DTU Management
Department of Technology, Management and Economics

Modelling Market Dynamics within the Maritime Sector

Towards Realistic Maritime Predictions: Enhancing NavigaTE with Market Dynamics

Mærsk Mc-Kinney Møller Center for Zero Carbon Shipping

Master Thesis

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June, 2025

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Cover photo: Vibeke Hempler, 2012
Published by: DTU, Department of Technology, Management and Economics, Brovej, Building 258, 2800 Kgs. Lyngby Denmark
www.byg.dtu.dk

Approval

This thesis was conducted as part of the Master of Science in Business Analytics (MSc Eng.) programme at the Technical University of Denmark (DTU), under the Department of Technology, Management and Economics, during a six-month period.

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23rd of June 2025

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Abstract

This thesis introduces an original integration of market dynamics into the bunker optimization module of the NavigaTE algorithm, developed within the Mærsk Mc-Kinney Møller Center for Zero Carbon Shipping. By replacing static fuel cost assumptions with a dynamic pricing mechanism informed by shadow prices and iterative convergence, the model captures fuel allocation decisions under realistic market constraints. This enhancement enables a more responsive and economically grounded representation of fuel distribution in the context of maritime decarbonisation, improving the fidelity of system level assessments under regulatory and supply limitations.

Acknowledgements

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This thesis has made use of AI for assistance in writing clarity, code documentation, and structural organization, serving as a support tool under the author's full supervision and direction.

List of Abbreviations

Abbreviation	Definition
ETS	Emission Trading System
IMO	International Maritime Organization
HFO	Heavy Fuel Oil
MGO	Marine Gas Oil
LNG	Liquefied Natural Gas
GHG	Greenhouse Gas
MMMCZCS	Mærsk Mc-Kinney Møller Center for Zero Carbon Shipping
EEXI	Energy Efficiency Existing Ship Index
CII	Carbon Intensity Indicator
MBMs	Market Based Measures
EUAs	European Union Allowances
EU ETS	European Union Emissions Trading System
GCAM	Global Change Assessment Model
LP	Linear Programming
IDE	Integrated Development Environment
ABM	Agent-Based Model
MCP	Market Clearing Price
MSA	Method of Succesive Averages
MVP	Minimum Viable Product
MACC	Marginal Abatement Cost Curve
LHV	Lower Heating Value
WTP	Wilingness to Pay
WTW	Well-to-Wake
WTT	Well-to-Tank
TTW	Tank-to-Wake
GFS	Goal-based Fuel Standard
LCoF	Levelised cost of Fuel

Abbreviations used throughout the thesis.

Contents

1 Introduction

1.1 Background and Motivation

The maritime industry accounts for nearly 3% of global CO_2 emissions, and with increasing global trade, this figure is expected to rise unless significant mitigation measures are implemented. In response, regulatory bodies such as the International Maritime Organisation (IMO) have adopted increasingly ambitious targets. In its 2023 revised strategy, the IMO called for a 20% reduction in greenhouse gas (GHG) emissions by 2030, a 70–80% reduction by 2040, and net-zero emissions by 2050, relative to 2008 levels [1].

Meeting these targets demands a structural shift away from conventional fossil fuels such as heavy fuel oil (HFO), marine gas oil (MGO), and liquefied natural gas (LNG) toward low-carbon and zero-carbon alternatives. These include fuels like ammonia, methanol, hydrogen, and methane. It is important to distinguish between fuel *types*, referring to the chemical molecules used (e.g., methanol, ammonia), and fuel *pathways*, which indicate the production method (e.g., blue ammonia, e-ammonia, bio-methanol) [2, 3]. These distinctions are necessary because production methods directly affect the life-cycle emissions and marginal costs of the fuel.

Despite being technically viable, the transition to zero emission fuels is constrained by significant economic and logistical challenges. These fuels remain considerably more expensive than conventional fossil options [4], and the global port infrastructure is not yet equipped to handle widespread distribution and bunkering of alternative fuels. As a result, the maritime industry must balance regulatory requirements, market incentives, and the current state of technological development to approach a realistic path toward decarbonisation.

The Mærsk Mc-Kinney Møller Center for Zero Carbon Shipping (MMMCZCS) is a leading independent research center dedicated to enabling a climate neutral shipping industry. This thesis contributes directly to the modelling infrastructure used at the Center, specifically by extending the NavigaTE tool, with a market-based pricing mechanism. NavigaTE allows for dynamic simulation of ship level fuel allocation across a range of regulatory and market configurations. This makes it a suitable testing ground for simulation models in maritime decarbonisation.

