al. (2022) [51].

$$\text{MultiHead}(Q,K,V) = \text{Concat}(head_1,\ldots,head_h)W^O \tag{20}$$

$$head_i = Attention\left(QW_i^Q, KW_i^K, VW_i^V\right) \tag{21}$$

where, $W^o \in R^{h\times d_{model}\times d_k}$, h denotes the number of parallel attention layers. QW, KW, and VW are weight matrices, $W_i^Q \in R^{d_{model}\times d_k}, W_i^k \in R^{d_{model}\times d_k}, W_i^v \in R^{d_{model}\times d_k}$.

(2) Add & Norm layers

To incorporate the output vector from the hidden multi-head attention layer with the original positional input embedding of the ship's time domain motion, Add & Norm layers are utilized. The Add layer consists of a residual network or residual connection, which enables the learning of residual functions for the inputs, as shown in Equation (22). The output of the Add layer then passes through a Norm layer, which applies layer normalization to enhance performance and training efficiency, as described in Eqs. (22)-(25). These layers facilitate the integration and normalization of the input and output vectors in the model.

$$F(x) = \mathrm{H}(x) - x \tag{22}$$

$$\mu^{l} = \frac{1}{h}\sum_{i=1}^{h} a_i^{l} \tag{23}$$

$$\sigma^{l} = \sqrt{\frac{1}{h}\sum_{i=1}^{h} (a_i^{l} - \sigma_{\mu}^{l})^2} \tag{24}$$

$$\widehat{a^{l}} = \frac{a^{l} - \sigma_{\mu}^{l}}{\sqrt{\left(\sigma^{l}\right)^2 + \mu}} \tag{25}$$

In the above equations $H(x)$ is the desired mapping, $F(x)$ denotes the stacked nonlinear layers, and the original mapping reconstructed as $F(x)+x$; h denotes the number of nodes of the hidden layer; l denotes the number of layers. The σ^l and μ^l are the parameters of layer normalization; σ_{μ}^{l} is the mean value; $\widehat{a^{l}}$ denotes the results of layer normalization and ε denotes a very small number that can be used to avoid $\sqrt{\left(\sigma^{l}\right)^2 + \mu} = 0$, see Equation (25).

(3) Feed-forward network

The output from the Add & Norm layers is then passed through feed-forward networks for additional processing. The Feed-Forward Network (FFN) is employed to enhance network stability and reduce training time. It consists of multiple linear layers, with a Rectified Linear Units (ReLU) activation function, connecting each sub-layer. Further details can be found in the work by Li et al. (2019).

$$FFN(x) = \max(0, xW_1 + b_1)W_2 + b_2 \tag{26}$$

$$ReLU(x) = (x)^{+} = \max(0, x) = \begin{cases} x & if \quad x > 0 \\ 0 & if \quad x \leq 0 \end{cases} \tag{27}$$

where, the function max () denotes the ReLU function as per Equation (27); W_1, and W_2 represent the value of slope; b_1, and b_2 represent the value of intercept.

(4) Linear layer

The decoder is capped off with a linear layer that acts as a classifier to present the predicted outputs. The linear function is the linear transformation of data streams [50]

$$y = xA^{T} + b \tag{28}$$

where, A^T represents the value of slope; b represents the value of intercept.

The complex architecture of the transformer allows learning different ship motion dynamics in real conditions, potentially boosting the predictive ability of the ship manoeuvring features of the selected ship, see testing and validation in Sections 4.2 and 5.2. To evaluate the performance and quantify the errors between the real and digital twin, Root Mean Square Error (RMSE), Mean Square Error (RMSE), and error rate e_n are used as shown in Eqs. (29-31).

$$RMSE = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2} \tag{29}$$

$$\mathrm{MSE} = \frac{1}{N}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2 \tag{30}$$

$$e_n = (y_n - \hat{y}_n) / (y_n) \tag{31}$$

where, y_n is the actual value, $\hat{y}_n$ denotes the predicted value, $\overline{y_n}$ is the mean value.

AI-Based Digital Twin Models

This section demonstrates the use of multi-objective AI-based digital twin models [9, 12]. Layer 1 of the digital twin model is trained by utilising extensive data streams derived from high-frequency full scale measurements data of a Kamsarmax bulk carrier owned by Laskaridis Shipping Co. Ltd. (see Table 2). Figure 10 illustrates voyages from full scale measurements data collected for this vessel from February 2021 to February 2023. Layer 2 of the digital twin model was trained using operational data obtained from the Ro-Pax ship owned by Viking Line Co. Ltd (see Table 3). Trajectories and hydro-meteorological

Table 2. Ship specification of the KAMSARMAX class bulk carrier

Information		Real
IMO	9843405	
Vessel Type	Bulk Carrier	
DWT	81 600.0 t	Digital Twin
Length x Breadth	229.0 x 32.0 m	
Year Built	2020	

Figure 10. Full scale measurment data of the selected bulk carrier from 02.2021 to 02.2023

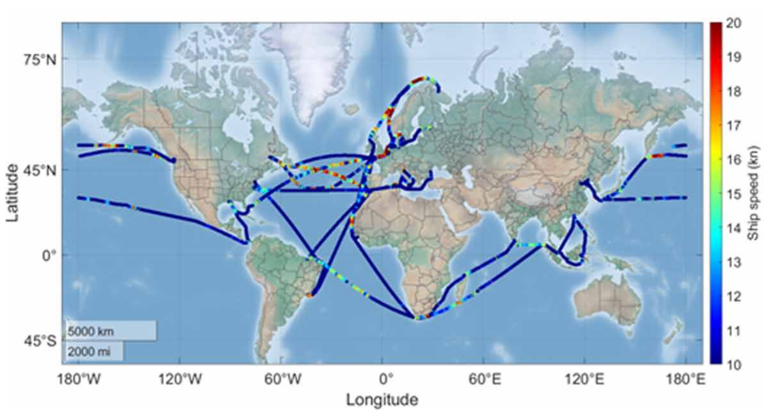


Table 3. The ship specification of the selected Ro-Pax ship

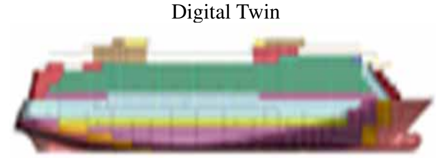
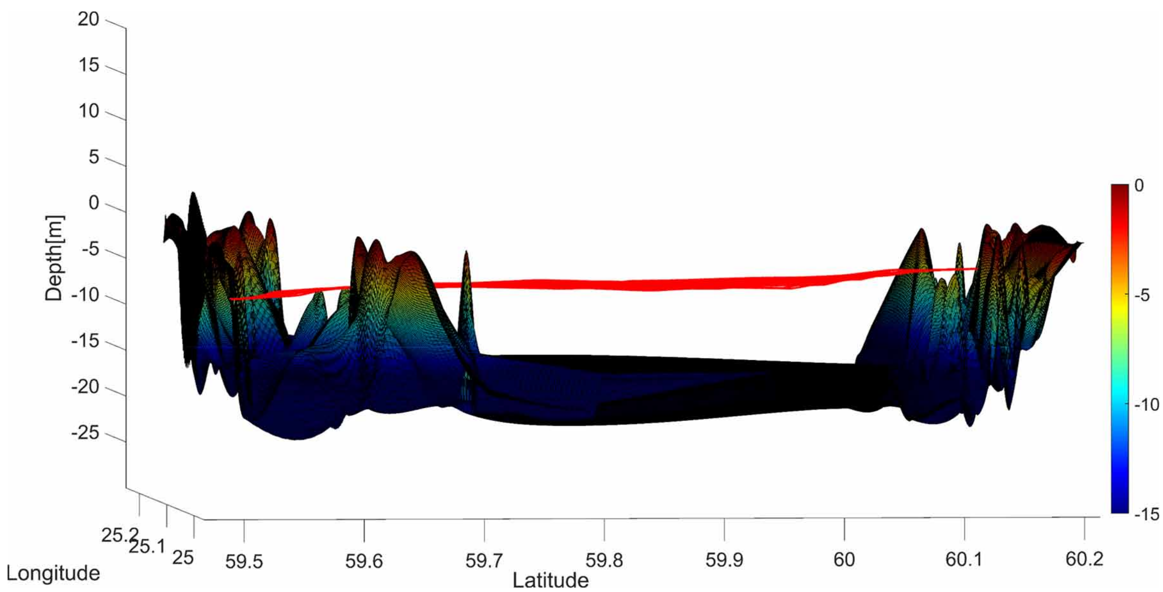
Information		Real
IMO	9773064	
Vessel Type	Ro-Pax ship	
DWT	49 134.0 t	Digital Twin
Length x Breadth	212.0 x 30.6 m	
Year Built	2017	

Figure 11. Ship voyages from Helsinki to Tallinn



conditions were observed between two ports situated in the Gulf of Finland as shown in Figure 11 [9]. This approach was adopted due to the inherent challenge of collecting all the required data from a single ship.

Ship Fuel Consumption Predictive Analytics

A bi-LSTM architecture was employed to train a digital twin of the ship energy systems. Inputs to the model encompassed ship navigation data such as ship speed, course and heading, operational conditions (e.g., ship mean draft and trim, main engine shaft power and temperature), and Metocean data encompassing wave characteristics, wind conditions, current information, and air temperature. These inputs were carefully selected based on their relevance to fuel consumption prediction. The output of the model was the ship fuel consumption represented in the time domain. This information was utilized to drive the predictions generated by the digital twin A visual representation of the model architecture and its components can be found in Figure 12. To train the digital twin of the ship energy system, the digital twin of the ship energy system employed an architecture consisting of an input layer, three bi-LSTM layers, three attention layers, and an output layer. The bi-LSTM layer had 128 hidden units. The model characteristics and the selected hyperparameters are presented in Table 4.

The training loss and validation loss were calculated using the training (80%) and validation (20%) datasets, respectively. The curves shown in Figure 13 illustrate that both of those decrease and stabilize around the 178th epoch. Therefore, if no improvement in the validation performance is observed beyond this point, the training process is terminated early to prevent overfitting. After completing 178 epochs, the deep learning model achieves an optimal fitting state, indicating a balanced convergence between the model's performance and the training data. This optimal fitting state implies that the model does not suffer from overfitting, characterized by excessive complexity and high accuracy on the training data but poor generalization to testing data. It also avoids underfitting, which occurs when the model fails to capture underlying patterns in the data, resulting in subpar performance on both training and testing

Figure 12. The digital twin processing of ship fuel consumption prediction for model training, testing and application (Zhang, Tsoulakos, Kujala et al, 2023)

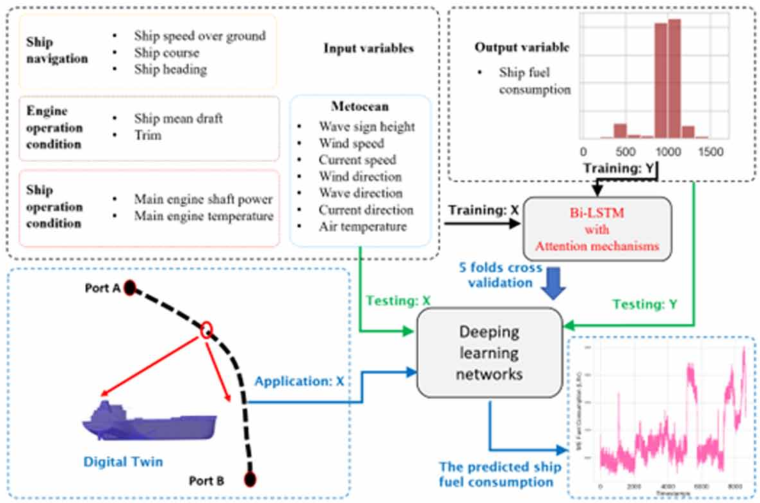
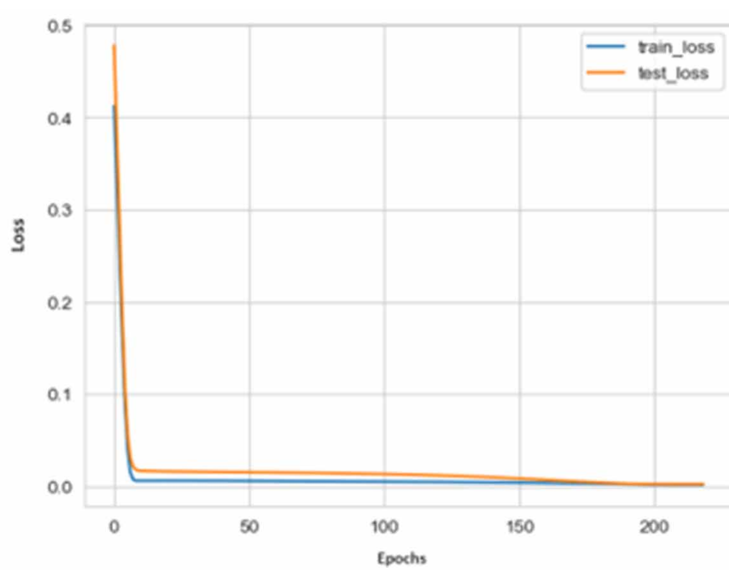


Table 4. The model characteristics and the optimal hyperparameters

Model	Input variables	output variable	layers
Bi-LSTM	14	1	7
Hidden units per layer	Optimizer	Batch Size	Early stopping
128	Adam	48	Patience=10
Dropout rate	Leaning rate	Epochs	Regularization param
0.2	5e-05	178	0.1

Figure 13. The model performance evaluation



data. The digital twin of the ship energy system built using the deep learning model achieves a desirable equilibrium by effectively capturing the intricacies of the training data while also generalizing well to new data streams.

As depicted in Figure 13, the training process demonstrates that the deep learning model can achieve an optimal fit, effectively addressing both overfitting and underfitting. Furthermore, the average validation loss using Mean Squared Error (MSE) is determined to be 2.04e-2. To further evaluate the trained deep learning model, new inputs were selected from the testing database, as illustrated in Figure 12. The model was used to predict ship fuel consumption in the time domain, and the resulting error rates were calculated using Equation (31), as shown in Figure 14. The results of ship fuel consumption prediction are illustrated in the upper figure. The red line represents the real values of ship fuel consumption, while the green line represents the predicted results. The alignment and deviation between the two lines indicate the accuracy of the digital twin. In the bottom figure, the blue line represents the error rate in the time domain. It shows the magnitude and direction of the errors between the predicted and actual fuel consumption values at different points in time. These findings indicate that the trained deep learning model can effectively capture the characteristics of the ship energy system under real operational conditions. Further analysis of the prediction errors is presented in Figure 15. Over 90% of errors are below 4%, with an average error rate of 0.98%. It is important to note that the proposed model has limitations in effectively capturing abnormal fluctuations present in the sensor-collected data. This is also reflected in the significant errors indicated by the peak values in lower Figure 14.

Figure 15. The analysis of prediction errors using the proposed model

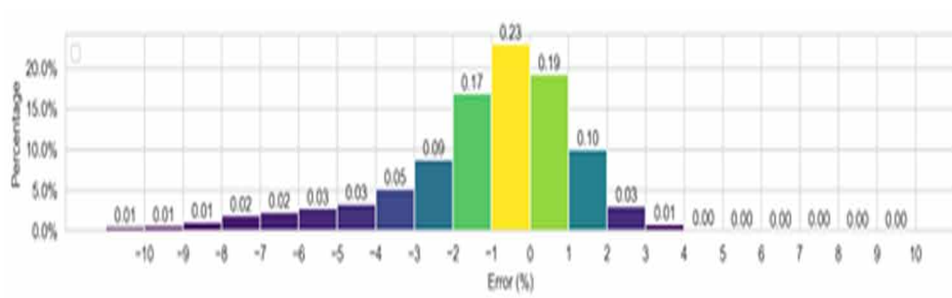
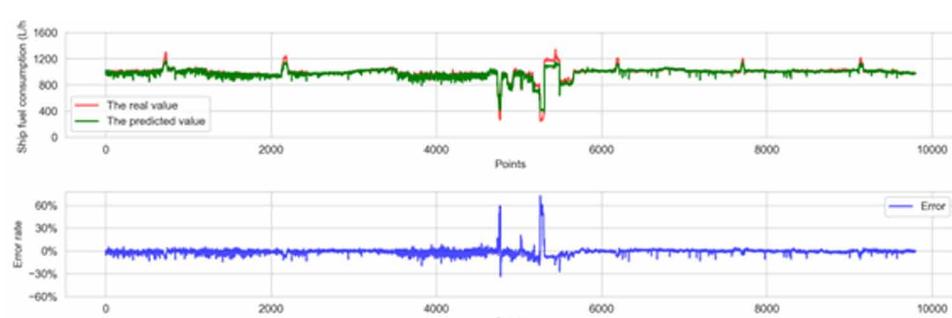


Figure 14. The comparison of real and predicted ship fuel consumption



Ship Motions Predictive Analytics

For the typical Ro-Pax ship shown in Table 3, ship trajectories were collected during the ice-free period between 2018 and 2019. The waterway between Helsinki and Tallinn may freeze during the winter months of December, January, and February. However, this aspect is not considered in the present analysis.

A 6-DoF ship dynamics model (Taimuri et al., 2020) was utilized to generate time-domain input parameters (rudder angle, propeller rpm) and time-domain output results (6-DoF ship motion dynamics) for 500 voyages between Helsinki and Tallinn, see Figure 11. Subsequently, a transformer architecture was developed to train a deep-learning model that maps the inputs to the outputs. Inputs $\{X\}$ encompass rudder angle, propeller rpm, speed, heading, wind information, and wave information. Outputs $\{Y\}$ comprise surge, sway, heave, roll, pitch, and yaw. This information was employed to guide the predictions produced by the digital twin of the ship motion system. A visual representation of the model architecture and its components can be found in Figure 16. To capture the key features of historical ship motion dynamics, a complex architecture of the transformer was designed. Model characteristics and selected hyperparameters are presented in Table 5.

The total dataset comprised a total of 500 voyages divided into three parts: 80% for training (400 ship voyages), 10% for validation (50 voyages), and 10% (50 voyages) for testing. The curves shown in Figure 17 demonstrate that both the training and validation losses decrease and stabilize at the 38th epoch. The results of the training process indicate that the deep learning model achieves an optimal fit, indicating that it neither overfits nor underfits the data. To test the digital twin of the ship motion system, the future inputs of ship control actions, desired inputs, and environmental conditions were considered. The 6-DoF ship motions were then predicted, as depicted in Figure 18. The ground truth represents the

Figure 16. The digital twin processing of 6-DoF ship motion prediction for the long-term voyage in real conditions and turning circle in calm conditions (Zhang, Taimuri, Zhang et al, 2023)

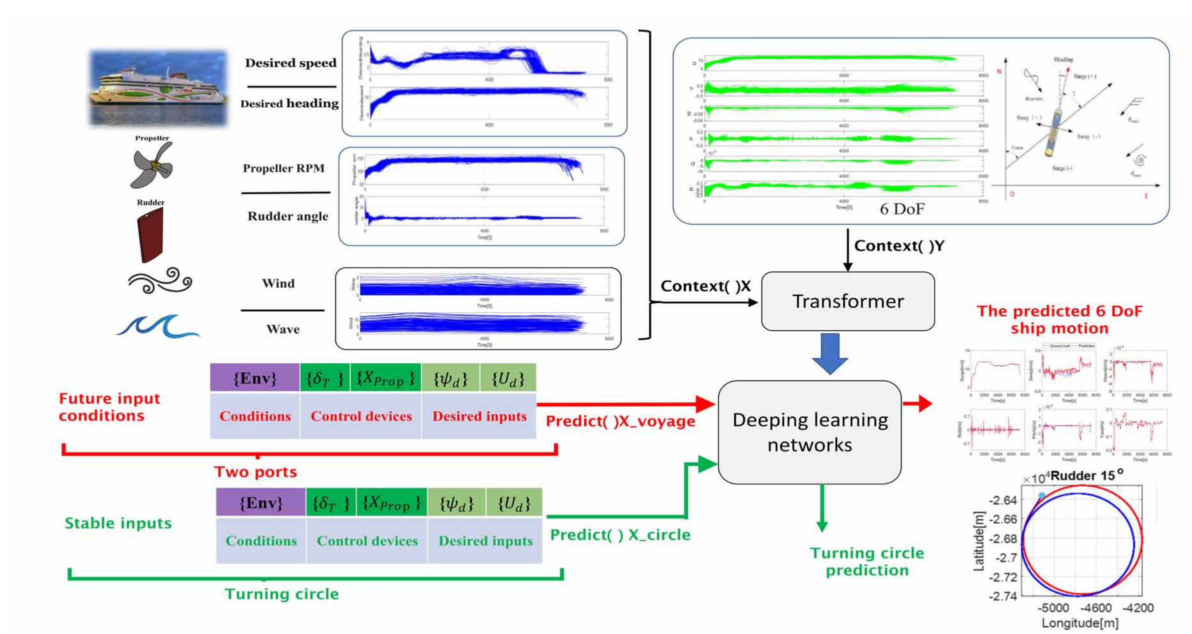


Table 5. The model characteristics and hyperparameters of the transformer

Model	Input variables	Output variable	Encoder
Transformer	8	6	6 blocks
Decoder	Optimizer	Batch Size	Dimension
6 blocks	Adam	8	256
Encoder	Encoder module	Inner layers	Epochs
1 parallel attention layer	3 parallel attention layers	1,024 dimensions	48

Figure 17. The model performance evaluation

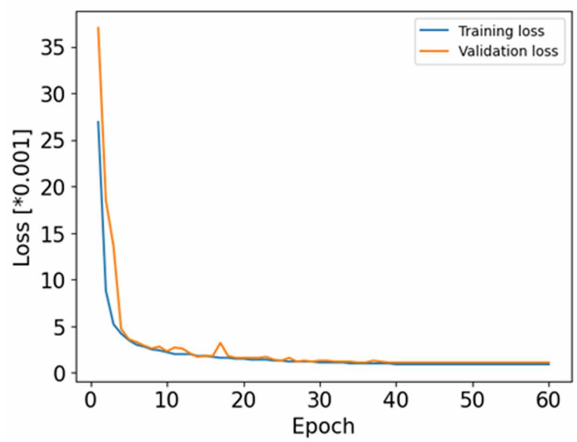


Figure 18. The comparison of real and predicted ship motions

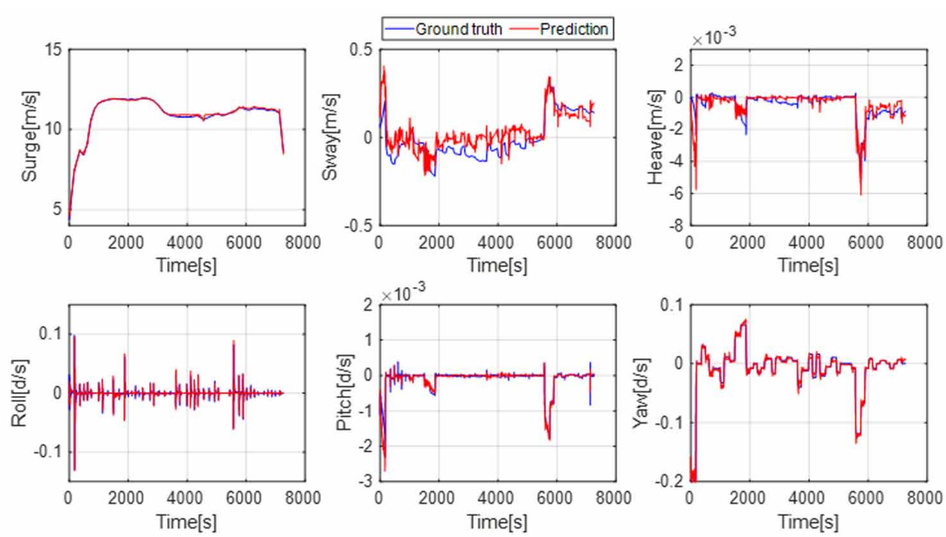
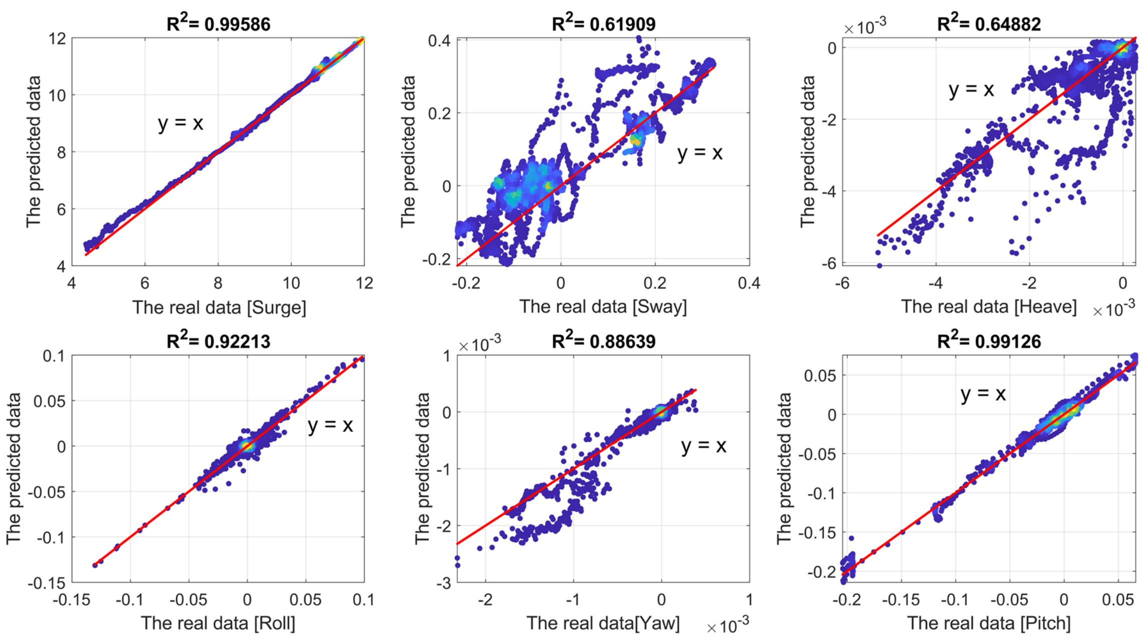


Figure 19. The results of the performance evaluation using R^2 value



real data in blue. The prediction denotes the predicted results in red. These results demonstrate that the digital twin model can effectively capture the ship motion features in real-world conditions.