1.2 Research Objectives

The core objective of this thesis is to develop and implement in the NavigaTE framework a realistic market-based fuel pricing mechanism and to evaluate how this addition affects fuel allocation, operational cost, and emission outcomes in maritime shipping. The work combines methodological development with practical analysis, bringing together optimisation, economic logic, and scenario simulation.

The research is structured around four objectives:

1. **Design and implement a market driven pricing mechanism**: Develop a pricing routine that captures how fuel prices emerge from supply and demand interactions under different market structures, including global, local, and emerging configurations.
2. **Integrate the pricing routine into the NavigaTE environment**: The pricing mechanism is written in Python and incorporated directly into the main simulation flow of NavigaTE. It works together with the existing fair-share linear programming model and uses the Gurobi solver to compute results.
3. **Evaluate system level impacts of pricing**: A total of 16 scenarios are analysed, representing all combinations of four regulatory environments and four market typologies. Of

these, 12 scenarios include dynamic pricing mechanisms, while 4 serve as cost reference cases. Model outputs include fuel switching trends, total GHG emissions, and overall cost outcomes for the system over the 2025 to 2050 simulation period.

4. **Extract insights for policy and industry**: Use the results to compare the effect of market signals and regulations on fuel choices in the different regions, and to identify which vessel types or operations are most sensitive to price changes or limited supply.

Together, these objectives ensure this thesis offers both a methodological contribution, a new pricing mechanism, and a practical one, insights into how market signals impact decarbonisation.

1.3 Initial Thesis Hypothesis

This thesis begins with the hypothesis that it is possible to model fuel prices in the maritime sector as the result of competitive mechanisms based on the market, where different fuel types interact through a system of supply constraints, carbon regulations, and vessel preferences. It is expected that prices will not be set externally, but rather will emerge from the optimisation behaviour of vessels competing for limited fuel resources.

To explore this, the model was initially designed to test different fuel market typologies (global, local, and emerging), each with its own implications for pricing, allocation, and regulation. It was also assumed that these market structures would influence how prices are formed and how fuels compete with one another in terms of cost-effectiveness and accessibility.

Given uncertainty in future fuel costs and carbon policies, an early modelling direction considered the use of techniques based on scenarios to simulate vessel behaviour under different economic conditions. Additionally, it was hypothesised that market-clearing prices might need to be computed using external convergence algorithms, such as the bisection method, to match fuel supply with demand dynamically.

Another key objective was to explore the role of agent-based decision making. It was assumed that the vessels would act individually based on cost and regulatory exposure, making it necessary to use iterative algorithms to simulate interaction between agents and new price signals.

Two main academic hypotheses guide the structure and focus of the work:

1. **Analytical hypothesis:** Once naturally computed, prices will reveal deeper information about the maritime fuel system. By observing how prices evolve under constraints, levies, and regulations, we gain insight into the underlying market dynamics and potential stress points in fuel availability. These price signals serve as indicators of economic tension in the system and allow for a more transparent interpretation of allocation outcomes.

2. **Mathematical hypothesis:** Most maritime models used today rely exclusively on cost minimisation and do not incorporate natural price formation. This thesis tests whether explicitly modelling prices lead to significantly different allocation decisions, and whether the added complexity is justified by improved results and analytical power. The goal is to assess if prices can act as an effective modelling layer beyond costs, capturing interactions that are otherwise invisible in purely cost-driven frameworks.

Overall, the thesis was designed as an exploratory framework to test how market-driven pricing mechanisms could be integrated into a maritime fuel allocation model, and how fuel types would interact under realistic policy and supply conditions.

2 Literature Review

2.1 The Maritime Sector Decarbonisation Challenge

This section aims to provide the reader with essential background information to support the understanding of key concepts and modelling choices used throughout this thesis.

2.1.1 From IMO 2018 to IMO 2023 and FuelEU Maritime

The *International Maritime Organisation* (IMO) is the United Nations agency that sets global safety and environmental rules for shipping. In 2018 the IMO adopted its first global greenhouse gas (GHG) strategy. The plan calls for a 40% reduction in the average carbon intensity of shipping work by 2030 and at least a 50% cut in total annual emissions by 2050, both relative to the 2008 baseline [5]. Two technical measures, the Energy Efficiency Existing Ship Index (EEXI), which assigns each ship an efficiency score based on design, and the Carbon Intensity Indicator (CII), that rates the yearly operational performance of each vessel on a simple A–E scale, went into effect in 2023 to establish a consistent efficiency benchmark for the global fleet.

In 2023, the Marine Environment Protection Committee, the branch of the IMO in charge of pollution regulations, revised its strategy and increased its ambition to reach net zero greenhouse gas emissions *"by or around 2050"* [6]. The revision also introduced preliminary targets for 2030 and 2040 and encouraged member states to reach agreement on pricing and regulatory reforms by 2025. In parallel, the European Union adopted FuelEU Maritime (Regulation EU 2023/1805), which fixes a gradual cut in the carbon intensity of energy used on board ships that visit EU ports, starting with a 2% reduction in 2025 and reaching an 80% cut in 2050 [7]. Taken together, the global and regional standards indicate a strong and growing legislative push for low carbon marine fuels.

2.1.2 The Cost Gap between Fossil and Alternative Fuels

Fossil marine fuels remain significantly cheaper than their zero-carbon alternatives. Heavy fuel oil and marine diesel cost 50–70% less per unit of energy than green ammonia, methanol, or hydrogen [8, 9]. This gap derives from expensive inputs, low production volumes, and undeveloped supply chains. Additional costs arise from storage, distribution, and vessel retrofitting.

A carbon price between 150 and 250 € per tonne of CO_2 has been cited as necessary to bring green fuels closer to parity [10], though more recent estimates suggest 350–450 €/tCO_2 for full competitiveness, especially for synthetic fuels [11, 12]. In the absence of such signals, fuel switching remains commercially unattractive, indicating the need for regulatory instruments such as levies or mandates.

2.2 Market Typologies for Bunker Fuels

Fuel prices in shipping vary widely across ports due to differences in infrastructure, geography, and regulation. Unlike global commodity markets with uniform pricing, maritime fuel markets are shaped by local conditions and policy. This section highlights how standard economic market types apply to bunkering and why this matters when modelling price signals and fuel choices, providing the economic context needed to understand the new pricing mechanism implemented.

2.2.1 Economic Theory on Market Types

Classical microeconomic theory categorises market structures based on how connected the trading nodes are and the extent of frictions that prevent prices from aligning [13, 14]. In perfectly integrated markets, where trade flows freely and information is transparent, arbitrage leads to a single, shared price. However, when logistical or regulatory barriers exist, markets become segmented, and price differences emerge across regions. A third scenario arises when public policies like quotas, mandates, or taxes intervene in supply and demand, adding non-market forces to the way prices are formed.

Table 2.1 presents a simplified taxonomy of market types, organised by whether markets are integrated or segmented and whether policy influences price setting.

Market label	**Price formation rule**	**Dominant drivers**
Global (integrated)	World supply meets world demand. Arbitrage keeps local quotes close to an international benchmark.	Many suppliers, transparent trade, low transport cost
Local (segmented)	Each node clears its own balance. The local price equals the highest bid that satisfies demand.	Port size, draft limits, regional regulation, limited storage
Emerging (policy driven)	Public quota or subsidy prevents a pure cost clearing. The observed quote combines the recent trade average with the explicit policy charge.	Early technology rollout, carbon levy, blending mandate

Table 2.1: Classification of market types based on price formation mechanisms and dominant economic drivers. Adapted from [13, 14].

In global or integrated fuel markets, prices are determined globally and marginal cost logic dominates. In local or segmented markets, local scarcities and transport barriers can drive significant price divergence. In emerging markets, price signals are influenced as much by policy design as by underlying supply-demand dynamics. All three market types are relevant in maritime bunkering, depending on geography, infrastructure, and regulatory maturity.

2.2.2 Market Types in Bunker Fuel Pricing

The theoretical market differences discussed above translate directly to observed practices in marine fuel supply. Table 2.2 illustrates how global, local, and emerging market conditions shape price formation at different types of ports.

Market label	**Illustrative ports**	**Observed bunker pricing method**	**Key constraint**
Global	Singapore, Rotterdam	Daily quote set at *Platts* or *Argus* benchmark plus barge cost.	None; deep water and extensive storage
Local	Baltic minor ports, small Caribbean hubs	Premium of twenty to eighty USD over hub quote, varies with seasonal demand.	Draft limits, ice season, limited tank capacity
Emerging	Green-corridor pilots in Norway or Japan	Contract price equals weighted average of recent sales plus national carbon levy or direct subsidy.	Short supply chain, mandatory blend share

Table 2.2: Mapping of market typologies to specific ports, including observed pricing strategies and dominant structural constraints in bunker fuel logistics. Adapted from [15, 16, 17].