To accurately evaluate the performance of the trained model, R^2 values were calculated and assessed (Figure 19). The R^2 values for surge, roll, and pitch predictions exceeded 0.9, thus indicating a strong correlation between the predicted and real values. The R^2 values for sway and heave predictions are 0.62 and 0.65, respectively. These results suggest that the predicted and real values are in close agreement. The model demonstrated good performance in predicting all 6-DoF ship motions. However, the agreement for sway and heave predictions is slightly lower as compared to surge, roll, and pitch. This discrepancy may be attributed to the adopted method, which is based on an auto-regression model that may underestimate certain influential factors in ship sway and heave, such as swell, current, etc.

APPLICATIONS OF MULTI-OBJECTIVE AI-BASED DIGITAL TWIN MODELS

As a first step toward demonstrating the benefits of an AI-based digital twin in this section, the models outlined in Section 4 are utilized to predict ship fuel consumption and to estimate ship turning circles in calm sea conditions.

Ship Fuel Consumption Prediction

To expand the usage of the trained digital twin model to a subsequent voyage of the ship indicated in Table 2, which begins in Canada and ends at Attu Island as shown in Figure 20. The ship is operating in

Figure 20. Ship fuel consumption prediction by calling the trained digital twin model

```
Save model: model.save('Ship fuel consumption model.h5')
Load model: loaded_model = load_model('Ship fuel consumption model.h5')
Use the model: Predictions = loaded_model.predict(New_inputs)
```

a loaded condition, with a deadweight tonnage (DWT) of 76,528 metric tons, and the estimated distance of the voyage is approximately 3,994 nautical miles.

The error analysis of ship fuel consumption prediction for an entire voyage is presented in Figure 21. In the upper figure, the red line represents the real values of ship fuel consumption, while the green line represents the predicted results. In the middle figure, the blue line represents the error rate in the time domain. The bottom figure displays the prediction error distributions. It provides a visual representation of the distribution of errors across different ranges or intervals. Examining the error distributions can offer insights into the overall performance and identify any systematic biases or patterns in the prediction errors. The findings, unveil the outcome of the fuel consumption prediction using the trained digital twin. They highlight that more than 90% of the prediction errors are below 5%, and the average error of the ship fuel consumption of the whole voyage is measured at 2.54%. These results serve to affirm the viability of deploying the trained digital twin model as an efficacious tool for forecasting fuel consumption during comparable voyages. Consequently, the application of the model holds the potential to furnish valuable insights and facilitate efficient fuel management and optimization endeavours in real operational conditions.

Turning Circles Prediction Using the Digital Twin of the Ship Motion System

To demonstrate the generalization capability of the digital twin of the ship motion system, the prediction of ship motion dynamics was conducted by setting stable rudder angles as new inputs to generate turning circles. The selected stable rudder angles were set at 1°, 5°, 10°, and 15° (starboard), while the propeller revolutions were fixed at 109 rpm. Figure 22 illustrates the predicted turning circles for different rudder angles (1°, 5°, 10°, and 15°). The results indicate that the trained digital twin model can capture the turning characteristics of the ship accurately, despite not being explicitly trained on ship turning circle data. This suggests that the model has effectively "learned" the ship maneuvering features and can generalize well to new scenarios. Figure 23 presents an error analysis of turning circle predictions

Figure 21. The error analysis of ship fuel consumption prediction using the trained digital twin model

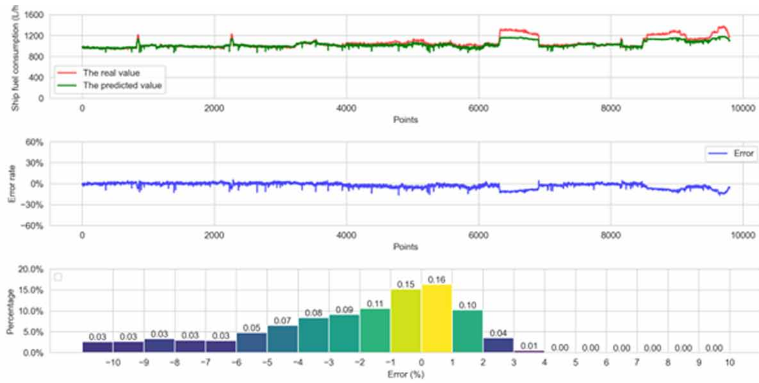
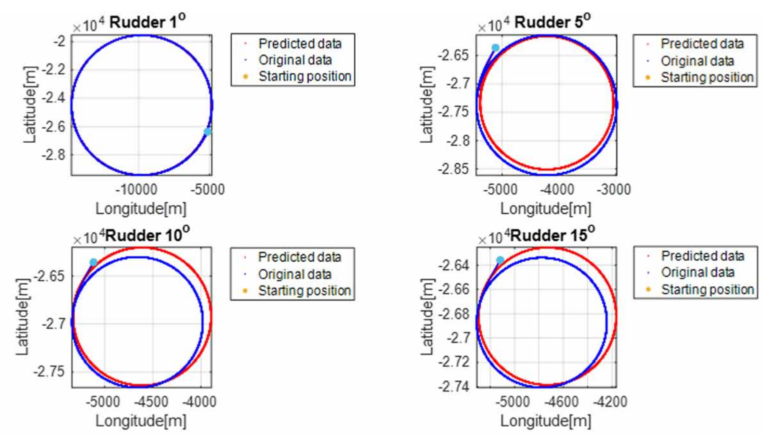


Figure 22. The prediction of the ship turning circle using the designed digital twin model



for various rudder angles (1°, 5°, 10°, and 15°). The analysis reveals that the predicted error increases as the rudder angle increases. This can be attributed to the fact that a significant majority (96.8%) of the rudder angles in the trained datasets fall within the range of -1° to 1°, as depicted in Figure 24. Consequently, as the rudder angle deviates from this range, the number of available training data points decreases, resulting in lower accuracy for turning circle predictions with higher rudder angles. To further improve the accuracy of the digital twin of the ship motion system in predicting turning circles for high rudder angles, it is suggested to train the model with more complex voyages that involve ship motion dynamics in real conditions. By incorporating such data into the training process, the model can learn to handle the complexities and variations associated with higher rudder angles, thereby enhancing its accuracy and performance.

Figure 23. The error analysis of turning circle prediction at different rudder angles

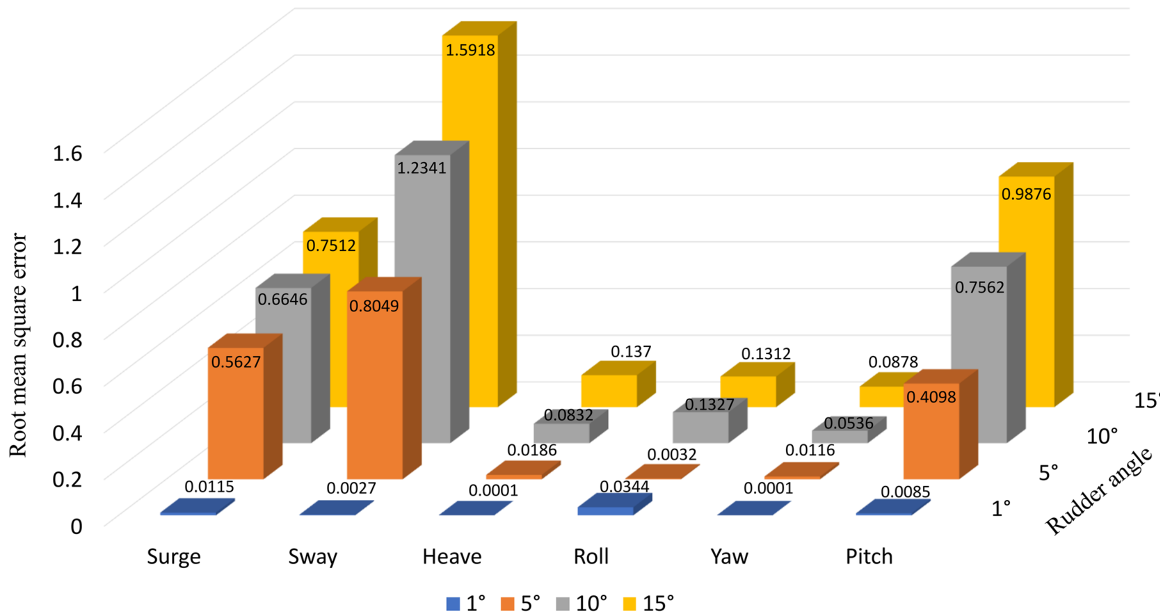
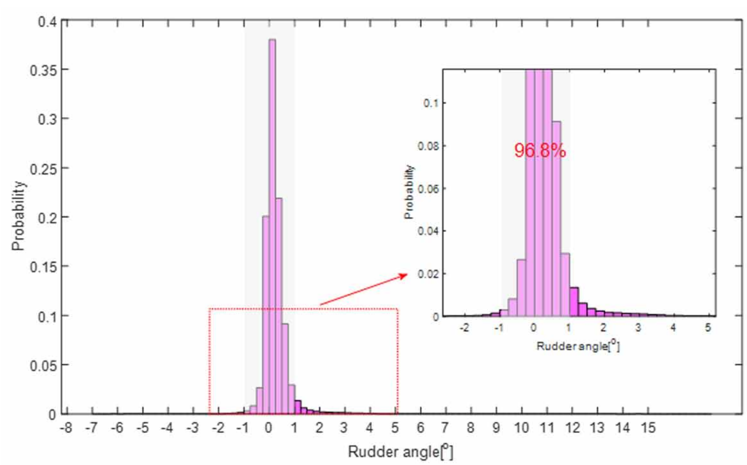


Figure 24. The distribution of the rudder angles of the trained data. The window demonstrates that distribution ranges from [-1 to 1]



CONCLUSION

This chapter introduced a ship digital twin model designed to enhance safe and sustainable ship operations. The digital twin presented consisted of two distinct layers: (a) Layer 1 that incorporates a bi-directional LSTM network with attention mechanisms to replicate the ship's energy system and estimate ship fuel consumption in real operational conditions; (b) Layer 2 that employs a transformer neural network to construct a digital twin model of the ship's motion system, thus enabling analysis of ship motions in relation to hydro-meteorological conditions. The ship digital twin was trained, validated, and tested using bulk carriers and Ro-Pax ships as focal points. Key conclusions derived from the study can be summarized as follows:

The innovative use of multi-objective AI-based digital twin models for predicting ship motions and ship fuel consumption holds significant promise and utility in ensuring safe and sustainable ship operations.

High-frequency sea tail data streams are invaluable for constructing ship digital twins, and the proposed deep learning methods effectively capture the complex relationships between external conditions, internal conditions, and ship performance.

Layer 1 of the AI-based ship digital twin learns the ship's energy systems and can be utilized to estimate long-term ship fuel consumption under real operational conditions.

Layer 2 of the AI-based ship digital twin identifies the ship's motions accounting for realistic hydro-meteorological conditions. It can accurately predict dynamics in real conditions between two ports, as well as ship turning circles with various rudder angles under calm conditions.

While the preliminary results presented in this chapter are promising, it is important to note that they are limited to specific ship types. Extensive testing is necessary to generalise the suitability of the methods and with the ultimate goal to develop a comprehensive framework for the appropriate utilization of digital twin technology in fleet management.

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Chapter 10
Shipping Applications of Digital Twins

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ABSTRACT

This chapter presents three applications of digital twin in shipping, namely the predictive maintenance of ship machinery, cargo load area cleaning, and hull biofouling treatment. The chapter discusses the business importance of each of these applications and surveys the current state of the art practices. The chapter then illustrates novel approaches that utilise digital twins and bring improvements in terms of costs, safety, and environmental impact.

INTRODUCTION

Chapter Aims and Objectives

In this chapter we discuss applications of digital twin (DT) technologies to specific shipping operations in shipping and maritime. The overall aim of the shipping industry is to operate in a cost efficient, profitable, safe, and environmentally sound manner. This in turn requires the use of special purpose technologies to support to ship operation and maintenance. The ambition is to introduce new, more sophisticated information technologies that improve performance and reduce costs. As it increasingly happens in other business domains, such technologies are underpinned by Digital Twins (DTs). DTs

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that incorporate digital models of the ship allow the use of data driven decision making that improves speed, precision or accuracy in ship operations. Broadly, these include:

- Ensuring that the ship machinery is operating smoothly and efficiently and no failures occur during operation.
- Time and labour-intensive operations take place as efficiently as possible by utilising ship knowledge and advanced IT and automation.
- All ship outstructures (e.g. hull) are maintained in clean condition in order to operate smoothly and efficiently.

More specifically, we are discussing three shipping business operations of particular significance:

Predictive engine maintenance. Analysing sensor signals to predict the failure of equipment in order to prevent potentially catastrophic failures.

Cargo hold cleaning: Making the task of cleaning cargo holds safe, efficient and more environmentally friendly.

Antifouling hull cleaning: Improving the hydrodynamic efficiency of the ship in a cost efficient and environmentally friendly manner through treatment of biofouling.

Apart from the business benefits, this Chapter emphasises the direct environmental benefits that application of DTs has on ship operations. More specifically:

Predictive machinery maintenance has beneficial effects on the smooth running of the ship, resulting in lower fuel consumption and fewer harmful emissions.

More efficient cargo hold cleaning has the direct important consequence that it produces fewer chemical pollutants- byproducts of the cleaning process which are usually dumped at the sea.

Finally, biofouling monitoring and treatment improves the hydro performance of the ship which results in lower fuel consumption and hence lower emissions.

Chapter Organisation

The Chapter is organised as follows: The next section presents the business case for predictive ship machinery maintenance and how DT aids that. Section 3 introduces the problem of cleaning cargo hold in bulk cargo ships and discusses ways about how DTs can aid the efficient, safe and environmentally friendly cargo hold cleaning. Section 4 discusses the antifouling treatment of underwater ship hulls, its benefits and how DT based approaches can improve its effectiveness and environmental efficiency. Finally, Section 5 discusses benefits and pitfalls of the proposed approaches and presents a future outlook of the evolution of the discussed systems and technologies.

PREDICTIVE MAINTENANCE OF SHIP MACHINERY WITH THE HELP OF DTS

Shipping Maintenance, Its Importance, and Its Variants

Effective ship machinery maintenance is important as it minimises equipment failure and unexpected disruptions to ship operations which in tun hamper the profitability of the shipping company. (Jimenez et al., 2020). In manufacturing, the goals of maintenance are high availability, quality, safety, the achieve-ment of production target and the optimised use of energy and resources. (Mobley, 2002), (Dekker, 1996) Over time, with continuous improvements in technology, different maintenance practices have emerged. These include:

Periodic or Scheduled Maintenance This is the practice of overhauling or replacing machinery or components on regular intervals, according to a maintenance schedule. This practice however has been criticised as being wasteful, while at the same time does not guarantee protection from unexpected equipment failures.

Preventive Maintenance: This practice involves regular inspection, and maintenance (e.g. cleaning, lubrication, reassembly), according to a maintenance schedule, as well as condition analysis. While this practice ensures a longer lifecycle of the equipment, but similar to the practice of periodic maintenance, it does not guarantee protection from unexpected failures.

Emergency Maintenance: In emergency maintenance, repair or replacement of components or equipment is carried out as soon as they have failed or as soon as it is detected that their failure is imminent.

Regarding maintenance of ship equipment, the practice of scheduled and preventive maintenance is followed, i.e. at regular intervals when the ship is taken out of operation. Emergency maintenance is in general more difficult and expensive to apply when the ship is at sea, and usually is carried out only on critical equipment.

The main benefit of preventive maintenance on ships is the ability to schedule corrective maintenance before ships enter open water, where repairs are more difficult and expensive.

Condition based monitoring (ISO 17359: Condition monitoring and diagnostics of machines – General guidelines) is part of a maintenance strategy where an attribute of some machinery or equipment that correlates with its correct functioning or malfunctioning is monitored in order to detect an impending failure. Once an abnormal reading of such variable or parameter is detected (such as for example, a rise in the component's temperature) indicating impending failure,, the maintenance team is alerted in order to carry out preventive or emergency maintenance actions.

Condition based monitoring is more efficient than preventive, temporary and emergency maintenance. Predictive maintenance is a promising strategy for avoiding catastrophic failures by acting before they occur, as emergency maintenance can mitigate or minimise the potentially catastrophic effects of machinery and equipment failure.

Maintenance in shipping has often adopted a preventive or scheduled maintenance system, which does not always include a condition-monitoring scheme. (Shorten, 2012) According to Shorten (2012), the shipping industry has been slow to adopt the latest maintenance practices, with only 17 percent of classed ships operate with an approved preventive maintenance system, 12 percent of those using condition monitoring, and only around 2 percent of ships operating a condition based monitoring scheme.

Due to the costs and risks associated with unexpected machinery and component failures, the practice of *predictive maintenance* has been gaining popularity in manufacturing, aerospace, and more recently in shipping. Predictive machinery maintenance is essentially the estimation of the probability of defect, by incorporating the analysis of signals from the component, system and/or from its environment.

For instance, if there is increase in exhaust gas temperature then there is a chance of imminent engine failure (Mishra & Ali, 2017). Thus, the reading from the exhaust gases can be used as an indicator for the detection of imminent failures. There is usually a threshold limit in the data value before a failure alarm is triggered, for instance in the engine failure a reading of 520 degree Celsius for the exhaust gas temperature is the threshold value (Mishra & Ali, 2017).

Therefore, since the classification of sensor signals as normal or abnormal requires statistical analysis, predictive maintenance and condition monitoring are effectively data *driven* techniques.

Research in data driven predictive maintenance has therefore utilised machine learning and other Artificial Intelligence techniques, to predict equipment failure, such as for example, engine failure (Goksu, 2020) (Mohanty & Paul, 2022). Artificial Neural Networks (ANNs) have for instance been proposed for predictive maintenance. The ANN is first trained with historical machinery failure data, and then it becomes capable to detect upcoming failures with a given degree of probability.

The Role of DTs in Predictive Maintenance

Condition based monitoring and predictive maintenance requires the receipt and fusion of signals from multiple sensors onboard the ship and its surrounding environment.

Sensors are installed on components and machinery by the machinery manufacturers, resulting in a multitude of sensors and data types and formats that need to be homogenised and fused in order to be used by the predictive maintenance algorithms. The sensors are not only from different manufacturers but also of different type as they measure different physical properties such as temperature, vibrations, voltage and so on. This leads to an increased complexity in detecting the true health status of the component or machinery, due to the existing interdependencies.

The role of the digital twin is therefore manyfold in supporting predictive maintenance, as:

The DT is an all encompassing model of the ship, describing all components, subsystems and systems, their interrelationships and interdependencies (e.g. energy, electrical or mechanical interconnections).

DTs can present standardised and unified interfaces to the sensor data, using for example standards such as those promoted by the International Data Spaces association (https://internationaldataspaces.org)

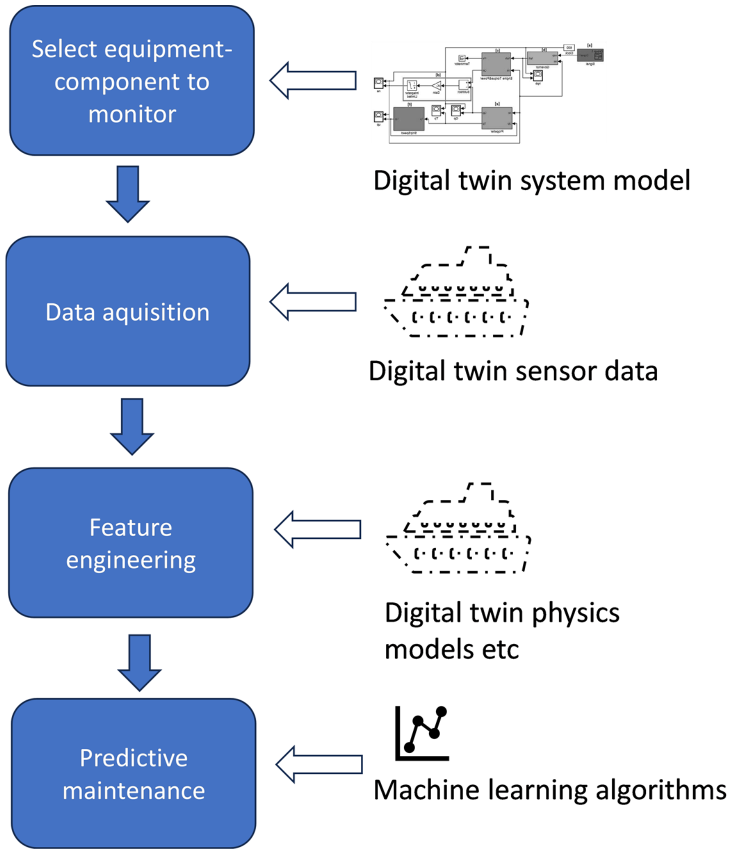
DT holds historical values of variables measured by the sensors. This is important for the predictive maintenance algorithms, for instance for training and validating the ANNs that carry out the predictions.

Method for Developing a DT Based Predictive Maintenance System

While predictive maintenance is a very wide area and depends on the specifics of the equipment monitored and its context, the diagram of Figure 1 illustrates a generic predictive maintenance workflow underpinned by DTs.

More specifically, the following steps are involved: First, the component or equipment to be monitored needs to be selected within the DT model(s). This will lead to the identification of sensors attached to the component/equipment. Access to the sensors' current and historical data will be made available through the standardised interfaces made available by the DT. By evaluating all the sensor signals that are available, using a feature engineering process, the signals that are most indicative for the condition that is monitored are selected. This ensures that the size of the predictive model that will need to be considered is manageable. The process of feature engineering is undertaken by domain experts (e.g. ship equipment engineers, electrical, process engineers and modelling experts and supported by the DT that provides models of the physical properties of the equipment component and of all required physics models to simulate and analyse the behaviour and interdependencies of the modelled variables. Experiences from other prediction models and/or similar DTs may also be utilised here.