- **Global markets:** Large hubs like Singapore and Rotterdam see frequent trading and prices closely tied to international benchmarks. Competition and infrastructure keep price variation minimal, making them central to global fuel pricing.
- **Local markets:** Smaller or remote ports face higher prices due to limited access, storage, or seasonal demand. These premiums, often \$20–\$80 per tonne above benchmark, reflect logistical and infrastructure constraints.
- **Emerging markets:** In early-stage green fuel ports, prices are shaped by both market activity and policy tools like subsidies or carbon levies. These interventions are essential for making low-carbon fuels viable in the short term.

From a modelling point of view, each market type requires a tailored approach to price formation. In global hubs, a single benchmark per fuel is usually enough due to competitive alignment. In contrast, smaller or more isolated ports may face higher local costs driven by infrastructure limitations or seasonal changes. Emerging markets introduce further complexity, as prices are shaped not only by market forces but also by policy tools like subsidies or levies. Accounting for these differences helps the model better reflect the real world variability in fuel availability and pricing across regions.

2.3 Linear Programming and Shadow Pricing Fundamentals

2.3.1 Linear Programming

Linear programming (LP) is a widely used tool for solving optimisation problems that involve allocating limited resources under a set of constraints. It has found broad application in fields like economics, transport planning, and energy systems, where decisions often involve balancing cost, capacity, and feasibility. Within the NavigaTE framework, LP serves this exact purpose: optimising fuel allocation across vessels and ports while adhering to technical, regulatory, and resource constraints.

The method was established in the 1940s with the introduction of the simplex algorithm by George Dantzig [18]. This algorithm works by moving along the edges of the feasible region defined by linear constraints, searching for the solution that optimises the objective function. Aged but proven, it remains a top method for structured decision problems.

Key components of the method include:

- **Pivoting Rules**: These guide how the simplex method transitions between corner points of the feasible region, determining which variables enter or leave the basis [19, 20].
- **Slack Variables**: Inequality constraints are converted into equalities using slack variables, allowing the problem to be solved using matrix methods while preserving economic interpretation [21].
- **Duality**: Every LP problem has a corresponding dual that provides insight into the value of relaxing constraints and the trade-offs between different objectives [22].

This mathematical structure is especially relevant in constrained environments, such as maritime fuel markets, where supply bottlenecks, infrastructure limits, or emissions policies shape the feasible set of decisions.

2.3.2 Duality Theory and Shadow Prices

Duality offers an alternative perspective on optimisation problems. While the *primal* problem focuses on minimising costs under given physical or regulatory constraints, the *dual* problem assigns value to those constraints, effectively capturing their economic implication. The relationship between the two formulations is essential for understanding the underlying structure of the solution and interpreting the trade-offs involved.

Let the primal problem be defined as:

$$\begin{aligned} \textbf{Primal Problem:} \quad & \text{Minimise} \quad && c^T x \\ & \text{subject to} \quad && Ax \geq b, \\ & && x \geq 0 \end{aligned}$$

The corresponding dual problem is:

$$\begin{aligned} \textbf{Dual Problem:} \quad & \text{Maximise} \quad && b^T y \\ & \text{subject to} \quad && A^T y \leq c \end{aligned}$$

The strong duality theorem ensures that, under certain conditions, the optimal values of a linear program and its dual are equal. This property allows one to validate solutions and extract meaningful economic insights. As shown in Anstee [23], for a standard primal-dual pair, the optimal solutions satisfy $c \cdot x^* = b \cdot y^*$, reinforcing the equivalence of primal and dual formulations.

Shadow Prices and Scarcity Rents

The dual variables y, known as shadow prices, indicate how much the objective function would improve if a specific constraint was slightly relaxed. In practical terms, they show the value of gaining access to one more unit of a limited resource. This makes them especially useful in policy design, operational planning, and resource allocation models [24, 25, 26].

In systems shaped by regulations or capacity limits, such as emissions caps, fuel mandates, or infrastructure constraints, shadow prices reveal which bottlenecks are most economically binding. Their values can vary over time, reflecting shifts in technology, regulation, or market behaviour. As shown by *Kagan et al.* [27], shadow prices in climate policy can reflect strategic behaviour and expectations about future rules, not just present-day scarcity.

In constrained systems like maritime decarbonisation, these prices provide a link between mathematical outcomes and economic meaning. They help identify where and when policy or supply constraints make low-carbon transitions more costly, offering a way to track the economic pressure points that shape real-world adoption patterns.

The NavigaTE model applies linear programming to allocate marine fuels under several physical and policy constraints. The optimisation routine determines the most cost-effective distribution of fuels across vessels and ports, while staying within limits such as fuel supply, port capacity, and emissions targets. The shadow prices that emerge from this process reflect the economic value of relaxing each constraint, they effectively act as market signals, indicating where fuel is scarce or where regulations are tight. These values are then used within the pricing mechanism to adjust fuel costs dynamically across the network.

2.4 Agent-Based and Fair Share Allocation Models

2.4.1 Agent-Based Models in the Maritime Sector

Agent-Based Models (ABMs) offer a decentralised alternative to system-optimal approaches by simulating the behavior of individual actors, such as shipowners, fuel suppliers, and regulators, each responding to local conditions, constraints, and incentives. Rather than assuming a central planner with perfect foresight, ABMs reflect the diversity and imperfect information that characterise real-world decision-making.

This perspective is particularly relevant for maritime decarbonisation. The shipping sector includes a wide variety of actors, from large international carriers to small regional operators, each facing different fuel options, regulatory exposure, and risk preferences. ABMs can capture how these differences influence fuel adoption, especially under uncertain or evolving policy regimes.

An outstanding example is the MarPEM model by *Bas et al.* [28], which simulates the shift away from HFO under various policy interventions. By accounting for feedback loops between agents and policies, the model illustrates how regulatory tools, such as carbon pricing or subsidies, can produce divergent outcomes depending on how agents perceive costs and benefits.

For NavigaTE, which is grounded in a centralised optimisation framework, integrating ABM logic adds an important behavioral layer. While the core model solves for efficient fuel allocation under constraints, agent-based extensions would allow for more realistic dynamics by reflecting how different actors may respond to the same shadow price or policy signal in diverse ways. This hybrid structure helps close the gap between theoretical efficiency and the political and commercial realities of fuel transition.

2.4.2 Shadow Prices under Agent-Specific Constraints

In traditional optimisation, shadow prices reflect the uniform marginal value of relaxing a constraint, assuming all decision makers face the same conditions. However, in agent-based models, where agents differ in objectives, constraints, and information, shadow prices become agent-specific. The same constraint may have different implications depending on an agent's fleet, routes, or regulatory exposure, meaning no single "correct" marginal value exists across the system.

Parker and Filatova [29] illustrate this through a land market model where agents interact locally and make decisions based on their specific circumstances. Rather than converging to a uniform price, the model shows how different land uses and preferences result in a patchwork of local valuations. Likewise, Arslan [30] examines traditional maize farming in Mexico, showing that smallholder farmers assign higher implicit value to certain crops, not because of market prices, but due to cultural ties and household food security.

In the context of NavigaTE, this has direct implications for how the model interprets and applies shadow prices. While the core framework identifies a system optimal solution, real world actors are unlikely to respond uniformly to a given price signal. By incorporating agent specific constraints, such as differing fuel access, risk tolerance, or regulatory exposure, NavigaTE can better reflect the fragmented nature of the maritime sector. This allows the model not only to estimate aggregate outcomes but also to explore distributional effects, identify which actors are most vulnerable to policy shifts, and test targeted interventions that support more inclusive and realistic fuel transition pathways.

2.5 Market Clearing Equilibrium Theory

Market equilibrium occurs when the amount supplied matches the amount demanded at a certain price. At this point, no buyer or seller can improve their outcome by changing quantity or price. This principle is fundamental in economic theory and underlies the structure of many energy markets. The developed feature roots rise from this concept, adapting it to the NavigaTE and maritime framework.

Let:

$$S(p) = \text{total supply at price } p, \quad D(p) = \text{total demand at price } p,$$

and define the excess demand function as:

$$Z(p) = D(p) - S(p).$$

A market-clearing price p^* satisfies:

$$Z(p^*) = 0,$$

meaning that the market clears without surplus or shortage. At this price, all buyers and sellers are matched, and the total value created in the market is maximised [31, 32].

2.5.1 Market Clearing in Energy Exchanges

In electricity and gas markets, prices are often set through central auction systems. Buyers submit bids, and sellers submit offers. These are collected to form supply and demand curves. The market-clearing price $\bar{p}$ is the value at which they intersect :

$$\tilde{D}(\bar{p}) = \tilde{S}(\bar{p}).$$

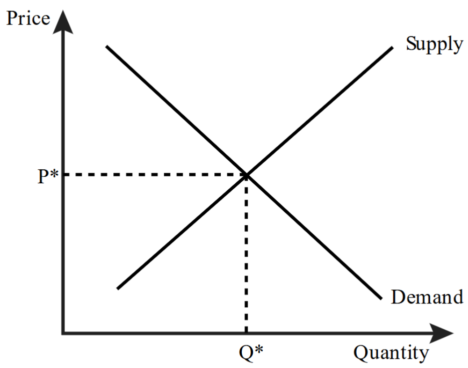


Figure 2.1: Basic supply and demand curves intersecting at the equilibrium point (p^*, q^*).