Figure 1. Workflow for predictive maintenance



Once the predictive model is finalised, its implementation in a suitable Artificial Neural Network (ANN) is carried out, followed by the steps of testing using historical data provided by the DT, validation and deployment.

Potentially the predictive maintenance system can be integrated with other monitoring and management systems such as engine room monitoring systems in order to receive contextual data (e.g., ship operational data) in order to make accurate diagnoses of the equipment/component's health state under varied external conditions.

If the system detects abnormal patterns in the incoming sensor data that lead to a failure prediction, the central monitoring/maintenance system will be alerted, and the source of the failure will be localised, its criticality will be assessed and a mitigating action will be decided such as emergency maintenance, changing the operational parameters of the equipment, shutting down the equipment, and so on.

In addition to supporting predictive maintenance, DTS can support additional functionalities such as the ability to analyse and simulate how an equipment/component would behave under different operating conditions, for instance under higher or lower temperatures, stresses, etc. This in turn provides the ability to test different maintenance scenarios, i.e. determining whether the equipment/component would continue to operate under the different scenarios, or an intervention would be required, for instance preventive maintenance (InformationWeek, 2018).

This ability is also very important from an efficiency viewpoint as physical interventions on the equipment that would be costly but ineffective can be avoided.

In conclusion, DTs can play a pivotal role in implementing predictive maintenance in shipping. A DT maintains a history of the equipment/component change in parameter values, and therefore allows an assessment of its current age and condition. Moreover, information about the context of the component, both current and historical is available, allowing an accurate diagnosis and interpretation of the current state or behaviour of the component. Additionally, as the equipment or component ages different sensors/ measurements may be required, and these can also be retrieved from the DT.

CLEANING OPTIMISATION OF CARGO HOLDS WITH HELP FROM DTS

Background

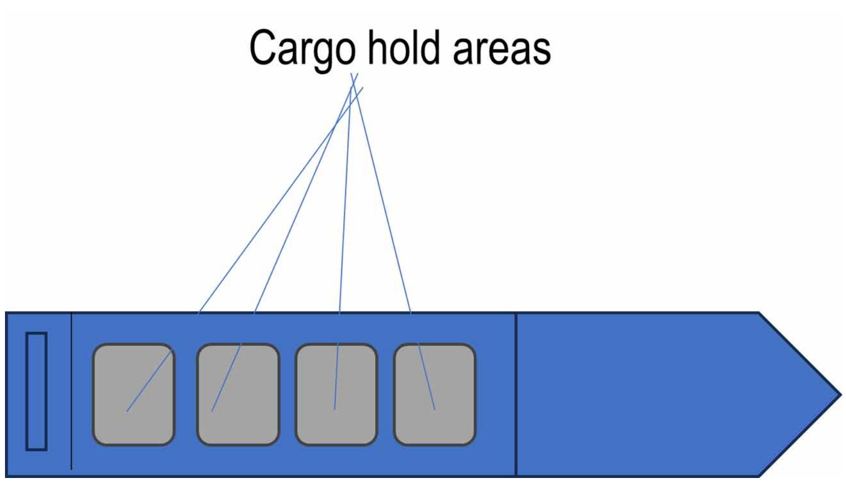
Bulk carriers are ship designs optimised to allow the efficient loading, transportation and unloading of bulk cargo (Fig. 2). Their efficiency therefore is measured by their ability to transport the largest quantities of cargo at the shortest possible time.

The loading and unloading of the cargo, and the subsequent reloading with different cargo is a complex procedure requiring preparation, a key part of which is cargo hold cleaning. (SAFETY4SEA, 2023)

Cargo, in particular loose cargo is susceptible to deterioration when transported in the ship's holds, as a result of its own characteristics (e.g. chemistry) as well as the characteristics of the containing environment, such as temperature. (DNV, 2019)

As a result, the inappropriate transport of cargo can result in its deterioration, causing a drop in its value or even making it non merchandisable. One of the frequent causes of such problems is the inadequate cleaning of the cargo hold after the cargo has been unloaded and prior to the new cargo been loaded. The contact of the new cargo with areas where traces of the old cargo remain can cause contamination and other chemical interactions that affect the quality of the new cargo. For instance, the loading of cement in areas that previously contained water can cause its hardening, rendering it unusable.

Figure 2. Cargo storage areas in bulk cargo ship



The inadequate cleaning of cargo hold areas can therefore have financial consequences for the shipping company as shippers will often claim compensation when their cargo becomes spoiled. Ships can be held at port until the surveyors are satisfied that the cargo areas are cleaned adequately. All these translate to loss of revenue for the shipping company.

Moreover, inadequate removal of traces of cargo from the loading area surfaces can cause their deterioration, such as rusting.

The difficulty of effective cleaning of cargo hold areas is caused mainly by its shape and size which makes the use of access equipment (e.g. ladders and platforms) essential. In turn this can create health and safety issues for the crew that performs the cleaning operation.

Another issue relates to the type and intensity of cleaning required. For instance some cargo residues will require the use of detergents, while others will simply require rinsing with sea water. The unnecessary or excessive usage of detergents and other chemicals (that are subsequently get dumped to the sea) creates however an environmental hazard.

Cargo Hold Cleaning Using Robots

Robotics have been receiving the attention of researchers as a technology that is applicable to shipping. For instance research projects such as MINOAS (Marine Inspection Robotic Assistant System) and INCAAS (Inspection Capabilities for Enhanced Ship Safety), two EU-funded projects, researched the use of robots to support the inspection process of large marine vessels.

In more recent years, robots have started to be utilised in shipping applications such as hull cleaning, as well as for vessel inspection (Markus et al., 2014)

Regarding cargo hold cleaning some commercial products have recently been reported in the industry. These employ mainly magnets in order to attach themselves to the cargo hold walls,, as well as cameras that transmit images of the cargo hold areas to their human operators. Deployment of robots to at least partially automate the cargo hold cleaning process claims to protect the marine environment by preventing the dumping of chemicals being released into the oceans during the cleaning operation. Additionally, robots can reduce the need for strong chemicals, as they substitute them for milder detergents or plain water, further reducing the environmental impact. Lastly, the use of robots reduce the need of seafarers to use access equipment to clean the cargo holds and also reduces their exposure to potentially harmful cleaning chemicals, thus improving their health and safety.

Application of DT to Cargo Hold Cleaning

Although the use of robots can reduce the time required to clean cargo holds, this still remains a time intensive operation as robots need to be guided by human operators. A fully autonomous robot instead could potentially carry out the process quicker while requiring less or no human crew attendance.

An autonomous robot needs to be programmed with an operational path in order to execute the cleaning process as efficiently as possible. Information to construct such path can be obtained from the ship's DT.

Indeed, a ship's DT includes amongst other 3D models of the ship and its subassemblies. 3D models of the different cargo holds on the ship contain not only information about the geometric properties of the cargo hold area but also of its connections to other ship subassemblies and components, for instance the hatches as well as the bilge (lower part of the ship hull below the cargo hold area).

The information provided by the cargo hold 3D map can therefore be used as direct input for the robot's path planning. Indeed, it has been demonstrated that a robot path can be programmed directly from a CAD model {Bedakaa & Lin, 2018). Moreover, the 3D model of the cargo hold obtained from the DT allows to plan:

- The order in which the different cargo hold areas will be cleaned
- The types of cleaning chemicals to be used as well as cleaning attachments such as hoses allowing the robot to effectively reach all areas of the cargo hold.
- Identification of areas that are difficult or impossible to clean by the robot and thus will require human operators.

Robots equipped with suitable sensors such as cameras and chemical detection sensors can also act as aid for the surveyor that needs to verify that the cargo hold has been cleaned adequately. The robots can convey to the surveyor not only an image of the cleaned area but also its location on a map (obtained from the DT), assisting the surveyor to verify that all cargo hold areas have been cleaned.

UNDERWATER SHIP HULLS BIOFOULING TREATMENT

Background

To minimize the energy footprint of shipping, various approaches are being explored, such as transitioning to cleaner fuels (such as liquefied natural gas, hydrogen, ammonia, etc.), incorporating energy-saving devices on ships, and optimizing ship routes to enhance efficiency. Biofouling, the accumulation of marine organisms on the submerged surface of ship hulls, also has a significant impact on a ship's hydrodynamic performance (Demirel et al., 2017; Schultz, 2007). The roughness of the hull surface resulting from bio-fouling leads to increased friction and, as a result, higher power requirements and fuel consumption (Demirel et al., 2017; Hakim et al., 2019), and therefore increase in vessel fuel consumption and emissions and the accrual of cleaning costs.

As already mentioned, biofouling can have negative effects on vessel performance, fuel consumption, and manoeuvrability. Therefore, regular cleaning is of great importance in maintaining hull performance. Biofouling leads to increased hydrodynamic resistance, as the presence of organisms disrupts the flow of water around the hull, creating eddies or increased turbulent flow. Additionally, the deposition of organisms on the ship's propellers can cause mechanical stress on the propeller shaft, leading to reduced performance and, in extreme cases, destruction. Thus, regular cleaning operations are necessary to remove these organisms, minimizing hydrodynamic resistance and restoring the vessel's original design performance.

Adhering to a systematic cleaning program tailored to the ship's needs, planned voyages, and the specific biofouling rates observed ensures timely removal of accumulated organisms before they reach critical levels and cause negative effects on ship performance. It also prevents the deterioration of the ship's hull coatings due to secretions and toxins excreted by organisms, which can cause structural damage and increased maintenance requirements. This approach allows for the inspection of the hull's condition, facilitating the early identification of coating wear or corrosion issues that require further attention.

Finally, it is important to note that regular cleaning contributes to environmental sustainability by preventing the introduction of non-native species into new environments when ships travel to different areas, thus reducing the ecological impact on marine ecosystems.

The growth of biological organisms not only increases fuel consumption but also reduces the manoeuvrability and operational efficiency of vessels. Additionally, it can lead to the introduction of invasive species into new ecosystems, causing ecological disturbances. Hence, it is imperative to effectively mitigate the impact of biofouling through appropriate monitoring and measurement techniques. These techniques can provide accurate and timely determinations of biofouling levels and species composition, enabling informed decisions regarding the implementation of preventive measures. By understanding the patterns and types of biofouling present in different marine environments, ship owners and operators can tailor their approach to effectively combat fouling. Furthermore, reliable monitoring methods allow for data collection to evaluate the effectiveness of various antifouling techniques and optimize the planning of vessel maintenance and cleaning operations. These measurements provide critical information about the extent of pollution, its impact on vessel performance, and the potential risk of transporting invasive species. On the other hand, ship owners can adopt proactive fouling management actions to maintain optimal hydrodynamic performance, extend coating life, and reduce fuel and maintenance costs. It is important to mention that effective monitoring and measurement techniques support compliance with environmental regulations and help preserve marine ecosystems by preventing the spread of non-native species.

Biofouling in Marine Environments

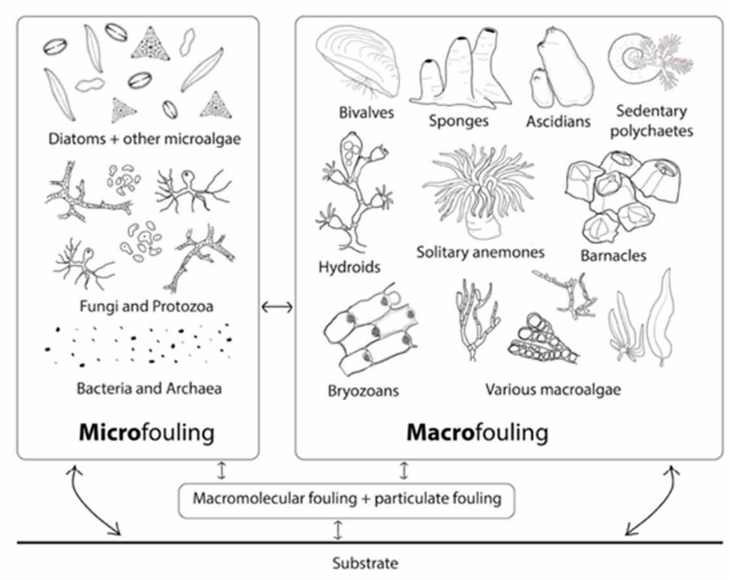
Definition and Types of Biofoulings

Marine biofouling refers to the colonization and growth of marine organisms on submerged surfaces. This phenomenon has been recognized since ancient times, dating back to the earliest seafaring ventures (Alghamdi & Quijada, 2019). In the present day, biofouling stemming from human constructions poses detrimental effects on various sectors, particularly shipping. The performance of maritime transport is significantly hampered by the accumulation of noxious organisms on the hulls of ships, leading to concurrent harm to the environment and biodiversity.

Globally, over 4,000 species of marine biofouling organisms have been reported, with the majority of them predominantly inhabiting coastal areas and harbours that offer favourable conditions for their growth (Cao et al., 2011). The advancement of more efficient, safe, and sustainable methods to mitigate biofouling relies on a comprehensive understanding of the development and characteristics of fouling communities. This includes discerning their species composition at different stages, growth rates, and reproductive patterns. Fouling communities encompass a diverse array of organisms, encompassing bacteria, fungi, algae, bryozoans, hydrozoans, sponges, mollusks, and crustaceans, among others (Chava et al., 2021).

The main components of fouling communities can be defined as (Cao et al., 2011; Chava, et al., 2021), as per Figure 3 diagram.

Figure 3. Principal framework of major components within fouling communities
Source: Chava et al. (2021)



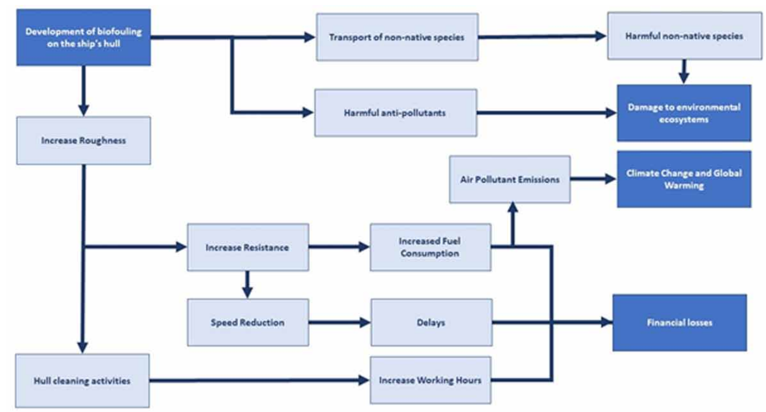
- **Macromolecular and particulate fouling**: This category pertains to the adherence of diverse biological macromolecules and organic and inorganic particles, predominantly influenced by natural forces.
- **Micro-fouling**: Micro-fouling encompasses the presence of bacteria, diatoms, unicellular algae, fungi, archaea, and protozoa, which collectively form intricate three-dimensional structures known as biofilms.
- **Macro-fouling**: Macro-fouling encompasses various types of macroalgae, alongside a wide range of sessile animals, including hydroids, bryozoans, sea anemones, barnacles, other ciliates, sessile polychaetas, bivalves, sponges, and ascidians.

The adhesion of marine fouling organisms involves a complex biochemical process. Generally, the biofouling of marine structures can be characterized by two crucial events (a) the formation of biofilms, which entails reversible physical adsorption, followed by irreversible secondary adhesion and subsequent proliferation of microorganisms, and (b) the settlement and growth of spores or larvae of macro-organisms (Cao et al., 2011). The fouling process can be divided into five main stages, starting with the adsorption of organic and inorganic macromolecules forming the primary film, followed by microbial cell transport and immobilization, bacterial attachment and biofilm formation, community development with the presence of various organisms, and finally the attachment of larger marine invertebrates (Delauney et al., 2010).

Impact of Biofouling on Ship Performance and Efficiency

The phenomenon of marine organism biofouling on the outer hull of ships has significant implications for their performance, as evidenced by studies conducted by Demirel et al. (2017) and Schultz (2007). The presence of biofouling organisms on the hull surface leads to heightened surface roughness, re-

Figure 4. Correlation between various problems caused by biofouling
Source and adapted from Hakim et al. (2019)



sulting in increased frictional resistance. Consequently, ships experience a rise in power requirements and fuel consumption, as reported in the studies by Demirel et al. (2017) and Hakim et al. (2019), and therefore put the integrity of the ship and the cargo at great risk (Alonso, 2011). The consequences of biofouling extend beyond economic concerns and encompass adverse environmental effects. Increased fuel consumption arising from heightened frictional resistance contributes to elevated air pollutant emissions. Moreover, the attachment of biofouling organisms facilitates the transportation of non-indigenous species from one biogeographical region to another. These introductions of potentially harmful species have negative implications for ecosystems (Demirel et al., 2017; Hakim et al., 2019; Schultz, 2007). In addition to its impact on shipping, biofouling has far-reaching consequences across various domains. The marine environment holds significant importance as it offers essential services, such as sustenance through food and water resources, safeguards biodiversity by mitigating storm waves to protect terrestrial organisms and enriches cultural activities like recreation and spiritual pursuits. The effects of biofouling on the economy extend beyond the realm of shipping, affecting interventions in fishing practices, the associated costs of control and cleaning, as well as the infrastructure that supports fishing activities, leading to potential reductions in fish stocks. From an environmental standpoint, biofouling poses a threat to the habitats it colonizes, primarily through the consumption of native species, competition for resources and space, and the introduction of diseases.

In Figure 4, the effects of biofouling are presented.

The development of biofouling on ships can be divided into four distinct phases, each characterized by different factors influencing the formation and persistence of biofouling (IMO et al., 2022).

- **Port of Departure:** In this phase, biofouling depends on various factors such as the duration of the ship's stay in the departure maritime area, the type and condition of the antifouling coating applied on the hull.
- **Travel:** During the travel phase, biofouling is influenced by factors including the ship's speed, duration and route of travel, location of biofouling on the hull, and the type of antifouling coating used.

- **Port of Arrival:** The biofouling in the port of arrival is influenced by the ship's stay in the maritime area, environmental conditions, availability of space for organisms to settle, and the level of biotic resistance.
- **Biofouling attachment area:** In this phase, the attachment and growth of biofouling depend on environmental conditions, availability of space for organisms to attach, level of biotic resistance, and the potential introduction of organisms from other ships.

Factors Influencing Biofouling Development

The development of fouling communities is significantly influenced by several factors, as shown in equation (1). These factors include seawater surface temperature (SST), salinity (psu), acidity (pH), water flow speed (v), light intensity (I), nutrient concentration (S), exposure time (t), micro-texture of the surface (m_t), surface potential (σ), contact angle (θc) as a measure of wettability, roughness parameter (Rt), and the performance parameter (ηc) of an antifouling coating (representing the efficiency and chemical contents, including leaching rate). In addition, surface colour and contour are believed to have various effects on biofouling growth, although their influence is not yet well-established (Uzun et al., 2019).

$$BG = f_1(SST, psu, pH, v, I, S, t, m_t, \sigma, \theta c, Rt, \eta c) \quad (1)$$

The surface characteristics of a ship, including micro-texture (mt), surface potential (σ), contact angle (θc), and roughness (Rt), exert a profound influence on the growth of biofouling. These properties play a significant role in the settlement and attachment of organisms such as hydroids, bryozoans, and ascidians. Micro-texture, characterized by its presence of grooves, pits, cracks, and crevices, provides sheltered habitats that attract these organisms by offering protection against strong water flow. Surface roughness (Rt) plays a critical role in bio-adhesion, as it creates crevices where extracellular polymeric substances can flow, facilitating strong attachment. In contrast, smooth surfaces only provide adhesive contact on the peaks of surface irregularities, resulting in weaker bio-adhesion. Researchers have confirmed the correlation between surface roughness and attachment strength. Surface potential (σ), which represents the surface charge, also influences the attachment process of microorganisms. Kerr et al., (1998) have demonstrated the impact of negative surface potential on the attachment process. Surface properties, such as mt, Rt, and σ, directly impact the colonization and adhesion of biofouling organisms on ship surfaces. Light intensity (I) plays a pivotal role in shaping the biofouling community, particularly the growth of plant-based fouling organisms ranging from microalgae to macrophytes. Light intensity is closely associated with water depth in existing models. Photosynthetic macrofouling, primarily comprising algae, thrives in nutrient-rich areas with high light levels within the depth range of 0–40 meters. However, other organisms such as mussels, barnacles, and tubeworms, which derive energy from sources within the marine environment, can grow at greater depths, unaffected by variations in light intensity (Babin et al., 2008). The availability of nutrients (S) and the velocity (v) of water flow are also significant factors influencing marine fouling. Nutrient abundance is closely linked to water flow rates and proximity to coastal areas, which tend to have higher nutrient levels due to human-related discharges (Cao et al., 2011). The impact of pH on biofouling development is an area that requires further research. Global seawater pH values typically range from 7.6 to 8.4, where it is predicted that in the coming years, due to ocean acidification resulting from increased atmospheric CO2, pH levels may drop between 7.6 and 7.8 (Clark et al., 2009). In this context, several studies indicate that pH levels ranging from 6.5 to 10 create favourable conditions for a wide range of biological fouling organisms. However, because of the relatively limited pH variations in the world's oceans, pH effects on biofouling development are not currently believed to play a significant role. Salinity (psu) holds significant influence over the growth of biofouling organisms, and different types of fouling organisms exhibit varied responses to changes in salinity. The salinity values observed in world seas typically range from 33 to 38 psu (Britannica, 2023), which falls within the salinity tolerance range of biofouling organisms (Qiu & Qian, 1998).

Finally, it is important to note that the performance of antifouling coatings can vary depending on the geographical region, mainly due to the significant influence of temperature on biofouling growth. Therefore, the model incorporates the change in sea surface temperature (ΔSST) as a parameter to predict the effects on the antifouling coating performance. Also, the model focused on the variations in sea surface temperature (SST) primarily based on latitude, while neglecting the relatively minor effects of changes in longitude. The authors recognized that the impact of longitude on SST is relatively small in comparison to the significant variations observed with latitude. Therefore, the model emphasized the more influential relationship between SST and latitude in predicting biofouling growth, as shown in equation (2) (Uzun et al., 2019).

$$SSTa = 12.5 + 15\left(\cos\left(\frac{latitudedegree}{28.64}\right)\right) \tag{2}$$

And

$$\eta_{ca} = \frac{\eta_{cy}\left(SST_a - SST_x\right) + \eta_{cx}\left(SST_y - SST_a\right)}{SST_y - SST_x} \tag{3}$$

The coating performance parameter at an arbitrary location is denoted as η_{ca}, in equation (3), while η_{cy} and η_{cx} represent the coating performance parameters at field test locations y and x, respectively. SSTa represents the sea surface temperature at the arbitrary location, while SSTy and SSTx indicate the sea surface temperatures at locations y and x. It's important to consider that the model takes into account the variations in coating performance and sea surface temperatures across different locations during the field tests.

Existing Methods for Biofouling Monitoring and Treatment

Biofouling caused by marine organisms on a ship's hull causes significant problems both in the environment and in the performance of maritime transport, with the increase in ship resistance leading to an increase in power requirement and fuel consumption. A study focused on commercial ships showed that a thin layer of sludge up to 50% on the surface of the hull, can cause about a 20 to 25% increase in fuel consumption and therefore emissions of gaseous pollutants. It is therefore clear that the implementation of activities to clean the hull of attached organisms and the use of antifouling systems are imperative (IMO et al., 2022).

But what is an antifouling system?

An antifouling system can be considered any colour or non-colour return coating, surface treatment or use of equipment on a ship that aims to control or prevent the attachment of undesirable marine organisms.

The predominant system employed by vessels at present is the utilization of antifouling coatings. Nevertheless, alternative methods exist, which can be implemented either in conjunction with the existing coatings or independently. These alternatives encompass the utilization of ultrasound, ultraviolet radiation, marine growth prevention systems, and robotic biofouling cleanup systems. The following paragraphs describe in detail the various ways of dealing with biofouling by category.

Biocidal Antifouling Systems

Biocidal antifouling systems encompass the use of paints that function by gradually releasing biocides from the hull surface's paint film, thereby impeding the attachment of marine organisms. These paints typically contain copper biocides, either with or without organic co-biocides or organic biocides. It is noteworthy that diverse biofouling develops at distinct rates of growth in different environments. Consequently, a judicious selection of the paint is imperative to effectively prevent the proliferation of microorganisms on the ship's hull. For instance, biofouling growth tends to be slower in freshwater compared to saltwater, prompting the incorporation of biocides with reduced concentrations and release rates in the paints intended for freshwater environments. The utilization of biocidal paints offers several advantages. They afford protection throughout various seasons, are facile to apply, and are readily accessible in the market. Nonetheless, concerns have been raised regarding their impact on marine ecosystems due to the release of biocides and metals into the marine environment, as well as the increased risks associated with their application and removal by human operators.

- **Soft biocidal antifouling paints.** Soft antifouling paints feature a paint film that gradually erodes, concurrent with the release of biocides. These paints are applicable for use on most vessels, barring those characterized by high performance and frequent hull treatments to maintain optimal performance. Nevertheless, their usage gives rise to concerns attributed to the discharge of biocides, metals, and microplastics into the marine environment.
- **Hard biocidal antifouling paints.** Hard biocidal antifouling paints function by releasing biocides from an insoluble paint film that remains intact over time. In comparison to soft antifouling paints, these hard variants discharge fewer toxic substances. They find application on ships that operate at speeds of up to 30 knots and are particularly well-suited for protecting propellers. However, to maintain their efficacy, regular cleaning is imperative.
- **Hard epoxy resin with copper.** The incorporation of copper within epoxy resin serves as an effective deterrent against fouling. While this approach yields high efficiency, its application demands precision, entails substantial costs, and proves ineffective against fouling species that have developed resistance to copper-based treatments.

Improper use of personal protective equipment during the application and removal of non-biocidal antifouling paints can pose health risks, while the wash water containing paint residue must be carefully collected and disposed of according to waste management regulations. These methods include the use of non-biocidal antifouling paints, silicone elastomer-based coatings, ultrasonics, water dock systems, reactive cleaning in water, and preventive cleaning in water (hull care).

- **Antifouling paints without biocides**: Biocide-free antifouling paints provide hull and propeller protection but their effectiveness in highly polluted waters is unverified.
- **Coatings based on silicone elastomer**: These coatings create a non-stick surface, preventing organism adhesion, but application is complex and may emit volatile organic compounds or risk oil leakage.
- **Ultrasonics**: Ultrasonic waves disrupt and prevent biofouling without chemicals, but require substantial investment, power source, lifting of the ship, and multiple transducers for larger vessels.
- **Water dock**: Isolated from outside water, water docks prevent organism sedimentation, but are limited to motor and pleasure boats, excluding larger vessels.
- **Reactive cleaning in water**: Fast cleaning with brushes, water jets, or robots while anchored, but requires waste collection to prevent harmful organism and microplastic release.
- **Preventive cleaning in water (hull care)**: Grooming the hull removes surface biofilms, effective for small biofouling thickness, but lacks organism collection equipment and requires regular implementation.

Methods for cleaning up biofouling in water can be categorized into three groups:

(1) Manual cleaning is typically used for small vessels; manual cleaning involves using brushes or scraping devices to remove biological fouling organisms. However, complete removal of biofouling is challenging. In a survey conducted by Song & Cui (2020), it was found that approximately 60% of organisms were removed using a hand brush during manual cleaning,

(2) Electric cleaning systems with rotating brush: Mechatronic technology has advanced underwater cleaning techniques for larger vessels. Robot cleaning systems, large cleaning devices, and hand cleaners have been developed. Systems with large rotary brushes driven by hydraulic motors are commonly used for fast cleaning of flat or slightly curved areas, while smaller brushes are suitable for propeller cleaning. It is important to choose the appropriate brush based on the characteristics of the biofouling.

(3) Non-contact cleaning methods have been proposed to avoid damaging welds, protrusions, and the mechanical integrity of the hull. These methods include high-pressure water jet, cavitation water jet, and ultrasonic cleaning. Compared to rotating brushes, these techniques cause less damage to the hull coating. Under the category of non-contact cleaning technologies, subcategories for cleaning biofouling in water include:

- **Ultrasound method**: Utilizing ultrasonic pulses at different frequencies, this method generates alternating positive and negative pressures that create tiny bubbles, effectively removing biofouling from the hull.
- **Laser method**: This approach involves using high-energy rays to clean the hull by targeting and removing biofouling.
- **High-pressure water jet method**: Using the force of high-pressure water, this method removes biofouling from the hull. Examples include the HullWiper, which collects biopollutants and sprays water at pressures of 50-450 bar (HullWiper, 2022), and the Magnetic Hull Crawler, a remote-controlled system with high-pressure jets reaching up to 1000 bar (Cybernetix, 2022).

- **Water jetting method with cavitation**: This method employs specially designed nozzles that convert high-pressure water into cavitation water. The resulting bubbles burst near the hull, generating high local stresses for enhanced cleaning power compared to conventional high-pressure water jets. Currently, there are no autonomous robotic systems available on the market that incorporate nozzles for cavitation water jets.

These subcategories offer diverse approaches to non-contact cleaning technologies, providing options for efficiently removing biofouling from ship hulls while minimizing damage to the hull coating.

The Rapid, Automated Inspection System for Biofouling Assessment

Description of System for Hull Biofouling Assessment

The proposed inspection system for hull biofouling assessment is a technological advancement in underwater monitoring, combining underwater robotic platforms, image analysis, and AI algorithms to provide a highly efficient and accurate assessment of biofouling development on ship hulls. The center of this system is an autonomous underwater robot specifically designed for biofouling inspection, equipped with advanced sensors, cameras, and mapping capabilities. In this way, the robot can navigate along predetermined paths on the hull, meticulously scanning and analyzing every surface. Therefore, the mapping and pattern recognition techniques ensures that all affected areas are identified.

Integration of Underwater Robotics, Image Analysis, and AI Algorithms

The integration of underwater robotics, image analysis, and AI algorithms is key to the rapid and precise evaluation of sea growth on the ship's hull. As the robot explores the underwater environment, it captures high-resolution images of the hull surface. These images are then processed using advanced image analysis algorithms that leverage AI techniques to accurately identify and measure biofouling organisms. In more details, by leveraging extensive datasets, the AI algorithms integrated into the system

Table 1. Advantages of the proposed system compared to traditional methods

Advantages	Rapid, Automated Inspection System	Traditional Methods
Efficiency	Reduces time and labour required for inspection	Time-consuming and physically demanding processes
Accuracy	Relies on objective data and sophisticated algorithms, minimizing subjective interpretation and human error	Subjective interpretation and higher chances of human error
Coverage	Covers larger areas in less time	Limited coverage due to manual processes
Data Quality	Provides detailed and accurate data on biofouling extent and types	Data may be less comprehensive and may lack detailed insights
Maintenance Optimization	Enables optimized hull cleaning schedules and improved coating performance	Limited data for proactive maintenance planning
Operational Efficiency	Facilitates proactive maintenance and enhances overall operational efficiency	Potential delays and reduced efficiency due to reactive maintenance
Health and Safety	Minimizes human involvement in potentially hazardous inspection tasks	Exposes workers to risks associated with underwater inspections

have been trained to accurately differentiate between various types and levels of sea growth, including algae, barnacles, and other marine organisms, enabling quick identification of biofouling presence and extent while providing detailed insights into the condition of the hull. Furthermore, with its capability for real-time data processing, the system enables on-site analysis of collected information, leading to immediate assessment, decision-making, and enhancing overall system efficiency and responsiveness to address biofouling issues promptly. The system's ability to perform on-site analysis and immediate assessment, coupled with its real-time data processing capability, further amplifies its advantages by enabling prompt decision-making, enhancing overall system efficiency, and bolstering its responsiveness in effectively addressing biofouling issues, as presented in Table 1.

It should be noticed that it not only offers the advantages mentioned earlier but also prioritizes health and safety by minimizing the need for human involvement in potentially hazardous inspection tasks.

Implementation of the Rapid, Automated Inspection System

Underwater Robotics Platforms Used in Biofouling Assessment

Leveraging robotic technology, outfitted with advanced sensors and equipment, not only eliminates the requirement for human divers to perform lengthy and dangerous underwater inspections but also enables navigation in underwater environments and captures detailed images of a ship's hull. As a result, it improves efficiency while reducing the risks associated with human involvement in such tasks.

In more details, high-resolution cameras capture detailed images of the ship's hull, providing valuable visual data for analysis and assessment of biofouling. Fluorescence spectrum sensors are employed to detect the fluorescence emitted by marine organisms on the hull's surface, aiding in the identification and quantification of specific biofouling agents. To ensure precise navigation and orientation, the robots are equipped with accelerometers that measure acceleration and provide information on motion in the underwater environment, and gyroscopes that measure angular velocity and assist in maintaining stability and orientation during underwater operations. To assess the structural integrity of the hull, the robots utilize LVDTs (Linear Variable Differential Transformers), which measure displacement or strain, and pressure sensors to monitor the pressure exerted on the hull, providing insights into its condition and integrity. Additionally, LIDAR (Light Detection and Ranging) technology is employed to generate three-dimensional models of the hull's surface. By utilizing laser beams, LIDAR facilitates accurate mapping and identification of biofouling areas, enhancing the system's ability to detect and address biofouling effectively.

While the integration of specialized sensors provides the necessary hardware for comprehensive inspections and evaluations of biofouling, it is equally essential to develop the appropriate software that will conduct the evaluation process. The software component plays a crucial role in analyzing the data captured by the sensors, employing advanced image analysis techniques and AI algorithms to accurately assess the levels and types of biofouling. By developing robust and intelligent software, the system can extract meaningful insights from the sensor data, enabling informed decision-making and optimizing maintenance strategies for the ship's hull. The synergy between hardware and software is crucial for a successful and effective biofouling evaluation system, ensuring a comprehensive and data-driven approach to hull assessment and maintenance.

Role of Digital Twins, Image Analysis and AI Algorithms in Evaluating Sea Growth

The heart of the system lies in its ability to analyze captured images and evaluate the extent of biofouling on the hull, using image analysis techniques, combined with powerful AI algorithms.

Fluorescence spectrum analysis is an image analysis technique which is used to assess and analyze biofouling on surfaces, particularly in the context of marine environments. It involves detecting and studying the fluorescence emitted by marine organisms present on the surface, providing valuable insights into the composition and extent of biofouling. In practice, fluorescence spectrum analysis is typically conducted using specialized sensors and equipment. The surface of interest is illuminated with specific wavelengths of electromagnetic radiation, known as excitation light. When the biofouling organisms on the surface are excited by this light, they emit fluorescence due to de-excitation of the atoms' electrons from the highest energy levels to the lowest, which is then captured and measured by fluorescence spectrum sensors. These sensors are designed to detect and quantify the emitted light across a range of wavelengths. Different types of marine organisms, such as algae, barnacles, or mollusks, emit distinct fluorescence patterns, allowing for the identification and differentiation of various biofouling species.

This analysis offers several advantages for biofouling assessment.

1. It is a non-intrusive and non-destructive analysis. There is no need for physical sampling or direct contact, and therefore reduces the risk of damage the surface of the hull/propeller.
2. Allows for rapid assessment over large areas.
3. Facilitates real-time monitoring of biofouling growth and enables efficient mapping and identification of biofouling hotspots on surfaces.
4. Aid in understanding the effectiveness of cleaning and antifouling treatments. By comparing fluorescence measurements before and after treatment, it becomes possible to evaluate the impact and efficacy of the applied interventions.

Fluorescence spectrum analysis, combined with the power of AI algorithms, further enhances the capabilities of biofouling assessment. While fluorescence analysis provides valuable data on the composition and extent of biofouling, AI algorithms take this information to the next level by leveraging machine learning techniques.

AI algorithms and machine learning are powerful tools that enable systems to learn from data, recognize patterns, and make intelligent decisions or predictions without explicit programming, driving advancements in various fields. The process of training algorithms involves several key steps. Firstly, a diverse dataset of images/samples representing various instances of sea growth, including a wide range of biofouling types, densities, and conditions, is collected to ensure comprehensive training. Then, each sample should carefully label or annotated with the corresponding biofouling type and level, providing ground truth information for reference during the training process. Then a categorization of the labelled samples is carried out according to their relevant characteristics, such as texture, shape, colour, or any other distinguishing properties that differentiate different types and levels of marine growth, to capture the basic characteristics of the biofouling. Depending on the nature of the data and the classification, appropriate machine learning algorithms (Convolutional Neural Networks (CNNs), Support Vector Machines (SVMs), or other classification algorithms are selected. During the next step of the process, the selected algorithm is trained using the labelled dataset and extracted features, enabling it to recognize patterns and correlations between features and the corresponding biofouling types and levels through iterative optimization techniques that adjust internal parameters to minimize classification errors and improve accuracy. In order to assess the performance of the trained algorithm, separate validation datasets are used, and if it is necessary iterative refinements are conducted, where adjustments (e.g., adjusting hyperparameters, or augmenting the training dataset with additional samples) are made to further improve the algorithm's performance.

Training the algorithms using previous data to recognize and classify different types and levels of sea growth brings significant advantages to the evaluation process. It ensures accuracy by exposing the algorithms to a diverse dataset encompassing various biofouling types and levels, enabling precise identification and classification of biofouling instances. The algorithms learn from patterns and characteristics present in the training data, facilitating accurate assessments in real-world scenarios. Furthermore, the trained algorithms exhibit generalization capabilities, allowing them to apply their learned knowledge to new instances of sea growth, thus making informed evaluations. The adaptability of the algorithms is crucial, as they continuously refine their evaluation process using newly collected data, leading to improved accuracy and performance over time. Additionally, the scalability of the algorithms enables efficient processing and analysis of large-scale datasets, facilitating comprehensive assessments across different hulls and environments. Lastly, as decision support tools, the trained algorithms provide valuable insights for maintenance operations and cleaning strategies, aiding operators in making informed decisions based on the severity and type of biofouling.

Mapping and Pattern Recognition Techniques for Navigation and Identification

Navigation and inspection of the hull's surface in a systematically way requires the utilization of mapping and pattern recognition techniques, which determine the predefined inspection paths and then the underwater robot follows a strategic route, ensuring comprehensive coverage of the hull.

Mapping techniques involve the generation of three-dimensional models of a ship's hull surface. Such models can be provided by the ship's DT. These models can be augmented through the utilization of advanced technologies such as LIDAR (Light Detection and Ranging), which enables the collection of precise measurements and data points. The acquired information allows for the creation of comprehensive and accurate representations of the topography of the ship's hull. Consequently, these models greatly aid in identifying areas affected by biofouling and facilitate targeted inspection and maintenance interventions.

Pattern recognition plays a crucial role in the system as it enables the identification and tracking of key reference points or objects in the underwater environment, thereby facilitating accurate positioning and navigation. These patterns may encompass landmarks, contours, or distinctive features that assist in precise navigation and localization. Consequently, the robotic platform can effectively adhere to predefined paths, systematically cover the hull's surface, and navigate around obstacles or challenging areas. This enables the system to make well-informed decisions concerning navigation adjustments, route optimization, collision avoidance, and adapt its navigation strategies to ensure the safe and efficient exploration of the hull's surface. Furthermore, they significantly contribute to the overall efficiency of the system by reducing the reliance on manual intervention. The automated recognition of patterns for navigation minimizes the necessity for human intervention or constant supervision, enabling continuous and uninterrupted inspection operations.

The combination of mapping and pattern recognition techniques simplify the inspection process by ensuring full coverage of the hull and accurate identification of biofouling hotspots. In addition, they support decision-making as they provide, together with other assessment parameters, information relevant to the assessment of severity, and therefore support the selection of appropriate response actions such as scheduling clean-up operations and applying targeted treatments.

Methods for Collecting and Analyzing Data on Hull Biofouling

In the context of the collection and analysis of data on hull biofouling a comprehensive approach is necessary to ensure accurate assessment and monitoring. This approach includes both data collection methods for bio-fouling assessment and data collection for monitoring robot performance during the inspection process. By combining these datasets, a holistic understanding of the hull's condition and the inspection process can be achieved.

For biofouling assessment, high-resolution cameras capture detailed images of the hull's surface, providing visual data that enables the assessment of biofouling growth and distribution. Fluorescence spectrum sensors detect and measure the fluorescence emitted by marine organisms, aiding in the identification and quantification of specific biofouling agents. These data sets are combined to provide insights into the extent, type, and distribution of biofouling on the hull. In parallel, data collection for monitoring the robot's performance involves sensors such as accelerometers and gyroscopes, which measure motion and orientation. LVDTs and pressure sensors assess the structural integrity of the hull. Three-dimensional mapping using LIDAR technology generates detailed models of the hull's surface, aiding in navigation and monitoring the robot's position.

- Correlation of Image Analysis and Motion Data: By correlating the captured images with the motion data from accelerometers and gyroscopes, it is possible to analyze the biofouling distribution in relation to the robot's movement, and thus providing insights into areas that were effectively covered during the inspection and areas that may require further attention.
- Integration of Biofouling and Structural Integrity Data: Combining the data from fluorescence spectrum sensors, LVDTs, and pressure sensors allows for a holistic assessment of the biofouling impact on the hull's structural integrity. As a result, correlations between biofouling levels and potential structural vulnerabilities can be revealed, assisting in the prioritization of maintenance and cleaning operations.
- Visualization of Biofouling Distribution on 3D Models: The three-dimensional models generated by LIDAR can be overlaid with the biofouling data collected through image analysis. This visualization provides a comprehensive view of the biofouling distribution, highlighting areas of significant growth and concentrated infestation.
- Data-Driven Reporting and Decision Support: By integrating all the collected data sets, including images, fluorescence spectrum measurements, motion data, and structural integrity data, comprehensive reports can be generated. These reports provide accurate information on the biofouling condition, hull integrity, and inspection performance. Data-driven decision support systems can leverage this information to optimize maintenance schedules, prioritize cleaning efforts, and enhance overall hull performance. This aspect will further be analyzed in section 0.

Taking all into consideration, a combination of data from both hull biofouling and robot performance monitoring ensures a holistic approach to understanding the hull's condition and inspection process, enabling enables accurate assessment, proactive maintenance planning, and optimized decision-making for effective biofouling management.

Utilization of Image Analysis and AI Algorithms for Precise Assessment

Utilization of image analysis and AI algorithms gives a precise assessment of hull biofouling. The collected data (specifically the images captured by high-resolution cameras and the fluorescence measurements obtained by spectrum sensors) can be harnessed, enhancing the accuracy and efficiency of the evaluation process. On the one hand, with image segmentation, feature extraction, and classification, the algorithms can distinguish different types and levels of marine organisms and encrustations, providing a more comprehensive understanding of the biofouling state on the hull. In this line, AI algorithms, powered by machine learning, are employed to analyze the collected data from the sensors, enabling a precise assessment by leveraging the algorithms' ability to recognize complex patterns and make informed decisions based on the data. Therefore, a synergistic effect is revealed, meaning that the accurately captured images, along with the precise fluorescence measurements, serve as inputs for the algorithms, which then utilize their learned knowledge to analyze and assess the biofouling state with enhanced accuracy and efficiency.

An example will now be provided, focusing on the assessment of biofouling caused by the macroalga species Ulva lactuca. Sea lettuce, scientifically known as Ulva lactuca (Ulvaceae, Chlorophyta), is a macroalga that is widely distributed in marine and estuarine environments. It is a prevalent species found in coastal benthic communities across the globe, exhibiting its ubiquity in these ecosystems (Cruz de Carvalho et al., 2022). When assessing hull biofouling, high-resolution cameras will capture detailed images of the ship's hull surface, revealing the presence of green patches, while image analysis techniques are used to identify and quantify the extent of Ulva lactuca biofouling. Additionally, fluorescence spectrum sensors will detect and measure the specific fluorescence spectrum emitted by Ulva lactuca, which is 681 nm (Cruz de Carvalho et al., 2022). This will then be analyzed by AI algorithms trained on previous data and will accurately quantify the abundance and distribution of Ulva lactuca. In this way, an accurate assessment of the impact of Ulva lactuca biofouling is achieved, allowing informed decisions to be made regarding appropriate mitigation measures.

Reporting Capability and Benefits of Accurate Information

The reporting capability of the system enables the generation of detailed and accurate reports that provide comprehensive information about the biofouling condition of the ship's hull. The reports are not only data presentations but analyzed data, ensuring an effective reporting.

This can be achieved by employing different kinds of techniques: Written reports present a holistic summary of the biofouling assessment, a detailed analysis of the collected data, results interpretation, and key findings. They can incorporate charts, graphs, and images to enhance the understanding of information. In contrast, visual representations utilize text, images, diagrams etc. to highlight the key findings, trends, and observations from the biofouling assessment. These can be used when a more dynamic and interactive approach is desired. When a more dynamic, user-friendly, and interactive approach is desired, data visualization tools such as infographics or interactive dashboards, can be utilized, allowing relevant stakeholders to gain a deeper understanding of the biofouling assessment. These include interactive charts, maps, and other visual elements, which enable the user to explore data, visualize trends, and extract

Table 2. Benefits of the accurate information compared to traditional methods

Benefits of Accurate Information	Modern Techniques	Traditional Methods
Informed Decision-Making	Enables data-driven decision-making	Relies on subjective observations
Proactive Maintenance Planning	Facilitates proactive planning	Reactive approach to maintenance
Cost Optimization	Optimizes resource allocation	May result in inefficient resource use
Performance Enhancement	Improves vessel efficiency	Potential performance degradation
Compliance with Regulations	Demonstrates adherence to standards	Potential non-compliance issues

insights. Finally, due to the rapid progress of information technology (IT), significant advancements have been made in the reporting capabilities for hull biofouling assessment. Specifically designed online platforms and software applications facilitate efficient and standardized reporting procedures, ensuring consistency and ease of use, by customizing templates, data input functionalities and automated report capabilities.

The choice of the best reporting technique depends on various factors, including the specific needs and preferences of the stakeholders, the nature of the data being reported, and the intended purpose of the report. Each technique has its advantages and considerations. However, in the context of hull biofouling assessment, a combination of techniques may be beneficial to cater to different audiences and enhance the effectiveness of communication.

Regardless of the specific type of reports utilized in hull biofouling assessment, there are numerous benefits associated with accurate information compared to traditional methods as presented in Table 2.

DISCUSSION AND FUTURE OUTLOOK

In this section we discuss the challenges and possible future directions with respect to predictive maintenance, cargo hold cleaning and hull antifouling treatment using digital twins. In all the above discussed applications, digital twins play a pivotal role. As emphasised in several chapters of this book, a digital twin is a faithful digital replica of a ship or a ship subsystem. The digital twin guides and streamlines the above operations by providing accurate and realistic representations of the ships engines (and their operational behavior), 3D models of the cargo holds which lead to more targeted cleaning operations, and also more accurate understanding of the fouling conditions of the hull which leads to more efficient cleaning operations.

However, as all the discussed DT applications are in their infancy there are potential strengths as well as pitfalls that are examined in this section.

Challenges of Predictive Maintenance With the Help of DTs

Predictive maintenance is all about anticipating to failures and taking the necessary preventive actions Overall, the DT supported predictive maintenance approach proposed in this Section shares similar benefits and pitfalls with other data driven maintenance operations that utilise AI/ML techniques. These can be summed up as data availability, coverage and quality.

Data availability is a crucial issue as equipment failures are rather rare phenomena. Thus, it is hard to find datasets that contain failure states as well as normal operating states of components and equipment. Datasets must therefore be collected over large periods of time, potentially over several years. Additionally, datasets can be borrowed from other DTs modelling ships with similar equipment.

In addition, not only data quality but also *model quality* is important. An accurate DT model should precisely reflect the properties of its physical counterpart. For individual subsystems and components such as ship engines, these models can be obtained from the manufacturers and are expected to be of sufficient quality, as manufacturers themselves dedicate substantial resources to develop accurate models (as well as digital twins) of their products. However, the quality of the models must also address subsystem assemblies and their interactions, for instance the faithful modelling of the behaviour of coupled engine, driveshaft and propeller subsystems.