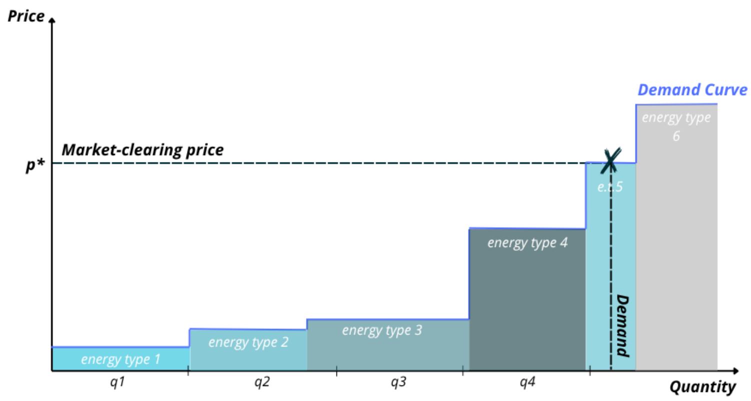


Figure 2.2: Market-clearing mechanism in electricity markets under the merit-order principle. The intersection of total demand with the last (most expensive) accepted bid sets the spot price for all dispatched units.

The market-clearing price is set at the point where aggregate demand intersects the last accepted supply bid, the marginal unit. This pricing approach aligns market prices with marginal costs and promotes transparency [33, 34].

2.5.2 Walrasian General Equilibrium

The idea of equilibrium can also be extended to a system with many agents and goods. Each agent i starts with an initial endowment ω_i and selects a consumption bundle q_i to maximise their utility:

$$\max_{q_i \geq 0} u_i(q_i) \quad \text{s.t.} \quad p \cdot q_i \leq p \cdot \omega_i.$$

A Walrasian equilibrium consists of a price vector p^* and allocation $\{q_i^*\}$ such that:

1. Each agent chooses the best option they can afford.

2. Total demand equals total supply: $\sum_i q_i^* = \sum_i \omega_i$.

Term	Definition
$u_i(q_i)$	Utility function of agent i
ω_i	Initial endowment of agent i
p	Vector of commodity prices
$q_i(p)$	Demand of agent i at price p
$Z(p)$	Excess demand: $\sum_i q_i(p) - \sum_i \omega_i$

Table 2.3: Core components of Walrasian equilibrium.

Under regular assumptions such as continuity and convex preferences, this system has a solution. The prices are unique up to a scale, and the allocation is Pareto efficient: no agent can be made better off without making another worse off [35, 36].

2.5.3 The Tâtonnement Adjustment Process

To describe how equilibrium might be reached in practice, Léon Walras proposed a process called tâtonnement, or "trial and error." Prices adjust over time based on the gap between supply and demand:

$$\dot{p} = \gamma Z(p), \quad \gamma > 0.$$

If the price is too low and there is excess demand, prices rise. If the price is too high, they fall. This process helps explain how markets might move toward equilibrium even without a central planner. Although purely theoretical, the concept gives useful insight into how decentralised decisions can coordinate through price signals [37, 38].

The NavigaTE model applies these ideas to simulate how fuel prices adjust under supply constraints and policy rules. Instead of setting prices directly, the model searches for the prices that clear the market across different ports and vessel types. This is done by embedding the concept of market equilibrium within an iterative optimisation routine. By doing so, NavigaTE reflects how prices emerge from the balance of supply and demand, shaped by both physical limits and regulatory signals.

2.6 Iterative Algorithms and Convergence Methods

In many large-scale optimisation problems, including those related to energy systems and transport models, standard solution methods may struggle to handle nonlinearity, decentralisation, or dynamic market feedback. To address these challenges, iterative algorithms, heuristics, and convergence methods are employed to gradually refine solutions over successive steps. This section reviews key approaches relevant to fuel pricing and allocation in maritime models, understanding this is crucial for grasping how the algorithm within NavigaTE operates.

2.6.1 Iterative Algorithms and the Simplex Method

Iterative algorithms approach optimisation problems by progressively refining solutions until convergence is achieved. A common example is the simplex method, widely applied in linear programming, which systematically moves between feasible solutions, improving the objective function at each step. Its robustness and transparency make it particularly well-suited for applications involving constrained resource allocation.

2.6.2 Heuristics

Heuristic methods provide practical alternatives in cases where exact optimisation is computationally infeasible. Instead of guaranteeing perfect optimality, they focus on delivering good enough solutions within reasonable time frames. These approaches are particularly valuable in large-scale or complex systems, such as logistics, scheduling, or market simulations, where quick decision-making can be more critical than absolute mathematical precision [39, 40].