A digital twin requires remodelling with any change in equipment's configuration or element state Any modification affecting equipment performance requires a change to its model and underlying algorithms. Such modifications – at a machine level (replacing original parts with made-to-order ones) or at a factory level (changes to the operational policy) - are not always reflected in factory specifications, thus, cannot be precisely simulated, which escalates the risk of errors. Although deploying a digital twin-based predictive maintenance is time-consuming and labour-intensive, the technology offers the ability to timely recognize disruptions in asset performance, forecast potential problems and simulate various maintenance scenarios. It helps enterprises eliminate machine downtime, reduce equipment maintenance costs, improve equipment reliability and extend its lifespan.

Challenges and Future Outlook of Cargo Hold Cleaning With the Use of Robots and DTs

The second use case presented in this Chapter pertained to the use of digital twins and other automation (such as robots) towards making the operation of cargo hold cleaning more safe, efficient and effective.

This use case argued about the pitfalls of the current cleaning method (mainly manually operated, slow and with safety risks for the operators). Instead, a robotics based operation can speed up the process, improve the quality of cargo hold cleaning and reduce safety risks for the crew.

The use of digital twins, automation and robotics in cargo hold cleaning can potentially improve safety by reducing the need for human entry into enclosed spaces and improving the accuracy and efficiency of cleaning processes. There are still significant risks and limitations that need to be addressed. For instance, a totally autonomous robot operation may not be feasible for every type of cargo hold and cleaning operation, and therefore a semi-automated approach with human participation is required. Also, new or existing sensing technologies need to be added to the cleaning robots in order to detect the cleanliness state of the surface in order to apply the correct type and/or quantity of the cleaning substance.

Therefore, more research is needed to fully understand the potential benefits and risks of the approach, as well as how to enhance the effectiveness of commercial robot based cleaning systems with DTs.

Challenges and Future Outlook of Automated Antifouling Hull Survey and Treatment

One of the three use cases presented in this Chapter is monitoring and measuring the biofouling development in underwater body of the ship using a rapid, automated inspection system for hull biofouling assessment. This cutting-edge system utilizes underwater robotics equipped with image analysis and AI algorithms designed to evaluate sea growth. The results of these assessments allow for a more optimized hull cleaning schedule and improved coating performance. The robot deployed to inspect the sea growth on the hull, makes use of mapping and pattern recognition techniques to guide its navigation along a pre-defined path in order to identify all affected areas. The system includes a reporting capability, providing detailed and accurate data on the state of the hull.

Biofouling assessment results can be used for developing an optimized cleaning schedule. Indeed, a regular scheduling of ship hull maintenance and cleaning plays an important role in maintaining hull performance and mitigating biofouling-related problems. For this reason, the data provided by the biofouling assessment makes it possible to optimize the cleaning program, determining the optimal frequency and schedule for cleaning operations and ensuring preventive and targeted interventions. Specifically, by monitoring and analyzing the rate of development and severity of biofouling, stakeholders can make more effective decisions regarding ship cleaning, minimizing financial burdens, excessive biofouling risks, drag, and energy consumption. This enhances hydrodynamic efficiency and overall boat performance. Additionally, the evaluation results provide valuable information about the effectiveness of different cleaning techniques under specific conditions.

The DT can play several roles in aiding antifouling treatment. One of the most important is the ability to maintain historical data of hydrodynamic performance, correlated with data about the ship voyages (locations, sea temperature, time of the year/season). This allows the identification of relationships between hull fouling parameters and ship voyage profile and allowing for a more effective future antifouling treatment based on the planned and expected voyage schedule.

Therefore, the development of an optimized cleaning program with the aid of DTs can support the execution of cleaning operations at appropriate time intervals, optimizing the use of resources, reducing operating costs, minimizing environmental impact, extending the life of hull coatings, and increasing the ship's performance. These outcomes contribute to sustainable maritime practices and the financial prosperity associated with them. However, further advances are required to sensing and robotic technologies in order to obtain clearly defined benefits over the alternative methods in use.

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Chapter 11
Enhancing a Digital Twin With a Multizone Combustion Model for Pollutant Emissions Estimation and Engine Operational Optimization

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ABSTRACT

Pollutant emissions constitute a critical aspect of vessel operation, impacting both environmental compliance and sustainability goals. However, direct measurement of pollutants is often a complex endeavor. The contemporary maritime landscape further complicates matters with the introduction of diverse fuel variants, rendering emissions prediction an intricate challenge. In this chapter, the author employs a sophisticated multizone combustion model as a powerful tool to estimate engine performance and NOx emissions. This model serves a dual purpose: it enables real-time assessment of emissions based on basic engine operational parameters and functions as a decision support system for forecasting emissions across various fuel types and engine operational schemes. By integrating this implementation into the digital twin framework, the author augments it with invaluable insights. These insights, in turn, facilitate the reduction of carbon emissions while ensuring compliance with stringent NOx regulations.

INTRODUCTION

The maritime sector's contribution to anthropogenic emissions of greenhouse gases (GHG) and especially NO_x and SO_x is high and remains a challenge compared to other sectors in terms of control and abatement methodologies. The contribution of vessel emissions to GHG global emissions was estimated at 2.89% in 2018 and is expected to increase towards 2050 unless mitigative measures are implemented

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(IMO., 2020). The level of CO_2 emissions, the primary GHG emitted from marine vessels, is directly proportional to fuel consumption and its carbon content. Similarly, SO_x emissions are dependent on the fuel amount consumed and sulphur content. The maritime sector used to account for 5-8% of total SO_x emissions globally (Grigoriadis et al., 2021). In the last years SO_x emissions are confirmed to have declined considerably, more than 82% (Zetterdahl et al., 2016). This was the result of the update of IMO regulations mandating the transition to low sulphur content fuels or use of scrubber systems for exhaust gas cleaning (IMO, 2016). NO_x emitted by marine vessels comprise about 15% global anthropogenic emissions, with high impact near coastal areas as confirmed for the European region (Fridell,, 2019; Viana et al., 2014). Among marine engines NO_x emissions are higher for the large slow speed 2-stroke ones (Grigoriadis et al., 2021), that are used for propulsion in the majority of commercial cargo vessels and comprise the greater proportion of installed power in the industry (De Lauretis et al., 2019). Currently NO_x emissions are regulated under the mandates of MARPOL ANNEX VI (International Maritime Organization, 2020) that includes three categories of NO_x emission limits, Tier-I to Tier-III, depending on vessel and engine, age.

In the process of monitoring and optimizing a vessel's operation, pollutant emissions constitute a critical aspect considering current regulations and the marine industry's state. Planning, optimizing or replicating in parallel the vessel schedule via the use of a digital twin can provide detailed information for engine loading profile, vessel speed and fuel consumption based on the ship specific data integrated into the digital twin model and, when available, past operation data. The application of advanced routing optimization allows minimization of vessel idling time and reduction of total fuel consumption (Fagerholt et al., 2017; Moradi et al., 2022). Apart from the financial benefit, minimization of fuel consumption per voyage provides immediate improvement of the vessel's environmental impact, as CO_2 and SO_x emissions are proportional to fuel consumption and its carbon and sulphur content respectively (Miller et al., 2012), unless abatement devices or techniques are used for the case of SO_x. The matter of NO_x emissions is more complex due to them being a result of the combustion process characteristics. While NO_x formation is affected by the amount of fuel consumption and its nitrogen content, this accounts only for a minor NO_x formation mechanism, and several factors are involved that supersede the previous in importance regarding final tailpipe emissions. There is wealth of publications regarding NO_x formation mechanisms in diesel engines and the capability of accurate predictions using various methodologies (Grigoriadis et al., 2021; Provataris et al., 2017). When considering NO_x emissions control and their possible reduction via voyage planning, the impact of engine efficiency should be also considered, which affects total fuel consumption and CO_2 and SO_x emissions. There are multiple methodologies for estimating pollutant emissions during a vessel's voyage and they can be utilized within the framework of a vessel's digital twin application that will handle the vessel scheduling and engine operating profile modelling.

Before delving into the specifics of NO_x emissions modelling and predictive methods a short description of their primary formation mechanisms and effect of engine operation and tuning on them is provided. Through this the main challenges and requirements of NO_x estimation can be better understood, as the multiple parameters, from engine design itself to fuel type used, governing NO_x formation are detailed.

NO_x EMISSIONS FORMATION

Fundamentals of NO_x Formation

NO_x formation in CI engines is classified in three categories, thermal NO as the main source, fuel NO_x and prompt NO_x. Fuel and prompt NO_x contribution to total emissions is rather limited, as the former results from the nitrogen content of the fuel and the latter is caused by attack on air content nitrogen from hydrocarbon radicals. The most significant formation mechanism is thermal NO, driven by the breakdown of atmospheric nitrogen due to high temperatures (Taylor, & Costall, 2017). As the name implies, thermal NO formation is highly dependent on temperature, rising exponentially above 1100°C. NO formation is kinetically controlled and driven mainly by O_2 availability and temperature level. The formation of thermal NO is described by the Zeldovich mechanism that proposes two main reaction paths for their formation:

$$O+N_2 \leftrightarrow NO+N \tag{2.1}$$

$$N+O_2 \leftrightarrow NO+O \tag{2.2}$$

The first reaction takes place when O_2 molecules are dissociated to atoms under very high temperatures. The O atoms react with N_2 molecules forming NO and N. The resulting N reacts with nearby O_2, and NO and O are formed. The overall process is mainly controlled by the first reaction's rate, as the second reaction is much faster and occurs immediately after the first reaction. In cases of low oxygen availability and fuel rich conditions the second reaction weakens, and a third reaction is included in the mechanism.

$$N+OH \leftrightarrow NO+H \tag{2.3}$$

The three reactions are known as the extended Zeldovich mechanism (Zeldovich, 1946). As mentioned, this process initiates at approximately 1100°C and is commonly maximized in the region of 1900 – 2000°C. Since this is the common temperature range for combustion processes thermal NO are the main source and most measures employed by manufacturers to limit emissions are focused in reducing the above reaction rates either by lowering the combustion chamber temperature or significantly lowering oxygen availability to control the first reaction's rate. It is noted that for diesel engines, when referring to NO_x, the primary pollutant is NO and NO_2 are a minimal percentage of the total emissions.

Fuel NO_x is formed by the oxidation of fuel nitric contents. As such the fuel's N content is rather proportional to the amount of NO_x formed. The general reaction for their formation is:

$$R_xN+O_2 \leftrightarrow NO, NO_2, CO_2, H_2O \tag{2.4}$$

The complete mechanism has not been defined, but it is based on two primary formation pathways. In the first during the initial stage of combustion, volatile nitrogen species are oxidized. The second pathway is the result of nitrogen combustion from the char portion produced, however it is a considerably slower reaction than the former pathway. Due to the reduction of most NO_x formed via the second pathway to N by the formed char, the fuel NO_x finally emitted are mostly attributed to the first pathway i.e., the oxidation of volatiles.

In-Engine Conditions Affecting NO_x Formation

The main factors affecting NO_x formation in the combustion chamber are peak temperature values reached and temperature distribution history. The availability of oxygen in these regions is also of major importance, as it can enhance or inhibit the dissociation phenomena that allow NO_x formation. Considering these factors, engine type and tuning have considerable effect on NO_x formation and emissions. It is noted again, that when referring to NO_x for these engines the primary species in the thermal NO, as the percentage of NO_2 is almost negligible. Thus, from here-on the two values NO_x and NO should be considered equivalent. In addition, multiple operating variables that can affect the previous to a considerable degree must be considered when conducting an in-depth analysis. A characteristic example of engine type effect is the difference of NO_x emissions between slow speed main propulsion 2-stroke engines and medium speed 4-stroke auxiliary generators. For the former, high surplus of air due to the scavenging process, combined with longer presence of combustion gases in the cylinder (due to the slow speed) promote the pollutant's formation (Celo et al., 2015). Beyond the engine type difference, variations can be found between different engine models and even in engines of the same family due to tuning variations. A known major parameter that affects NO_x emissions is the maximum in-cylinder pressure due to combustion (P_{max}) (Weigand et al., 2011) as it usually leads to increase of the maximum temperature values. P_{max} is mainly influenced by the start of fuel injection (SOI) and start of ignition (SOC) angles. The used fuel's calorific content (LCV) also affects pressure rise during combustion (ΔP) as it increases combustion intensity. Usually, early SOI i.e., before the top dead center (TDC) will result in higher P_{max} and increased NO_x emission levels. Fuel injection, and ignition, after TDC means that combustion initiates during the initiation of the expansion phase, so the peak pressure and temperature reached tend to be lower. The SOC angle is also affected by the fuel type, specifically its combustibility usually expressed by its cetane number (CN). Review of multiple studies shows that ignition delay has variable effect on NO_x formation (Suryawanshi, & Deshpande,, 2005; Weigand et al., 2011) and cases of early SOC may not always lead to high NO_x emissions, and same may apply to the effect on P_{max}. Very low ignition delay inhibits the fuel – air mixing process. This results in lower rate and intensity of premixed combustion and lower peak pressure and temperature in the cylinder. The opposite, long ignition delay, can result in very intense premixed combustion and multiple hot spots in-cylinder, that increase NO_x formation considerably and also cause high pressure rise due to combustion. The previous effect will also be affected by the fuel's LCV that can affect the intensity of the combustion process and NO_x formation, as demonstrated in the study on biofuels of Wei et al. (2018), which present considerable calorific content variation depending on their sourcing and production method. However, considering the previous, NO_x formation is promoted from all parameters resulting to local temperature increase and O_2 availability.

As engine tuning is of vital importance to NO_x formation there is a series of internal measures employed by manufacturers to achieve compliance with regulatory limits. These can be found in Tier-I and Tier-II engines, and they remain is use in tandem with other NO_x abatement technologies for the state-of-the-art Tier-III engines (American Burau of Shipping (ABS), 2020; Muzio & Quartucy, 1997). NO_x emission reduction using engine tuning is a process of compromise between fuel efficiency and regulation limits. The most common methods are retarded fuel injection timing, advanced fuel injection technologies (split injection, rate shaping, etc.) and variable effective compression ratio using variable valve timing (inlet

Table 1. Measures for optimising diesel engine combustion and their effects on emissions and consumption (Helmut, 2010)

Measure	NOx	HC/CO	Soot	bsfc	Noise
Retarded start of injection	+	–	–	–	+
Exhaust gas recirculation	+	–	–	–	+
Cooled EGR	+	–	+	+	0
Supercharging	–	+	+	+	0
Intercooling	+	–	+	+	0
Pilot injection	0	+	–	0	+
Added post-injection	+	0	+	–	0
Injection pressure increase	0	+	+	+	0
Lower compression ratio	+	–	+	0	–

Symbols: +: reduction; –: increase; 0: no change

for 2-stroke and exhaust for 4-stroke engines). The use of these techniques has resulted in the reduction of the bsfc penalty because of retarded injection timing. . The use of sophisticated tuning, especially in the last decade, following the advances in engine control capabilities via electronic systems, results to variations between even engines of the same model that affect both brake specific fuel consumption (bsfc) and emissions trends with engine load. This was verified in multiple studies both by individual researchers and organizations (De Lauretis et al., 2019; Grigoriadis et al., 2021). In these works, following extensive data collection, high deviations between bsfc and NO_x emissions were detected between older and newer type marine engines that were attributed to tuning choices for NO_x emissions control.

However, for NO_x control there exists a number of technologies that have been employed in CI engines some of which are currently applied to 2-stroke marine engines. In Table 2-1 a summary of the measures used generally in the most common diesel engines to control most common pollutant emissions is provided along with the methods' advantages and disadvantages.

One of the main measures applied is the adjustment of injection timing. Retarded start of injection will lead to lower NO_x emissions, but also possibly increase soot formation (Helmut, 2010) and bsfc. The goal of retarded injection is to limit the peak pressure and thus in-cylinder temperature. This occurs because fuel injection takes place closer to expansion, which lowers the pressure. Injection retard reduces peak temperature, however the fuel and air mixing are negatively affected which leads to higher soot and particulate formation (Helmut, 2010). The decreased oxidation of soot due to the lower temperatures further increases the soot emissions. For advanced injection timing, combustion initiates the pressure rise when the piston is still moving upwards, thus pressure also increases due to compression. The higher pressure results in higher peak temperature values, that drives NO_x formation.

The adverse effects of retarded injection timing, as mentioned above, can be partially compensated using advanced injection technologies. A common technique is the reduction of injection duration. Increasing injection pressure enhances fuel mass flow rate, shortening injection duration. This allows for better mixing of fuel and air so the number and range of fuel rich mixture regions is decreased, leading to lower soot formation. However, the shorter injection duration leads to faster combustion, placing the combustion around Top Dead Centre (TDC), increasing thus peak temperature. The effect of injection

Figure 1. Effect of injection timing in NOx, soot and peak pressure (Helmut, 2010)

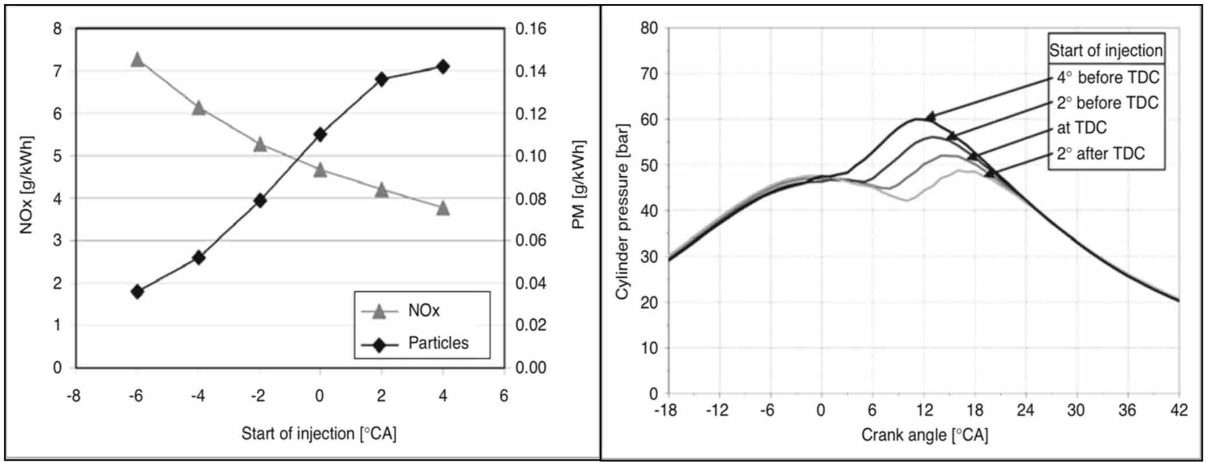
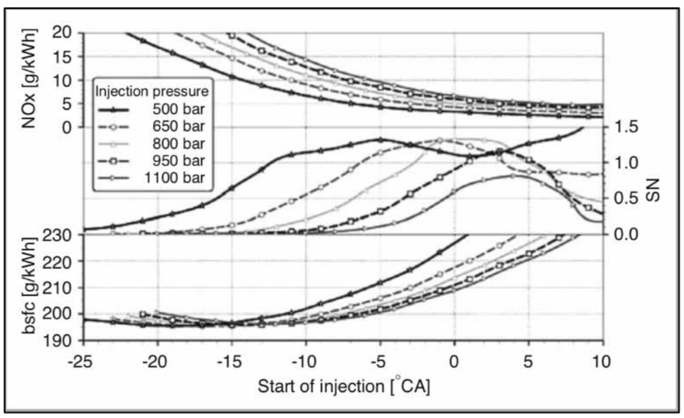


Figure 2. Effect of injection pressure relative to injection timing on soot and NOx formation (Helmut, 2010)



timing is presented in Figure 1 while the effect of injection pressure is presented in Figure 2 received from Helmut (2010) for a heavy duty diesel engine, as part of the above description. But the combination of reduced injection duration and retarded injection timing can finally result in NO_x reduction at an acceptable fuel penalty.

Other factors related to in-cylinder phenomena and operating parameters can also influence the final value of NO_x emissions, such as the effect of heat transfer, blowby, turbulence and fuel-air mixing that depend on detailed engine geometrical and operational data that are rarely available.

NOx Estimation and Modelling Applications in Maritime

Multiple approaches exist regarding the estimation of NO_x and other emissions from diesel engines. These involve various types of engines and combustion modelling for specific engine configurations or statistical approaches that provide information categorized by engine type.

Use of Standardized Emission Factors

The statistical approach can be found in the form of reference emissions factors, that rely on generating curves linking primary, and preferably readily available, engine operational parameters, such as power or fuel consumption to NO_x emissions (Duan et al., 2022). Normally the engine operating data are based on large databases of previous vessel voyages. The employment of a vessel digital twin model can provide state-of-the-art projections for engine power patterns and sailing speed (Kaklis et al., 2023) to be used in conjunction with emission factors. The use of standard emissions factors and engine power profiles is a typical approach adopted by both researchers and organizations (De Lauretis et al., 2019) and is a valuable tool for use in studies that consider a large number of vessels. For individual studies focused on single or low number of vessels considerable variations may be found due to specific engine characteristics, sailing patterns and type of fuel used, as can be verified by the results of various studies such as Duan et al. (2022), Grigoriadis et al. (2021), Huang et al. (2018). The error potential can be lessened by collection of data from similar type engines, however this is challenging for marine vessels, as on-board measurement procedures will be required for NO_x emissions. These measurements require considerable planning and also expertise to comply with the MARPOL ANNEX VI requirements (International Maritime Organization, 2020). This is further complicated by the increasing consideration of alternative fuels for use in marine engines, such as biofuels, that are recently attracting interest for use in marine engines as a drop-in fuel (IMO, 2023). The use of fuels with different physical and chemical properties can affect engine performance and combustion characteristics leading to variations in emissions of various species. Various testing campaigns involving on-board emissions measurements have been conducted in the last three years to examine and quantify the changes expected by widespread biofuel use in marine engines of commercial vessels, equipped with 2-stroke and 4-stroke engines. Based on the findings of regulatory body studies, such as Lloyd's Register (2022), and other studies by shipping companies and individual researchers (Chountalas, et al., 2023; Chountalas et al., 2023) the end effect of biofuel use on NO_x emissions can vary considerably between different engine models, despite belonging to the same category and is some cases engines that could be considered identical based on their design. Valuable information on the mechanisms affecting the previous is given in extensive reviews of past research projects on use of multiple fuels on diesel engines and their effect on emissions, such as Varatharajan and Cheralathan (2012). The studies included in the review conclude that the end effect of biofuels use on emissions cannot be predetermined due to several mechanisms influencing formation. This is also the conclusion of Mueller et al. (2009), in which the decisive factor is how close to stoichiometric the air–gas mixture is at ignition and in the standing premixed autoignition zone near the flame lift-off length. The combination of multiple factors affecting the final NO_x emissions is also mentioned in the works of Hoekman and Robbins (2012) and Sun et al. (2010). To satisfy the current and future requirements of a robust emissions prediction implementation, when examining capabilities of emission prediction and optimization of vessel voyage schedule a detailed source of emission data will be required. It is noted however, that for large fleet applications and studies on the level of country-wide fleets, the use of emissions factors is a quite viable approach, mainly due to data availability issues and other factors, as application of detailed models on a case-by-case basis will most probably not be feasible.

Finally, it has to be recognized that the use of emission factors alone cannot account for the effect of engine condition and settings on NO_x formation and emissions. The reason is that the effect of settings on NO_x emissions is considerable compared to the one on bsfc and thus fuel consumption.

Use of Detailed Engine Combustion Models

There are multiple engine models available, for commercial applications and academic use, that are used to predict exhaust emissions of diesel engines of various configurations. For the specific application the use of phenomenological models is the only option due to computational and time constraints. One of the more common configurations that has proven reliable for NO_x emissions predictions is the phenomenological multi-zone model (Abbe et al., 2015; Benajes et al., 2015; Hiroyasu,, 1985; Hountalas, et al., 2004; Jung, & Assanis,, 2001). Models of this type take into account the local mechanisms that drive mixture formation and combustion and can provide estimates of good accuracy, after a calibration procedure, to take into account the particulars of each application. The calibration requirement stems from the use of semi-empirical relations for various factors, that cannot be measured or be known with adequate accuracy, such as fuel spray penetration, air fuel mixing and various aspects of the combustion process. But an adequate calibration can be achieved using parameters that can be measured and are affected by these mechanisms. The same applies to most types of models attempting to describe complex physical processes. The phenomenological models used are divided into categories based on their complexity and calculation time demands, defined mostly by the number of zones employed for the simulation, with the simplest application being single-zone models. Due to their simplicity such models can be easily used as they have low computational power and time demands (Awad et al., 2013; Yasar et al., 2008). They are, however, not suitable for NO_x emissions calculations, due to only generating information for mean in-cylinder conditions. Considering the sensitivity of NO formation in terms of temperature and its distribution in the cylinder defined by the flame front, computational methodologies that do not account for localized phenomena cannot provide reliable predictions, especially for parametric analyses. Estimation of NO formation requires the utilization of at least zero-dimensional two-zone models or more detailed multi-zone ones (Provataris et al., 2017) or alternatively fully statistical models, semi-empirical models (based on combustion parameters such as the point of 50% fuel burnt) or results by the more recent neural network based ones, such as Oliveira et al. (2011). For applications that target marine engine modelling, semi-empirical methods are more commonly used due to the reliance of statistical and neural network models to comprehensive databases of emissions, that cannot be easily constructed by on-board measurements, as mentioned above, while real-time emissions monitoring installation on-board vessels are also a challenging implementation.

The most detailed approach to engine and combustion modelling is the use of computational fluid dynamics (CFD) simulations that can produce descriptions of the in-cylinder phenomena at a fundamental level (Reitz & Rutland, 1995). Their ability to calculate temperature distribution and chemical compositions in-cylinder with very high definition has been well proven (Jia et al., 2011; Mobasheri et al., 2012; Reitz & Rutland, 1995). This level of information can be utilized to generate detailed and accurate estimates of NO_x emissions on a case-by-case basis and achieve high sensitivity of the emission estimates to engine configurations and the particulars of each application. The main downside is the inability to employ these models for real-time applications, due to their high complexity. In addition, their highly complex structure adds high calibration requirements, similar to the problem with utilizing complex statistical methods in this particular application. Utilizing the results of statistical driven methods, such as AI, to improve CFD calculations speed or replace them outright, is an ongoing effort in other fields (Calzolari & Liu, 2021; Rościszewski et al., 2023), but is similarly hindered by the low data availability constraint. But even if this was possible, such models cannot be used for on-board applications.

The application examined in the next chapter is the use of a 2-dimensional multizone model to predict NO emissions of large slow speed 2-stroke marine engines with adequate accuracy for most applications, low calibration demands and low computational power requirements. This model can account for variations of performance parameters and fuel type. This allows for the emission values predicted to be customized to the tuning and state of the engine used in the vessel modelled by a digital twin. Following the description of the model, an example of the model's predictive capability for NO emissions during biofuel use on a marine 2-stroke engine is provided to demonstrate its capabilities in modern applications.

PHENOMENOLOGICAL MULTIZONE MODEL APPROACH-DESCRIPTION

The model described in this section can account for various engine operating parameters including variable injection timing variable valve timing, exhaust valve opening and closing angles featured in the electronically controlled implementations of modern engine types. Due to this capability the tuning of these engines can deviate even between same model engines. The use of automatic cylinder pressure control can also often lead to changes in engine operation resulting from environmental factors, fuel properties and other operational parameters. Unlike the past applications aimed at engines with mechanical control, incorporating tools to account for the aforementioned variations is important for studies that include the lifetime of a vessel as are the digital twins. The previous should also be taken into account not only for the emissions model but also for the digital twin modules that are used for condition monitoring such as Jiang, et al. (2022).

The model also utilizes fuel properties, specifically: density, LCV and chemical composition, including oxygen content. The use of LCV and oxygen content is of special importance when considering the use of the model for applications with biofuels. Last, the model is also able to accommodate other modern features of state of the art electronic 2-stroke marine engines, namely use of a cylinder bypass valve (CBV) and exhaust bypass valve (EGB). Their use affects the air mass trapped in the cylinder, and requires additional calculations compared to engines with conventional inlet and outlet systems. The use of the CBV and EGB alters performance and also NO formation levels, as it affects the air-fuel equivalence ratio. Furthermore, the specific model can also be modified for the use of EGR as a NO_x control technique and for its effect on engine performance. Below is provided a description of the model focusing on the main mechanism description.

Zone Formation Description

In the model, the fuel jet is divided into individual volumes or zones with different properties. The cylinder volume is treated separately and is attributed a uniform pressure value in each time step of the simulation, (215). The main approach of the model is the calculation of the conditions in each zone, by applying mass and momentum conservation equations and use of the first thermodynamic law to form a differential equation which provides the uniform in-cylinder pressure. Following the estimation of the mean cylinder pressure, the first thermodynamic law is employed for each zone to calculate the local temperature. The principle detailed below has been found to perform well in other studies using engine modelling, such as Kouremenos et al. (1997).

The consideration of zones is done to acquire a more realistic representation of the actual air-fuel mixing mechanism and the distribution of the investigated parameters inside the fuel jet. This is especially important for the prediction of NO which depends on temperature and species, mainly O_2, distribution. A single zone model cannot predict NO, as mentioned in the previous section, while a two zone model can offer NO predictions, but is limited regarding capability to predict the effect of load, speed and other parameters. The multizone approach offers enhanced prediction capability, important for practical applications.

It is common practice in phenomenological modelling to consider only one fuel jet and assume all others to be the same. The total number of fuel jets is thus equal to: N_{holes} x $N_{injectors}$. The number of zones in the circumferential direction was selected after a sensitivity analysis from the point where NO and performance predictions were stabilized. No zone mixing or jet interaction is considered. This is the suggested approach in phenomenological modelling, and also other more resource intensive modelling applications, as it is accounted for by the use of correction factors that are determined during the initial calibration procedure using reference (shop test) data.

Heat Transfer Model

For the heat transfer mechanism, a turbulent kinetic energy viscous dissipation rate $k\sim\varepsilon_t$ model is used to determine the characteristic velocity of heat transfer calculations (Hountalas et al., 2012). The mean flow kinetic energy E_m is supplied to the cylinder chamber during the gas exchange process. The kinetic energy is partially converted to turbulent kinetic energy k through a dissipation process at the rate of P_{tk} and finally to heat through viscous dissipation at a rate of $m\varepsilon_t$. The system of two differential equations for E_m and k can be written as:

$$\frac{dE_m}{dt} = \frac{1}{2}\frac{dm}{dt}u_{inl}^2 - P_{tk} - \frac{E_m}{m}\frac{dm}{dt} \tag{3.1}$$

$$\frac{dk}{dt} = P_{tk} - m\varepsilon_t - \frac{k}{m}\frac{dm}{dt} \tag{3.2}$$

with $E_m = \frac{1}{2}m\bar{u}^2$ and $k = \frac{3}{2}mu'^2$ for isotropic turbulence, and dm/dt the net mass flow rate into the combustion/cylinder chamber.

The turbulent kinetic energy production rate and the viscous dissipation rate ε_t are calculated from the known relations:

$$\varepsilon_t = \left(\frac{k}{1.5m}\right)^{1.5}\frac{1}{l_{car}}, P_{tk} = 0.09\mu_t\frac{\bar{u}^2}{l_{car}^2} \tag{3.3}$$

with l_{car} being the characteristic length equal to the combustion chamber height at each time step, or the cylinder radius depending on the piston position and μ_t the gas turbulent viscosity that is calculated using:

$$\mu_t = \rho l_{car} \left(\frac{k}{m} \right)^{0.5} \tag{3.4}$$

The heat transfer calculations additionally require the characteristic velocity calculated by:

$$u_{car} = \left(\bar{u}^2 + u'^2 \right)^{0.5} \tag{3.5}$$

The Nusselt number is calculated to be used for estimating the heat transfer coefficient:

$$Nu = cRe^{0.8} Pr^{0.33} \tag{3.6}$$

The heat transfer coefficient is calculated by eq. (3.7) and the instantaneous heat rate by eq. (3.8).

$$h_c = cRe^{0.8} Pr^{0.33} \frac{\lambda}{l_{car}} \tag{3.7}$$

$$\dot{Q} = A\left[h_c \left(T_g - T_w \right) + \sigma_r c_r \left(T_g^4 - T_w^4 \right) \right] \tag{3.8}$$

The above relation for heat transfer has been tested with very good results for this type of engine. Equation 3.8 contains two unknown parameters, the mean wall temperature T_w and the c constant of the previous eq. 3.7. During its application in the multi-zone model the T_w cannot be used for zones not in contact with the cylinder walls surface. To circumvent this difficulty the first part of eq. 3.8, referring to convective transfer phenomena, is calculated using the bulk average temperature of the jet, provided by:

$$T_g = \frac{\sum_{i=1}^{n_z} m_i c_{vi} T_i}{\sum_{i=1}^{n_z} m_i c_{vi}} \tag{3.9}$$

Then the heat exchange rate calculated in eq. 3.8 is distributed among the jet zones on using the individual zone mass, temperature and heat capacity as distribution basis:

$$d\dot{Q}_{i,d} = \frac{\dot{Q}\left(m_i c_{vi} T_i \right)}{\sum_{i=1}^{n_z} m_i c_{vi} T_i} \tag{3.10}$$

Regarding the radiative component of eq. 3.8, zone surface area is used so no further calculations are required and is used as described above.

Cylinder Blowby

Blow-by rate affects the compression pressure diagram. A detailed blowby model is embedded in the present simulation considering for the rings motion in their grooves. For the specific application, the blow-by rate can be modelled using a simplified approach assuming an equivalent blow-by area between the cylinder rings and the cylinder liner. The blow-by mass flow rate is calculated using the isentropic compressible flow assumption as follows.

$$\frac{dm}{dt} = C_d A \frac{P_u}{R_u T_u} \sqrt{\frac{2\gamma R_u T_u}{\gamma - 1} \left[\left(\frac{P_d}{P_u} \right)^{\frac{2}{\gamma}} - \left(\frac{P_d}{P_u} \right)^{\frac{\gamma+1}{\gamma}} \right]} \quad \text{for} \quad \frac{P_d}{P_u} \geq \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma - 1}} \tag{3.11a}$$

$$\frac{dm}{dt} = C_d A \frac{P_u}{R_u T_u} \sqrt{\frac{2\gamma R_u T_u}{\gamma - 1} \left[\left(\frac{P_d}{P_u} \right)^{\frac{2}{\gamma}} - \left(\frac{P_d}{P_u} \right)^{\frac{\gamma+1}{\gamma}} \right]} \quad \text{for} \quad \frac{P_d}{P_u} \leq \left(\frac{2}{\gamma + 1} \right)^{\frac{\gamma}{\gamma - 1}} \tag{3.11b}$$

where dm/dt is the blow-by mass flow rate, P is the pressure, T the temperature, γ is the ratio of the specific heat capacities under constant pressure and volume and C_d the discharge coefficient (index "u" denotes upstream of the flow and index "d" downstream).

The equivalent blow-by area A_{eq} is equal to:

$$A_{eq} = \pi D \delta r \tag{3.12}$$

where δr is referred to as the "equivalent" cylinder-ring clearance. This is considered as one of the model constants and its value should remain fairly the same with operating conditions. The equivalent blow-by area accounts also for the mass loss rate through the engine valves because no distinction is made, in the present analysis, between this mechanism and blow-by.

Air Swirl

Air swirl is required to achieve a high rate of air and injected fuel mixing in the cylinder. In the case of 2-stroke large scale marine engines the swirl motion of the cylinder charge is produced during the scavenging stroke as a result of the inlet port geometry. The effect of swirl on fuel mixing is lower for newer engines due to the advanced injection strategies used. Further to the promotion of fuel and air mixing the swirling motion of entry air assists the scavenging process and gas exchange improving efficiency of this stage of the engine cycles. The previous effect was researched and described in detail in Ramos (1989) and Willis et al. (1967). The swirling motion of the air is modelled assuming a hybrid scheme consisting of a solid body core surrounded by a potential flow region (Dent & Derham, 2006; Heywood, 2018). In this approach the air viscosity is taken into account, as it creates a boundary layer near the cylinder walls. This requires the use of tangential velocity profile for calculations, such as the one proposed by Heywood (2018):

$$u= W_p R \text{ for } 0 \leq R \leq R_c \tag{3.13}$$

$$u= W_p R_c (R_c/R)^{0.05} \text{ for } R_c \leq R \leq R_p$$

where R_c is the point to which the solid body rotation ends, given be the following empirical expression:

$$R_c= R_{in}(D_b/2R_p) \tag{3.14}$$

with R_p the cylinder radius, D_b the piston bowl diameter (for 2-stroke engine designs with no bowl D_b=D) and R_{in} the cylinder-valve axis distance. For the 2-stroke engine since air flows through the inlet ports Rin is equal to the cylinder radius, Rin=D/2.

The swirl ratio in the present case is considered to be an input and from the aforementioned modeling its variation during the engine cycle is determined. The calculation of swirl is based on the conservation of the flows angular momentum applied to the cylinder during the intake stroke. During the induction stroke angular momentum is continuously added to the cylinder, with a part of it lost due to friction and the remaining forming the flow field. The equation for angular momentum conservation is:

$$\frac{d(IW)}{dt} = I\frac{dW}{dt} + W\frac{dI}{dt} = -T_r \tag{3.15}$$

In eq. 3.15 W is the angular air velocity, I the moment of inertia of the mass trapped in the cylinder and T_r is the torque force acting on the flow field. T_r is equal to the force due to friction on the cylinder walls, piston crown and cylinder head. By integration of eq. 3.15 the instantaneous angular velocity of the cylinder charge is calculated.

Spray Model

The spray model used has been previously utilized in Amsden et al. (1985) and Nishida and Hiroyasu (1989). The main assumptions of this model are detailed presently. Empirical correlations are used to estimate the fuel jet angle and zone penetration in the cylinder. These correlations provide the velocity along the spray axis and its radial component (Amsden et al., 1985; Ramos, 1989). The air swirl effect is also considered by applying the approach of Amsden et al. (1985). Using the previous and the equations for mass and momentum conservation the position of each zone in the cylinder is estimated for each time step. The analytical model description is presented below.

Following injection, the fuel starts to penetrate into the combustion chamber and the individual zones of the model start to form. The initial conditions at injector nozzle exit are derived from the injection rate which can either be derived from a fuel injection system simulation model or can be predefined as input to the simulation. There are multiple approaches to model the initial behavior of the fuel spray before substantial breakup into droplets (Baumgarten Carsten, 2006) with a relatively simple but efficient approach The breakup length is calculated using the well tested test approach of Heywood (2018) and Ramos (1989):

$$L = u_{inj} t_{break} \cong c_1 \left(\frac{\rho_l}{\rho_a} \right)^{0.5} d_{inj} \tag{3.16}$$

with c_1 a constant and ρ_a and ρ_l the density of air and fuel respectively.

The distribution of spray velocity along its axis is calculated using correlations for spray penetration (Dent & Derham, 2006; Williams, 1973) with the following equations used in reference to time of penetration.

$$u = u_{inj} = c_d \left(\frac{2\Delta P}{\rho_l} \right)^{0.5} \text{for } x < L \tag{3.17}$$

$$u = u_{inj} \left(\frac{L}{x} \right)^n \text{for } x \geq L$$

with c_d above a constant. According to theoretical and experimental data the spray zones located at the fuel jet periphery will have lower axial penetration. To simulate this the following radial distribution of exponent n of eq. 3.16 is assumed:

$$n_i = n_{min} \exp\left[\log^{-1} \left(\frac{n_{max}}{n_{min}} \right) \left(\frac{r_i}{r_o} \right)^2 \right] \tag{3.18}$$

where n_i is the local zone exponent, r_i is its position relative to the axis and n_{min}, n_{max} are the minimum and maximum values for the exponent distribution. From a sensitivity analysis and considering the result from application of various engine designs the values are used are 0.7 and 1.0 respectively. For each time step the initial value of the radial velocity for all zones formed is given by:

$$u_{ri} = u_{inj} \tan\left(\frac{a}{r_o} r_i \right) \tag{3.19}$$

with r_o the nozzle hole radius and r_i the radial distance of each zone from the centerline. The angle "a" of the jet is estimated using the widely tested relation:

$$a = 0.05\left(\frac{d_{inj}^{2}\rho_{a}\Delta P}{\mu_{a}^{2}}\right)^{0.25} \tag{3.20}$$

To estimate the effect of the cylinder charge swirl on the fuel jet the local components of air velocity in the radial and axial directions are calculated using the conservation of momentum equations in both axes. The air swirl results to deflection of the zones from their original direction, which promotes air entrainment in the zones. Application of the momentum conservation equations shows that axial penetration of the jet decreases and this leads to increased air entrainment rate in the jet zone. The deflection of each zone is calculated using the local air velocity:

$$u_{ixt} = u_{ix} + u_{a}\sin(\varphi_{i}) \tag{3.21}$$

$$u_{irt} = u_{ir} - u_{a}\cos(\varphi_{i})$$

In the above equation, u_a is the local swirl velocity and φ_i the angular position of the zone inside the cylinder.

Wall Impingement

For wall impingement the most suitable approach is to assume that following impingement the zones follow a path parallel to the cylinder walls, even though such an approach would be non-realistic and is unlikely to provide a proper representation of the jet geometry. The wall jet theory of Glauert (1956) is used to estimate a zone's velocity after it reaches the combustion chamber walls.

$$w_{i} = w_{oi}\left(\frac{r_{oi}}{r_{i}}\right) \tag{3.22}$$

In the above eq. 3.22, r_{oi} is the initial radial position of the zone relative to the jet axis after impingement and w_{oi} its initial velocity. The zone is assumed to follow a path adjacent to the wall and its radial distance δ is used to define the thickness of the wall jet (Glauert, 1956; Kouremenos et al., 1997).

$$\delta_{i} = \delta_{oi}\left(\frac{r_{i}}{r_{oi}}\right) \tag{3.23}$$

where δ_{oi} is the initial distance of the zone from the wall following deflection. Before the zones collide with the combustion chamber walls, their velocity is divided into the normal one and one parallel to the cylinder walls. At impingement the parallel velocity component is deflected in total, while the normal component is assumed to be divided in two segments, left and right (Kouremenos et al., 1997). The portion of the zone with a velocity vector opposite to the parallel component will now be treated as a new zone created by the impingement. Its initial values for velocity and thickness are determined by applying conservation equations for mass and energy and accounting for the local jet geometry (Kouremenos et al., 1997).

Zone Air Entrainment

The most important parameter for multi-zone modeling is air entrainment into the fuel jet. This can be estimated either form the volume change of each zone through time or from momentum conservation. The typical approach for phenomenological multi-zone modeling is to use the momentum approach. But the volume change approach allows to circumvent the issues in accuracy that can be caused by the initial momentum loses due to friction that cannot be easily replicated directly in a model of this type. Furthermore, after a detailed analysis conducted, comparison of simulation results has revealed that with the volume approach no tuning of constant c_a which affects the peak combustion pressure is required with variation of engine operating conditions and load. The air entrainment rate for each zone is calculated by Kouremenos et al. (1997):

$$\frac{dm_{ia}}{dt} = c_a \rho \frac{dV_i}{dt} \tag{3.24}$$

with c_a above a constant specific to the model.

Droplet Breakup and Evaporation

There are multiple models and sub-variations for the modelling of droplet breakup utilizing relations within the multi-zone approach (Baumgarten Carsten, 2006; Jung et al., 2001; Kouremenos & Hountalas, 1994; Kumar et al., 2013), CFD direct numerical approach (Turner et al., 2012) and also approaches utilizing stochastic mathematic simulations (Karimi & Andersson, 2020) aiming to increase the accuracy of droplet size and distribution. For this application a conventional model was used that has been proven to work well with large 2-stroke marine engines.

The injected fuel is distributed into zones according to the injection rate and for each zone the fuel is divided into groups of droplets that have the same Sauter mean diameter. The formula used for the distribution of droplet diameters in the packages is given by Heywood (2018) and Ramos (1989):

$$\frac{dV}{V} = 13.5\left(\frac{D_d}{D_{SM}}\right)^3 \exp\left[-3\left(\frac{D_d}{D_{SM}}\right)\right] d\left(\frac{D_d}{D_{SM}}\right) \tag{3.25}$$

While a conventional approach, the use of the above relation gives a quite accurate prediction of the fuel-air equivalence ratio distribution inside the jet, (which is important for the present analysis) and the SMD packages approach is used in detailed analyses (with some variations to improve accuracy) that employ advanced flow simulations such as Lettieri Claudio (2010).

The Sauter mean diameter D_{SM} is obtained by the use of semi-empirical correlations derived by analysis of experimental data and is given as:

$$D_{SM,1} = 0.38 Re_{inj}^{0.25} We_{inj}^{-0.32} \left(\frac{v_l}{v_a}\right)^{0.37} \left(\frac{\rho_l}{\rho_a}\right)^{-0.47} d_{inj} \tag{3.26}$$

$$D_{SM,2} = 4.12 Re_{inj}^{0.12} We_{inj}^{-0.75} \left(\frac{v_l}{v_a}\right)^{0.54} \left(\frac{\rho_l}{\rho_a}\right)^{0.18} d_{inj} \tag{3.27}$$

where the 1 and 2 subscripts are used to refer to complete and incomplete sprays respectively. The required for calculations Reynolds and Weber number are given by:

$$Re_{inj} = \frac{u_{inj} d_{inj}}{v_l} \tag{3.28}$$

$$We_{inj} = \frac{u_{inj}^2 d_{inj} \rho_l}{\sigma} \tag{3.29}$$

The Sauter mean diameter is taken as the maximum of the two values received from equation 3.26 and 3.27.

For evaporation, similarly multiple modes are available (Baumgarten Carsten, 2006; Günter, 2006; Ramos, 1989) with one used in for the current model being the one of Borman and Johnson (1962). The rate of droplet mass change according to the model selected is given by:

$$\frac{dm}{dt} = -\frac{2\pi r D_v P}{R_{fv} T_m} \ln\left(\frac{P}{P - P_v}\right) Sh \tag{3.30}$$

The Sherwood number Sh is calculated as:

$$Sh = 2 + 0.6 Re^{0.5} Sc^{1/3} \tag{3.31}$$

In the above eq. 3.30 D_v is the mass transfer diffusivity for the fuel air mixture, T_m the mean temperature of the fuel-air mixture and P_v the partial pressure of the fuel vapor at the liquid surface. To obtain the temperature of the droplets the energy balance equation given below is integrated.

$$m_l c_{pl} \frac{dT_l}{dt} = 2\pi r \kappa_m \left(T_a - T_l\right) \left[\frac{z}{e^z - 1}\right] Nu + L_f \frac{dm}{dt} \tag{3.32}$$

The Nusselt number included in eq. 3.32 is given by:

$$Nu = 2 + 0.6Re^{0.5}Pr^{1/3} \tag{3.33}$$

and the z exponent is a dimensionless correction factor for heat transfer that includes the effect of the mass transfer in its formulation given in:

$$z = -c_{pf}\frac{dm}{dt}\frac{1}{2\pi r \kappa_m Nu} \tag{3.34}$$

In the last equation of this series, 3.34, κ_m is the thermal conductivity of the mixture and L_f is the fuel's latent heat of vaporization. The integration of equations 3.25 and 3.27, 3.28 provides the history of each droplet group inside the zones.

Combustion Model

For each zone the internal mixing rate is controlled by turbulent diffusion. The evaporated fuel and the entrained air mass of each zone are divided into two portions, macromixed one a micromixed one (Kouremenos et al., 1997). The corresponding mass rates are given by:

$$\dot{m}_{fmic} = D_t(u)\left(m_{fmac} - m_{fmic}\right) \tag{3.35}$$

$$\dot{m}_{amic} = D_t\left(m_{amac} - m_{amic}\right) \tag{3.36}$$

$$D_t(u) = a_{mix}u \tag{3.37}$$

with a_{mix} a constant and u the relative velocity of the burning zone element with respect to the surrounding air. The a_{mix} constant is used to control the overall intensity of the heat release rate and affects the estimated engine power. For this reason, it is used as a calibration constant to match the desired engine power output. The process of calibration is conducted as in Kouremenos et al. (1997).