In all cases, the appeal of heuristic methods lies in their flexibility and speed, making them ideal for real-time or exploratory simulations.

2.6.3 Convergence Methods

Convergence methods are designed to guide iterative processes toward a stable and reliable solution. In large-scale applications, both the speed and robustness of convergence play a critical role in determining whether an algorithm is practical and efficient in real-world settings.

Some **types of convergence** include *global convergence*, which guarantees convergence to the global optimum from any starting point [41]; *local convergence* that assures convergence only when the starting point is sufficiently close to a local optimum [42]. *Linear convergence* indicates that the error between the estimate and the true solution decreases by a constant ratio with each iteration [43]. In contrast, *superlinear* or *quadratic convergence*, often observed in Newton-type methods,describes an accelerating rate of convergence at each step [44].

Stopping criteria usually include a small change in the objective value, minimal updates in variables, or full satisfaction of constraints.

2.6.4 Bisection Method for Market Clearing

Originally a root-finding technique, the *bisection method* narrows an interval $[a, b]$ by evaluating the midpoint $c = \frac{a+b}{2}$, and iteratively reducing the interval based on the sign of the function at c [45]. In this project, the method is adapted to determine market-clearing prices: instead of locating a root, it finds the price at which supply roughly matches demand.

Though the classical requirement $f(a) \cdot f(b) < 0$ does not apply in this work, the principle of convergence still holds due to the monotonic relationship between price and supply-demand balance. High prices cause oversupply; low prices result in unmet demand. By narrowing the interval between a price floor and ceiling, the algorithm converges to a practical price, close to the equilibrium that supports market realism in the model.

2.6.5 Method of Successive Averages (MSA)

The Method of Successive Averages (MSA) is another iterative approach often used in traffic flow and energy systems. It incrementally blends previous and current estimates to smooth out fluctuations and avoid premature convergence [46].

The generic update formula is:

$$x^{(n+1)} = \alpha_n \cdot x^{(n)} + (1 - \alpha_n) \cdot \text{Calculation}(x^{(n)}), \tag{2.1}$$

where:

- $x^{(n)}$ is the estimate at iteration n,
- $\alpha_n = \frac{1}{n+1}$ is the averaging factor,
- Calculation$(x^{(n)})$ is the updated estimate based on the current state.

Variants of MSA include:

- **Standard MSA**: Uses a simple $1/n$ decay.
- **Weighted MSA**: Assigns higher importance to more recent updates.
- **Adaptive Averaging**: Adjusts weights dynamically to improve stability.
- **MSA with Memory Reset**: Periodically resets the average to prevent stagnation.
- **MSA with Polyak Step-Size**: Introduces adaptive step sizes for more controlled convergence, using the form $\alpha_k = \frac{1}{k^p}$ for $p > 0$.

MSA is particularly well-suited for equilibrium problems involving feedback loops and decentralised decisions, such as dynamic fuel pricing and multi-agent transport systems.

The iterative methods introduced in this section form the practical backbone of NavigaTE's fuel pricing and allocation logic. Techniques like the bisection method are used to find market-clearing prices by balancing supply and demand under real world constraints and regulatory signals. While this work focuses on bisection, more advanced methods, such as the Method of Successive Averages (MSA), are explored for future versions to handle more complex equilibrium behaviour.

3 NavigaTE Framework

3.1 Framework Overview

NavigaTE is a system-level modelling framework that combines vessel operations, fuel supply, and environmental regulations into a single optimisation platform. This chapter gives a clear description of the core structure of the existing bunkering module. It outlines the main purpose of the model, explains its key components, and describes the step-by-step sequence the model follows during each year of simulation.

Having this overview is important to better understand the new developments introduced in a later stage of this thesis. It also helps distinguish which parts of the model remain as originally designed, and which have been expanded to include these new market mechanisms.

3.1.1 Bunker Algorithm's Framework

The Bunker Algorithm is a key component of the NavigaTE framework, responsible for optimising fuel allocation across vessels and ports while considering market dynamics, emissions, and regulatory constraints. Its main functionalities include:

- **Fair-Share Allocation**: Ensures fair distribution across agents of fuel based on supply and demand constraints.
- **Shadow Prices**: Calculates marginal costs of relaxing supply constraints to guide optimal fuel allocation.
- **Market Dynamics**: Adjusts fuel prices dynamically for different market types (e.g., local, global, emerging).
- **Emission and Policy Integration**: Incorporates emissions, levy penalties, and regulatory constraints into the optimisation process.
- **Optimisation**: Uses linear programming (via Gurobi) to iteratively solve the bunkering problem and achieve convergence.