The fuel ignition delay can be determined by the correlation of Kadota et al. (1976):

$$S_{pr} = \int_0^t \frac{1}{a_{del}P_g^{-2.5}\Phi_{eq}^{-1.04}\exp\left(5000/T_g\right)}dt = 1 \tag{1.38}$$

In eq. 1.38, Φ_{eq} is the local equivalence ratio of the fuel air mixture inside the zone. The a_{del} is a constant calculated from the constants determination procedure of Kouremenos and Hountalas (1994) and the ignition quality of the fuel i.e., a function of its cetane number.

The combustion rate depends strongly on local temperature and on the concentration of O_2 and evaporated fuel. The local fuel combustion rate is modelled using an Arrhenius type equation (Heywood, 2018):

$$m_{fb} = K_b \frac{\left(m_{fmic} - m_{fb}\right)}{T^{0.5}} e^{\frac{-E_c}{T}} P_{O_2}\text{, for (AFR) > (AFR)}_{st} \tag{3.39}$$

$$m_{fb} = K_b \frac{\left(m_{fmic} - m_{fb}\right)}{\left(AFR\right)_{ST} T^{0.5}} e^{\frac{-E_c}{T}} P_{O_2}\text{, for (AFR) < (AFR)}_{st}$$

In the above K_b is a constant, E_c is the reduced activation energy, AFR the fuel air ratio and P_{O2} the partial pressure of oxygen in the zone. By using this approach, the effect of the EGR and also of the oxygen rich biofuels on the combustion rate are taken into account.

Fuel Injection System

For the estimation of the injection rate and the parameters governing droplet breakup and jet formation a simplified fuel injection model is used which considers for the following control volumes: high pressure pump chamber, delivery valve chamber, delivery pipe from pump to injector, and injector. This is preferred compared to the use of a simple injection rate shape.

The fuel is considered to be compressible, its compressibility defined by the following function,

$$K_f = -V_j \frac{dP_j}{dV_j} \tag{3.40}$$

The simulation of each control volume is accomplished by considering the previous equation and the incoming and outgoing volume flow rates, obtaining thus the following relation,

$$\frac{dP_j}{dt} = \frac{K_f}{V_j}\left(\frac{dV_j}{dt} - \dot{Q}_{tj}\right) \tag{3.41}$$

where $\dot{Q}_{tj}$ is the total net volume flow rate into the control volume and dV_j/dt is the rate of its volume change. The volumetric flow rate through orifices, various openings or ports is given by the formula,

$$\dot{Q}_j = A_j C_{dj}\left(\frac{2\Delta P_j}{\rho_j}\right)^{0.5} \tag{3.42}$$

and “j” is the corresponding volume. The delivery valve is modelled as a check valve allowing fuel flow only from the delivery chamber to the fuel pipe. The injector is modelled in a similar way, as a check valve, allowing fuel to flow towards the combustion chamber only when the pressure exceeds its opening pressure. The previous two approaches require the knowledge of minimum engine data and are more suitable for practical applications as the present one.

The pressure estimation in the control volumes is achieved by solving the unsteady flow equations inside the tube using the two basic principles of mass continuity and momentum conservation. The corresponding differential equations are solved using the method of characteristics (Kouremenos et al., 1991).

The injection profile is determined from the simple fuel injection simulation model using the actual fuel cam geometry. The model allows the use of this approach or the use of a predefined injection profile. A comparative analysis was performed using the simulated injection rate and a mean injection rate defined from the fuel consumption and injection duration at each operating condition to evaluate its effect on predicted values. The last was defined from the point of injection initiation and the peak combustion rate after significant analysis. As revealed, the qualitative results remained valid and only minor effect was observed for absolute performance and emission data, which is important for the needs of the proposed integration to a digital twin model that also includes engine operation particulars.

Gas Exchange System

For the simulation of the inlet and exhaust manifolds the method of filling and emptying technique is used (Heywood, 2018; Kouremenos & Hountalas, 1994). This allows the calculation of gas exchange rate between them and the engine cylinder. Good results have been found in other applications for large 2-stroke marine engines (Raptotasios et al., 2015). The model also includes the air cooler, EGR cooler, and turbocharger operation (Kouremenos & Hountalas, 1994).

Turbocharger:

As known from practice, characteristic charts for the compressor and the turbine are usually not available. For this reason the method of operation similarity (Kouremenos et al., 1995; Vavra,, 1960) is used from which the charts are reproduced using existing experimental data. The method is efficient for engine loads in the range of 40% to 100% and is as follows:

Using the least squares method, a set of constants is calculated for the polynomial curves that fit the following functions,

$$\eta_{is_C} = f_1(\varphi) \tag{3.43}$$

$$\eta_{is_T} = f_2(\varphi) \tag{3.44}$$

$$k_{is} = f_3(\varphi) = \Delta h_{is}/U^2 \tag{3.45}$$

where $\phi = m/(\rho AU)$ is the flow coefficient.

The data required for the calculation of the turbine and compressor characteristic maps in the previous form are:

- Pressure before and after the compressor.

- Pressure before and after the turbine.
- Air temperature before and after the compressor.
- Exhaust gas temperature before and after the turbine.
- Rotational speed of the turbocharger.

In the present application these data were obtained from the official engine shop tests.

Air-Cooler:

The air cooler is modelled using a simple approach that is based on the processing of shop test data. The pressure drop and the effectiveness are expressed as functions of the mass flow rate through it (Hountalas & Kouremenos, 1999; Watson & Janota, 1982) as follows,

$$\varepsilon = 1 - b\dot{m}^2 \tag{3.46}$$

$$\Delta P_{ac} = a_{ac}\dot{m}^2 \tag{3.47}$$

where "ε" is the effectiveness defined as,

$$\varepsilon = \frac{T_{a,in} - T_{a,out}}{T_{a,in} - T_{c,in}} \tag{3.48}$$

where subscripts "a, c, in, out" denote respectively: air, cooling medium, inlet and outlet from the air cooler. The mass flow rate of air is calculated from the engine simulation model using the measured data mentioned above. The same approach is applied for the simulation of the EGR cooler.

Exhaust Duct

The exhaust backpressure after the turbine at the exhaust duct is expressed in a way similar to the pressure drop at the air cooler as follows,

$$\Delta P_{exh} = a_{exh}\dot{m}^2 \tag{3.49}$$

Constant a_{exh} is estimated using the engine shop test data and the mass flow rate estimated from the simulation model.

Scavenging Model

Scavenging is of significant importance for 2-stroke engine operation and emission formation. It affects, beyond others, the temperature level inside the combustion chamber and the fuel jet and O_2 availability and thus NO_x formation. A two-zone model is used for simulating the scavenging process. One zone consists of the inlet charge mix of fresh air and recirculated gases and the second of the combustion products from the last combustion cycle. A description of the model is provided in Kouremenos et al. (1997). The scavenging model employs two zones so that for the gas exchange process the cylinder contents are divided in two parts, one for the fresh entrained air and the second for a mix for fresh air and combustion products of the previous engine cycle. During the scavenging process part of the intake air escapes directly to the exhaust manifold, which lower the temperature of the exhaust gas. The total amount of air entering the cylinder at a certain time step is divided in the part that enters the fresh air zone and the part that joins the combustion products zone. These amounts are given by the following equations:

$$dm_{a,fz} = dm_{a,inl}(1 - C_{1scav}) \tag{3.50}$$

$$dm_{a,cz} = dm_{g,exh}(1 - C_{2scav}) \tag{3.51}$$

The total amount of exhausted mass to exhaust manifold comprises of part of the fresh air zone and the combustion product zone as established above. The gas masses of the two zones are calculated by:

$$dm_{g,fz} = dm_{g,exh}C_{2scav} \tag{3.52}$$

$$dm_{g,cz} = dm_{g,exh}(1 - C_{2cav}) \tag{3.53}$$

In the above two equations the C_{iscav} are the constants of the scavenging model. At the end of scavenging perfect mixing between the two zones is assumed that results in a single zone comprised of fresh air and combustion products from the previous cycle.

Nitric Oxide Formation Modeling

The formation of nitric oxides is calculated using a chemical equilibrium scheme for each zone. Due to the very high temperatures inside the zones, chemical dissociation takes place. The contents of each zone are initially assumed to contain air and ideal combustion products (Raptotasios et al., 2015). Eleven chemical species are assumed in the complete chemical equilibrium scheme; O_2, N_2, CO_2, H_2O, H, H_2, N, NO, O, OH, CO.

The chemical reactions describing the species formation are:

$$\frac{1}{2}H_2 \leftrightarrow H,\ \frac{1}{2}O_2 \leftrightarrow O,\ \frac{1}{2}N_2 \leftrightarrow N,\ \frac{1}{2}H_2 \leftrightarrow H,\ 2H_2O \leftrightarrow 2H_2+O_2 \tag{3.54}$$

$$H_2O \leftrightarrow OH + \frac{1}{2}H_2, \quad H_2 + CO_2 \leftrightarrow H_2O + CO \tag{3.55}$$

$$H_2O + \frac{1}{2}N_2 \leftrightarrow H_2 + NO \tag{3.56}$$

Including the above equilibrium equations and the equations for the atom balance of C, H, N and O a system of eleven available equations is formed. The solution of these non-linear equations provides the concentration of the subject species in each zone.

The formation of NO_x is chemical kinetics controlled and for the present calculations the extended Zeldovich mechanism is applied (Lavole et al., 2007) that involves the below reactions:

$$O + N_2 \overset{k_{1f}}{\leftrightarrow} NO + N, \qquad k_{1f} = 1.6 \cdot 10^{10} \tag{3.57}$$

$$N + O_2 \overset{k_{2f}}{\leftrightarrow} NO + O, \qquad k_{2f} = 6.4 \cdot 10^{6} \cdot T \cdot \exp\left(\frac{-3125}{T}\right) \tag{3.58}$$

$$N + OH \overset{k_{3f}}{\leftrightarrow} NO + H, \qquad k_{3f} = 4.2 \cdot 10^{10} \tag{3.59}$$

with k_{if} the corresponding forward reaction rate constants.

Inside each zone the change of NO concentration is given by eq. 3.60:

$$\frac{1}{V} \cdot \frac{d([NO])V}{dt} = \frac{2(1-\beta^2)R_1}{1+\beta \cdot \frac{R_1}{R_2 + R_3}} \tag{3.60}$$

In eq. 3.60 $R_1 = k_{1f}[N]_e[NO]_e$, $R_2 = k_{2f}[N]_e[O_2]_e$, $R_3 = k_{3f}[N]_e[OH]_e$ and $\beta = \frac{[NO]}{[NO]_e}$. The "e" index denotes equilibrium. The NO concentration in each zone is obtained by the integration of eq. 3.60, as in Raptotasios et al. (2015).

MULTIZONE MODEL APPLICATION IN TWO-STROKE MARINE DIESEL ENGINES

In this chapter the use of the described model for performance and NO_x prediction is demonstrated for a typical modern marine 2-stroke propulsion engine. This includes the calibration procedure, evaluation of the model and real-world testing on a challenging application, the prediction of performance and NOx emissions when operating on multiple fuel types, including a biofuel mixture containing 30% biodiesel and 70% very low sulphur fuel oil (VLSFO). The emissions values were also measured on-board following the official Marpol guidelines (International Maritime Organization, 2020) to ensure good levels of accuracy, required for the comparison to the model's estimations.

Model Calibration and Initial Validation

The basis for the model's calibration was selected to be the official documentation of the engine, specifically the performance measurements during the factory acceptance tests (FAT) and emissions measurements of the official engine NO_x file. These included the main performance data, cylinder pressure data, air and exhaust gas flow rate and detailed information on fuel properties. The calibration process was performed in the four major points used for official emissions measurements under ISO 8178, as is common practice for such applications (Grigoriadis et al., 2021), specifically 25%, 50%, 75% and 100% load.

The calibration process involved estimation of the following parameters:

1. Air entrainment correction coefficient which affects the peak pressure values.
2. Estimation of EVC variation to match the measured P_{comp} values.
3. Turbine effective flow to match the measured exhaust manifold pressure.
4. Scavenging model calibration to match exhaust manifold mean exhaust gas temperature and measured mass flow rate.
5. Estimation of SOI and EVO settings at all loads corresponding.
6. NO_x scaling factor.

The above can be achieved using an automated procedure.

Following this, model constants were retained the same, and, most importantly, for constants 1, 4 and 6 the values were maintained the same regardless of engine load. After completion of the calibration procedure, the FAT results were reproduced, and the predicted values were compared with measured data.

In the following part, for the sake of space, detailed results are provided only for 25% and 75% load. In Figure 3 and Figure 4 the pressure traces are provided for the reference operation, which refer to use of marine gas oil (MGO). The calculated pressure traces present a very good match compared to the measured ones. During the FAT tests, peak compression and firing pressure values are practically the same and the same applies for the compression and expansion curves. The degree of pressure rise after fuel ignition is also replicated with good accuracy. While pressure trace replication is a good metric of the model's capabilities, accurate engine power and fuel consumption predictions are also required for the purpose of NOx emission prediction. In addition, for most digital twin implementation these values will most probably be the main inputs to the emissions model. The comparison results are given in Figure 5 and Figure 6. Engine power estimation presents practically no error and the bsfc values are also very close to the measured consumption of each load point. The level of error between estimated and measured specific fuel consumption is quite close to the total accuracy of the measurement procedure (that factors in both torquemeter and flowmeter accuracy), which is a very good result.

The calculated emissions also resulted in good accuracy levels, with overall low error for most load points, Figure 7. The results presented could be further improved by increasing correction factor use, but as mentioned in the chapter's start a philosophy of minimization of secondary corrections was elected to avoid possible high deviations when other conditions are used for the simulation. The engine air flow, Figure 8 was predicted with very good accuracy. Combined with the fuel consumption good prediction capability this mode can be used to estimate specific NO_x emissions using measured values of the pol-

Figure 3. Comparison between measured and calculated pressure traces, reference measurement 25% load

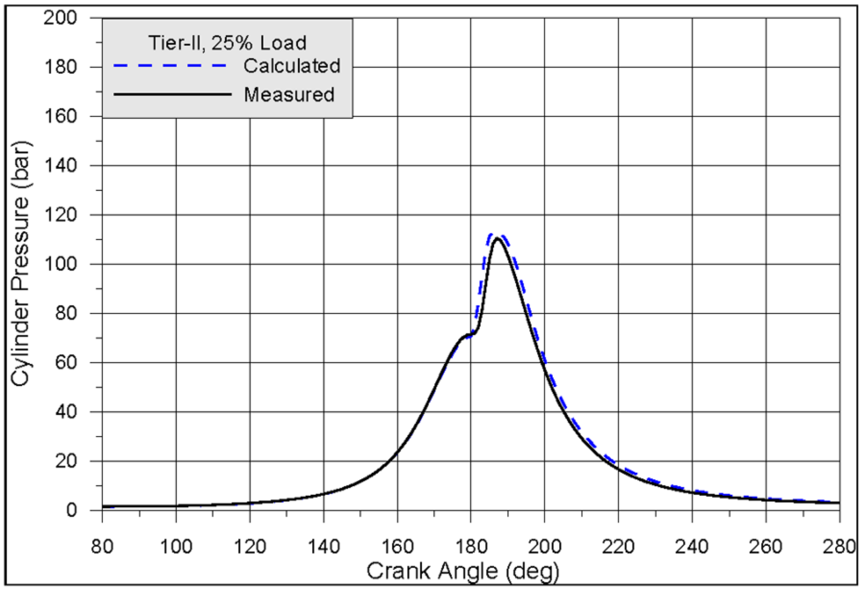


Figure 4. Comparison between measured and calculated pressure traces, reference measurement 75% load

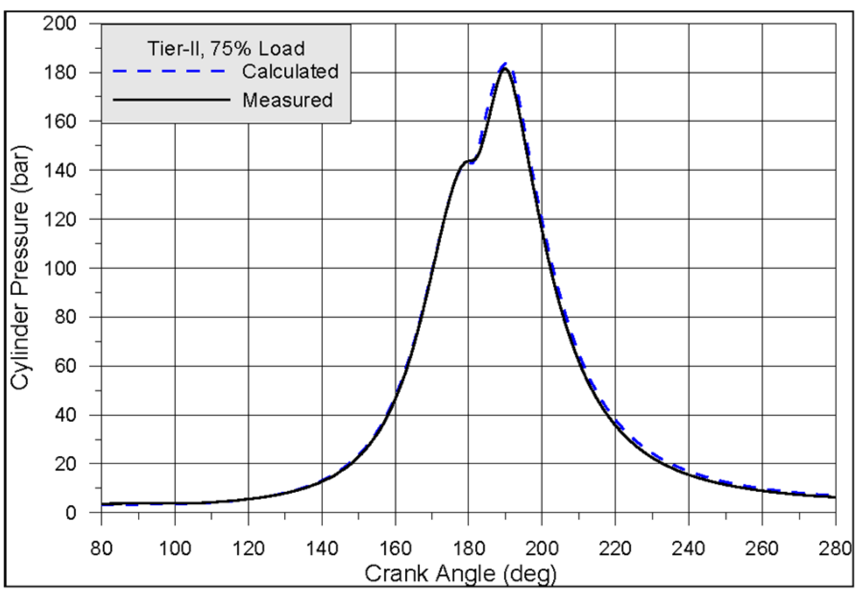


Figure 5. Calculated and measured power comparison, reference measurements

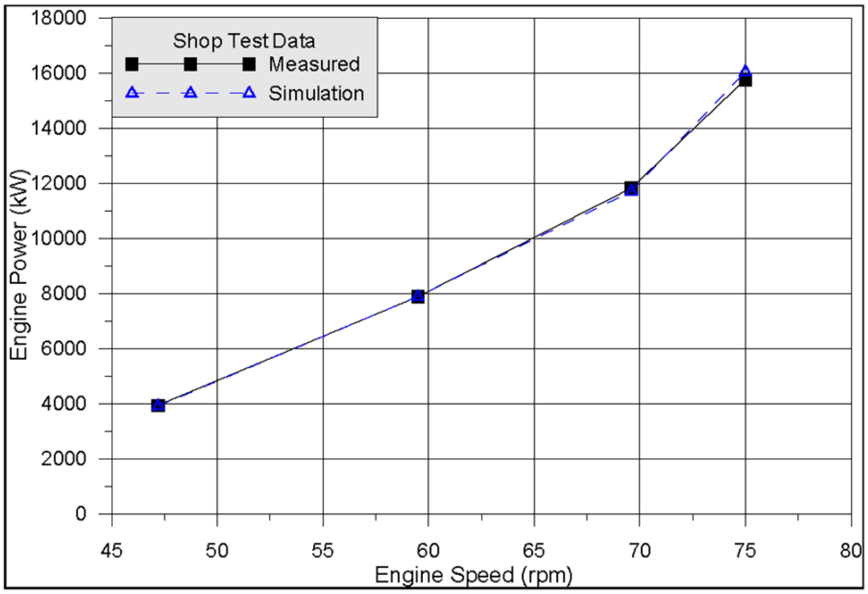


Figure 6. Calculated and measured bsfc comparison, reference measurements

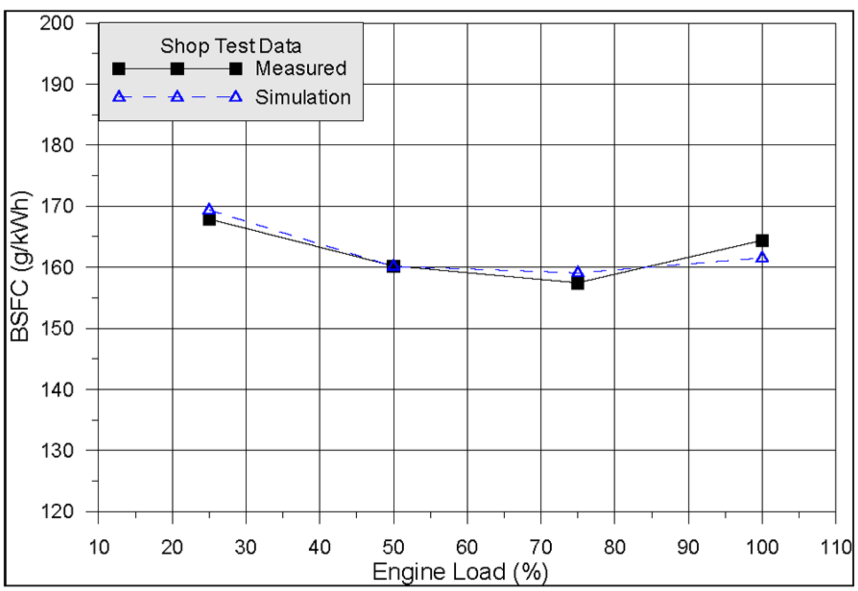


Figure 7. Calculated and measured NO_x specific emissions comparison, reference measurements

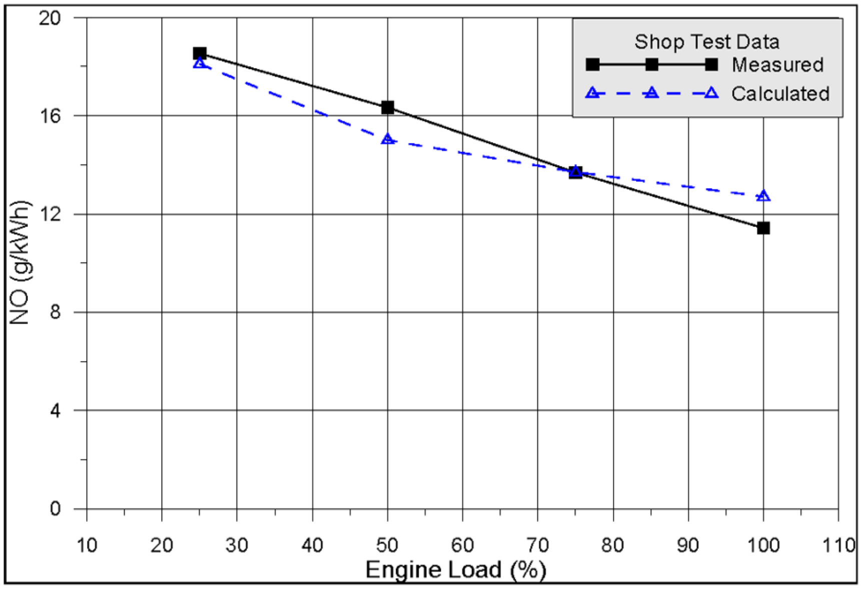
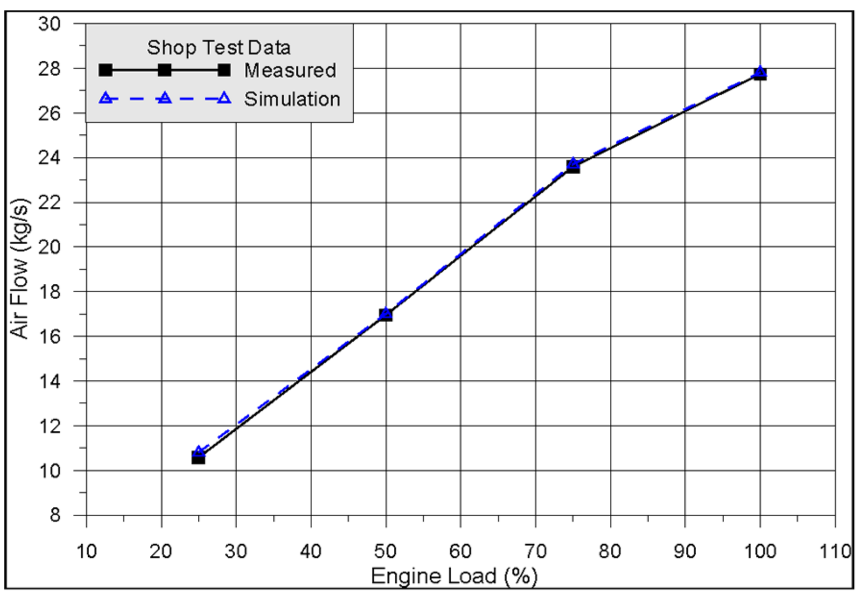


Figure 8. Calculated and measured exhaust gas flow rate, reference measurements



lutant's concentration in exhaust gases, which require exhaust gas mass flow (inlet air and consumed fuel) for the calculations.

Multizone Model Application for Modelling Biofuel Use in Two-Stroke Marine Engines

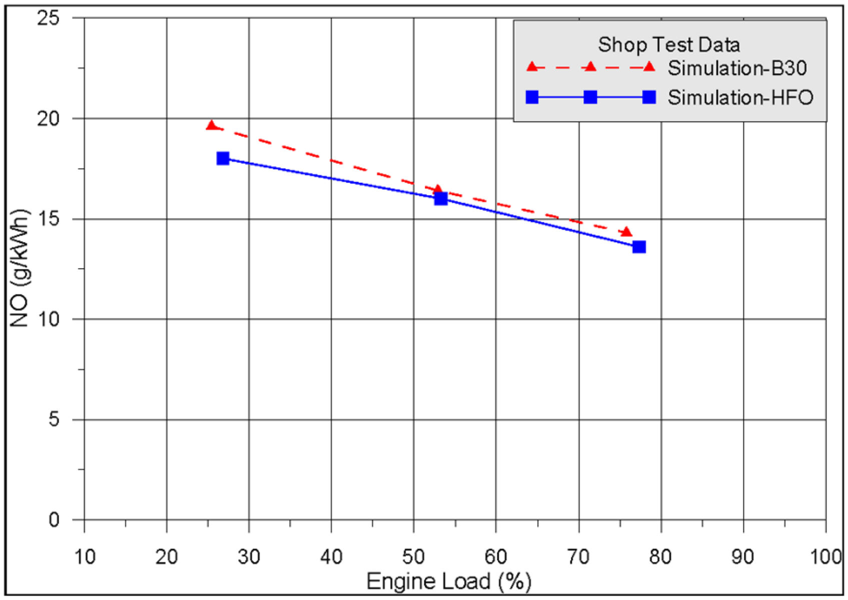
The results of the model application for B30 biofuel use in a 2-stroke marine engine are provided in this section. The model was calibrated using FAT data using MGO, as shown in section 5.1, and provided good results. It is noted that no secondary calibration was performed using up to date data, despite the engine being in operation for a considerable period between commissioning and the time of the biofuel tests. The data used for the model validation were collected during a detailed on-board measurement procedure. This included both exhaust gas composition measurements and comprehensive recording of engine performance parameters. The detailed engine performance data recorded were compared to the reference performance values during FAT tests. The comparison revealed that engine condition and tuning was close to the reference state. The main factor for this verification was comparison of fuel burn rate in the cylinder. This was derived by utilizing the measured cylinder pressure trace available from both the FAT and the biofuel tests, and conducting heat release rate analysis, as detailed in Chountalas et al. (2023). In cases of engines that present deviating operation a secondary calibration procedure may be required using the recently recorded data, when considerable deviations exist. This should also apply to the digital twin model assuming that it features engine operation replication for condition monitoring, which will not always be the case. This is further elaborated in the following chapter.

The model's prediction for NO emissions during operation with the B30 biofuel and the conventional HFO fuel are provided in Figure 9. The predicted values for the biofuel operation are then compared to the measurement results, with rather good agreement as the emissions trend with load is also replicated, Figure 10. The level of difference between the absolute values measured and estimated is well within the acceptable range, especially when considering the degree of deviations observed when performing such tests in multiple modern engines of this type, even the same model. The study currently providing the highest number of emission measurement data for B30 and conventional fuels, Chountalas et al. (2023) shows that NO_x emissions at each load can vary by more than 10% between the units tested. The findings of this study regarding NO_x emissions deviation are summarized in the below Figure 11.

The predicted NO formation history during the combustion process is given in Figure 12 for the same comparison. The loads included are 25%, 50% and 75%, the same as the ones for the actual exhaust gas composition measurements. The model predicts increased NO formation in-cylinder during the use of B30, with the effect being higher at low load, while the total increase is found rather moderate . The NO formation history shows that the slope of total NO formed remains rather steady with load increase, but the process of NO formation has longer duration for increased engine power output.

The predictive ability of the model relies in great part on reproducing in-cylinder conditions with good accuracy, especially in the regions of higher interest, near the flame front. The concentration of species, in this case primarily the oxygen content of the biofuel and the distribution of temperature are the major controlling parameters for NO formation. Through Figure 13 to Figure 18, the fuel-air equivalence ratio, temperature and NO formation distribution are compared for fuels of similar properties but different oxygen percentage, at 5^o crank angle (CA) after fuel injection for 50% engine load. The results show a clear and significant reduction of the fuel-air ratio inside the fuel jet for the B30 calculations that is the result of its O_2 content that is supplied directly in the flame front and inside the fuel jet. Normally, O_2 presence should be quite limited in the inner jet area until significant amount of air entrains the fuel spray, and this is indeed observed for the low oxygen fuel calculations. The increase of O_2 availability led to also to higher localized temperature values inside the jet for the simulations of biofuel operation

Figure 9. Comparison of calculated NO emissions, all loads on-board HFO and B30 operation



as surplus of O_2 drives combustion. The combination of higher temperature and O_2 for dissociation of N resulted in a higher rate of thermal NO formation. As expected, the higher NO values are formed in the jet periphery where fuel air equivalence ratio is close to stoichiometry and also slightly fuel lean.

Figure 10. Comparison of calculated and measured NO emissions, all loads B30

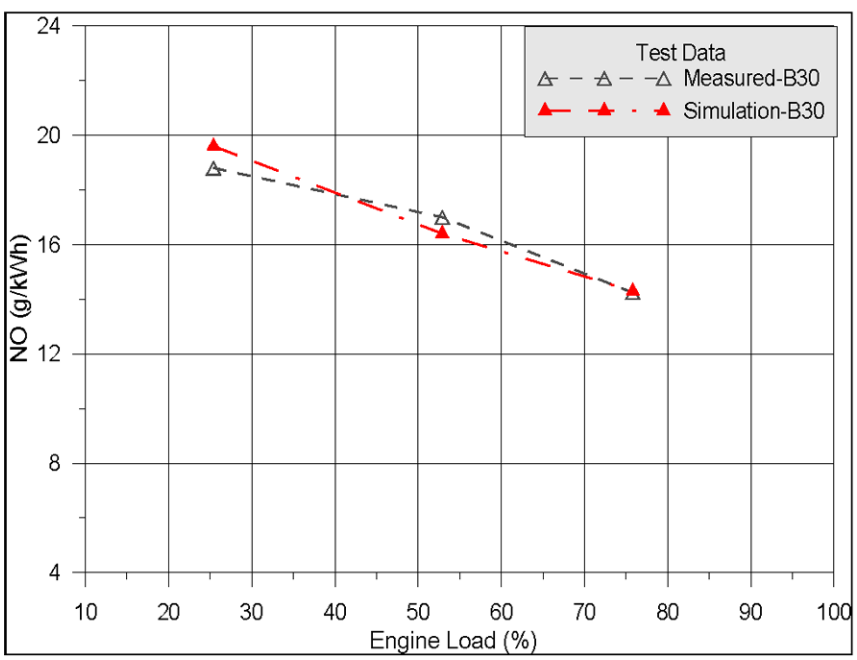
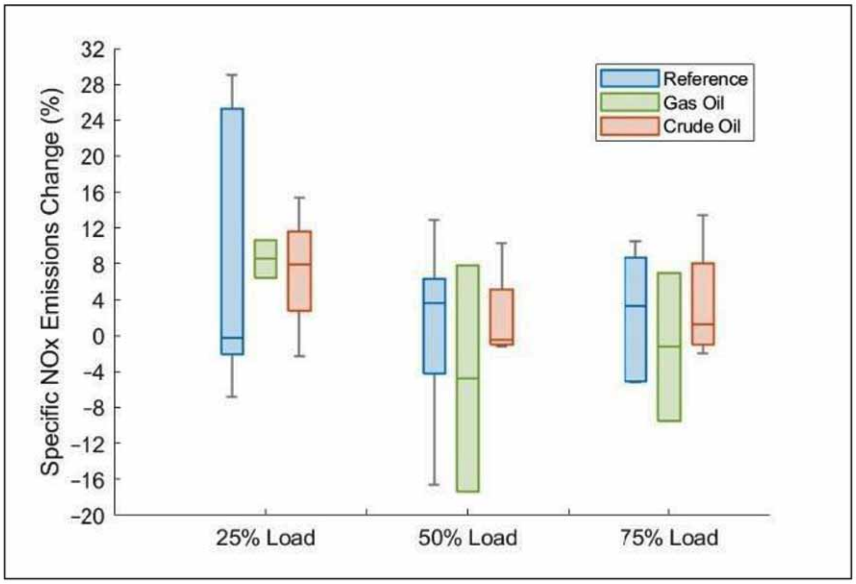


Figure 11. Specific NO_x emissions comparison, B30: Reference, gas oil, crude oil



The previous results show that the model can replicate the physics of NO formation and in turn provide a result that is close to the actual conditions without secondary calibration. Though it should be clarified that the model requires some degree of engine operating state feedback in order to retain good accuracy levels and should be regularly updated regarding tuning and overall performance for optimal results.

Figure 12. Calculated NO formation history, all loads, HFO and B30 operation

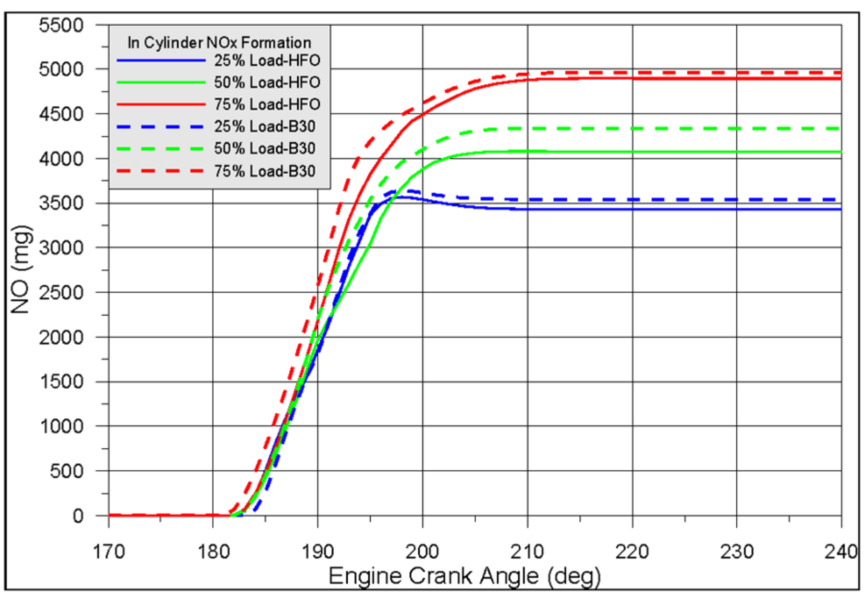


Figure 13. Fuel-Air equivalence ratio distribution in the jet area 5deg CA after injection, 50% load, B30

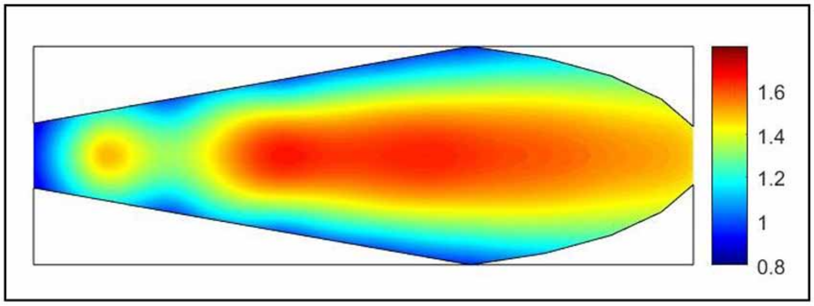


Figure 14. Fuel-Air equivalence ratio distribution in the jet area 5deg CA after injection, Low O_2 HFO

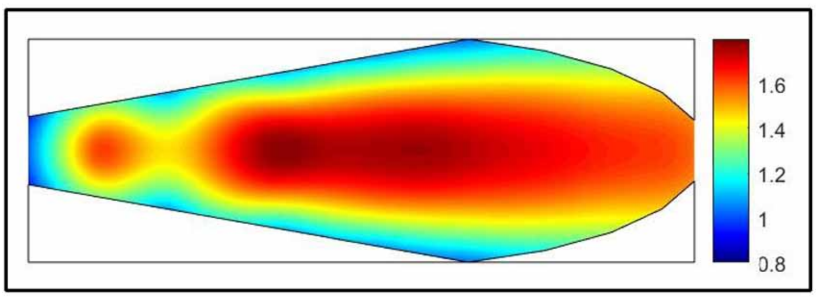


Figure 15. Temperature distribution in the jet area 5deg CA after injection, 50% load, B30

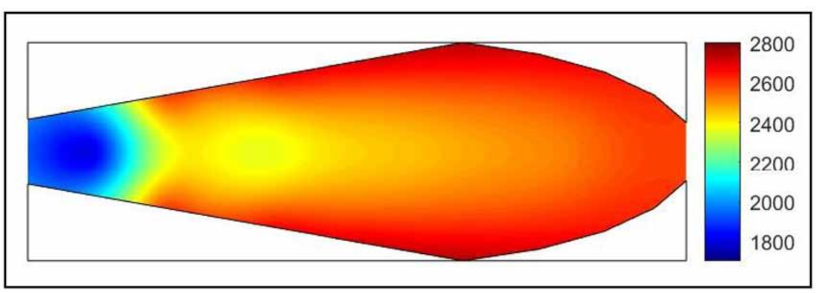


Figure 16. Temperature distribution in the jet area 5deg CA after injection, Low O_2 HFO

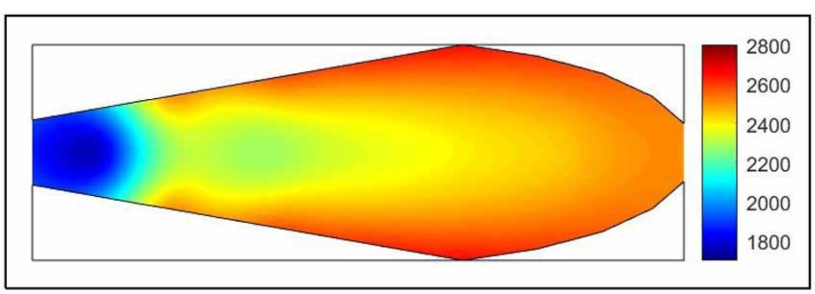
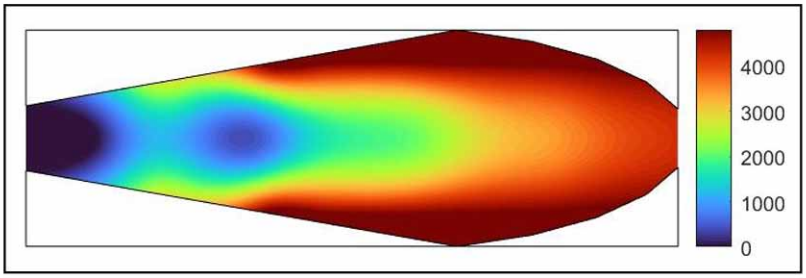


Figure 17. NO distribution in the jet area 5deg CA after injection, 50% load, B30



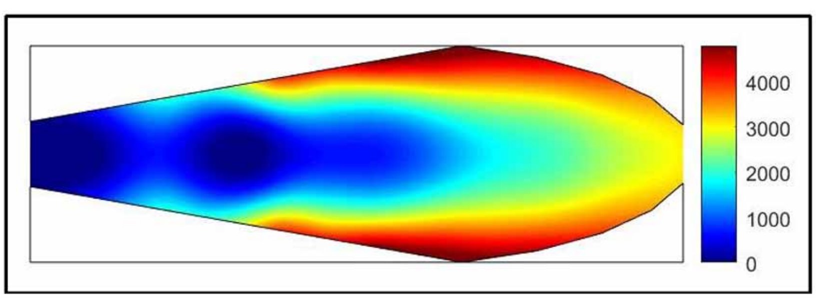
UTILIZATION OF MULTIZONE MODEL FOR DIGITAL TWIN APPLICATIONS

Emissions Model Use Based on Digital Twin Output

Following multi-zone model validation regarding its ability to predict both performance and NOx emissions there exist various possibilities, depending on the type of digital twin and multizone model used, for their use in digital twin applications.

The information provided by the emissions' model and its accuracy will be strongly dependent on the data generated by the digital twin and also the degree of feedback between the physical and digital system. In the simpler case, the digital system will estimate main operational data regarding the hull and overall vessel propulsion. The information about the engine(s) used for propulsion will be operating speed, power output and fuel consumption. The calculated values will be based on either past data of the same or similar vessels and/or the results of detailed and computationally expensive simulations, as theorized in the works of Botín-Sanabria et al. (2022), Madusanka et al. (2023), Raza et al. (2022), VanDerHorn and Mahadevan (2021), and Wei et al. (2023). In this case, the use of a multizone model integration would require simplified estimations of NO_x formation based on engine speed and load only, which is feasible and should be representable of the actual physical system unless engine operation is altered considerably, or factors such as ambient conditions reach extreme values. This can either be implemented with simplified real time computations, or with predetermined curves generated by the model during the implementation and integration stage. As briefly explained in the above chapters, the

Figure 18. NO distribution in the jet area 5deg CA after injection, 50% load, Low O_2 HFO



emission curves will be complemented by a series of correction factors to account for the specific vessel particulars under various operating scenarios regarding engine state.

It is possible to use the digital twin to generate more detailed engine operational data, but regular feedback between the physical and digital system will be required to ensure accuracy of predictions. Such data can be the result of the proposed multi-zone model or the result of simpler models having adequately low computational time. Since the engine operational values will be generated within the same simulation environment, they will not be considered as an input for the emissions calculations but be part of the overall process. This results in the aforementioned requirement for regular feedback from the physical system, that will be performed to verify that this part of the digital twin simulation is close to the actual conditions occurring at the physical system side. The use of a phenomenological combustion and cycle-mean value modelling for marine diesel engine digital twins is proposed in Bondarenko and Fukuda (n.d.) and mentioned as a probable approach in the recent extensive review of digital twin applications in maritime of Madusanka et al. (2023). This is also the suggested procedure according to digital twin researchers for system states and parameters that are not directly measurable due to technological limitations or cost concerns (VanDerHorn & Mahadevan, 2021). In the case of a marine vessel, regularly updating NO_x emissions data via on-board measurements is faced with both economical and scheduling challenges beyond the known technical challenges. For values that can be measured and recorded to generate a significant volume of information the digital twin model can use machine learning and artificial intelligence techniques for operation (VanDerHorn & Mahadevan, 2021). For values that cannot be determined or measured and not supported by relevant databases that can be used in the aforementioned advanced techniques it is common practice for the digital twin model to use simulation models such as the multizone one in this application (VanDerHorn & Mahadevan, 2021). Therefore for most applications there exists a significant overlap between the state-of-the-art digital twin and traditional modelling approaches (Jones et al., 2020). The major difference between the digital twin model and a conventional simulation one is that simulation models are used for predicting future states, while the digital twin tracks current and past states of the physical system.

For cases with very robust systems of telemetry implementation that record all major engine performance parameters, after an adequate data volume is recorded machine learning solutions could be alternatively used to predict engine performance, though this could prove highly challenging in the marine environment due to various factors (Wu et al., 2021) a major being the accuracy of recorded data.

Using Phenomenological Model to Estimate Emissions in Real Time

For digital twin simulations that do not include engine modelling or detailed physical system feedback for their operation and performance, the recommended application of the multizone model is generation of reference emissions curves. This can be performed during the digital twin design stage by simulating exhaust gas composition under different operating scenarios. These could include both CO_2 and NO_x, for various types of fuels, accounting for their physical and chemical properties. I addition, up-to-date information regarding engine operation, such as component condition and tuning differences from reference could be factored into the emission estimations via the use of correction factors. These curves could then be used for real-time monitoring of a vessel's environmental impact, without requiring constant measurements, which is not feasible for most marine vessels due to lack of suitable equipment. It is noted that lately vessels equipped with Tier-III engines are equipped with NO_x sensors that measure concentration in the exhaust gases continuously. In these cases, an emissions estimation application is still required, as the exhaust gas mass flow rate must be known to calculate the actual amount of NO_x emitted from the vessel. Direct calculation of exhaust gas mass flow using measured values would require both fuel consumption and CO_2 concentration, but the latter is not currently measured in any engine implementation. A multizone model can be used to calculate the exhaust gas mass flow to be used along the recorded NO_x concentration to estimate total emissions and also provide the predicted values for NO formation in-engine. These can be used for verification of the measured values by the installed sensors during the vessel's lifespan. Verification of sensor data is very important, and this requirement is further enhanced when the sensors operate in challenging environments. A discussed application of digital twin models in transport systems is their utilization to ensure the quality of telemetry systems using advanced sensor. As digital representations of physical systems, when feeding sensor data to the digital twin, the input values provided by sensors can be checked and even corrected according to the rules of the physical systems (Björkqvist et al., 2020). By the integration of a robust multizone model in the digital system engine specific data received by on-board sensors for emissions, when available, and performance can be evaluated when abnormal deviations are detected by the digital twin system.

Overall, in this approach the digital twin could be used to provide real-time estimations of a vessel's environmental impact during a voyage, based on the data received from the vessel for engine speed and power output, and, if available at a high accuracy, fuel oil consumption. In addition, projections can be made for optimization of vessel routing, based on economic and environmental impact factors, using the optimized engine load and rpm trend produced by the digital twin model. CO_2 emissions can also be included in the calculations (Wei et al., 2023) based on established methods such as the official EEXI formula provided by IMO (IMO, 2012) that applies to various fuel types via carbon conversion factors (CF). These can be either used as is or be updated with data from the multizone model and the on-board measurement equipment via telemetry in set time intervals or after major maintenance. Then, the NO_x emissions can be predicted using the multizone model results to provide the full environmental impact, along with possible SO_x emissions, of the studied journey.

Using Phenomenological Model to Estimate Emissions for Detailed Studies

Another potential use case of the multizone model integration to a digital twin can be investigation of scenarios that involve use of alternate fuels or engine tuning modifications. As demonstrated in the previous chapter 5, a detailed multizone model can successfully predict NO_x emissions for fuels of different physical and chemical properties, based on the initial calibration with the FAT data and utilizing information for current engine tuning and overall performance state. Furthermore, the sensitivity of such models, even less detailed versions, to tuning changes was confirmed in the detailed study of Provataris et al. (2017) for multiple applications. In the specific study phenomenological multizone models were found to accurately predict the effect of various factors, such as SOI timing on emissions. These capabilities, combined with the minimal computational resources and time required for modern computational systems can aid the use of the digital twin framework as a strategy planning tool. Before conducting cost intensive trials, the vessel's digital twin simulation can be used to generate estimations for the level of potential benefits expected by alternative fuel use or engine tuning modification, such as SOI timing to improve fuel consumption, while retaining NOx exhaust concentrations at acceptable values. Due to the sensitivity of both fuel consumption and NOx emissions to engine loading patterns, a projected vessel operational pattern that can be generated by the digital twin, factoring routes, probable weather conditions and sailing patterns will be able to provide detailed estimates for both cost and environmental impact under various scenarios. Implementing an analysis of this type for multiple vessels, for example a company's fleet in a brief time period and with minimal effort (personnel cost) will greatly enhance the capabilities of shipping company technical and chartering departments. Improving business processes and performance as well as quick design and decision making is one of the main expected benefits of a fully realized digital twin (Attaran & Gokhan Celik, 2023; Madusanka, et al., 2023).

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