3.1.2 Algorithm Workflow

The bunkering and market pricing routine follow four phases:

1. **Initialisation**
   Sets up the linear programming model with the required inputs (vessel data, fuel options, regulatory parameters). Dynamic properties such as policy states, emission factors and initial fair-share caps are also initialised at this stage.
2. **Build & Update**
   At every simulation step, the model is *built* (first step) or *updated* (subsequent steps). Decision variables, the objective function, and all constraints are created or modified to reflect the current system state. This process includes:
   - **Clean-Up**: redundant elements are removed, outdated vessels or fuels, obsolete constraints, and unused variables, to keep the model compact.
   - **Definition of Variables, Objectives and Constraints**
     – *Variables*: bunkered fuels, fuel consumption, emissions released or stored, regulation variables.

– *Objectives*: minimise total cost (fuel + emissions storage); secondary objectives enforce inter-port fuel consistency and regulatory compliance.

– *Constraints*: fuel mass balance, energy conservation, tank capacity, emission caps, regional bunkering limits, and equality constraints for fair distribution.

3. **Solve Methods**
By default, the model solves using fair-share allocation, iteratively adjusting allocations and active constraints until convergence. If market dynamics are activated, a two-stage algorithm is used: a ceiling iteration identifies binding constraints, followed by a bisection loop that resolves market-clearing prices through successive fair-share solves.

4. **Transfer Methods**
Outputs such as fuel allocations and emissions compliance are moved forward to the next time step. Vessel and port objects are updated with bunkering decisions and fuel consumption figures.

3.2 Core Frameworks: Fair-Share Allocation and Market-Clearing

3.2.1 Fair-Share in NavigaTE's Bunkering Algorithm

In the NavigaTE bunkering optimisation framework, the Fair-Share Allocation mechanism ensures that vessels initially receive fuel supply from ports based on a proportional, equitable distribution of available resources. This is particularly important in emerging markets where no real-time market price signal exists yet, and the allocation of fuel must respect supply constraints while also reflecting fair treatment across vessels.

These are the key characteristics that ensure this algorithm works:

- *Initialisation*: Each vessel is allocated a share of the available fuel at each port proportional to a precomputed fair-share factor and available supply.
- *Update Loop*: After solving the optimisation model, unused portions of allocated fair-share are released and reallocated to other vessels in need, iteratively improving the solution.
- *Convergence*: This loop continues until the allocation stabilises (within a defined numerical tolerance), ensuring supply is not wasted and allocations are as efficient as possible.
- *Adaptivity*: Fair-share is updated dynamically based on vessel behaviour (actual bunker use vs. allocation) and the global remaining fuel pool.

This approach ensures a fair distribution of resources while also laying the groundwork for price formation in interconnected markets. Once constraints become active, the system naturally moves toward an economically meaningful equilibrium.

This approach uses only the available supply and each vessel's fair share factor to guide allocation, ensuring that fuel is directed to vessels with greater operational needs. In cases where policies like emission caps restrict total fuel availability, the same fair share logic applies to the reduced supply. As a result, the system automatically redistributes fuel across vessels, allowing for a clear understanding of how regulatory limits affect distribution fairness, even before introducing any price mechanisms.

3.2.2 Market Clearing Mechanism

The market clearing mechanism implemented in this module draws inspiration from classical Walrasian equilibrium theory, as explained in section 2.5.2, where prices adjust iteratively to balance supply and demand across a decentralised system. In the context of multi-fuel maritime logistics, this translates into assigning implicit marginal prices π_{pf} to each port-fuel combination.

These prices act as coordination variables that guide the distribution of limited fuel resources across competing vessels.

The model handles allocation according to the selected market structure. In a *global* market, one uniform price per fuel applies across all ports and vessels. In a *local* market, prices vary by port but remain equal for all vessels bunkering at that location. In an *emerging* market, the system assigns prices at the most granular level, each vessel-port-fuel tuple, simulating a fragmented market where prices are shaped by bilateral constraints rather than centralised clearing. In each configuration, allocation decisions are governed by marginal valuations derived from the solution of a linear program. Fuel is allocated to the highest-valued users until supply is exhausted, mimicking competitive bidding behaviour in real-world exchanges. These marginal valuations are not pre assumed; instead, they emerge endogenously from the shadow prices of the optimisation, which reflect local scarcity and the economic cost of diverting fuel elsewhere.

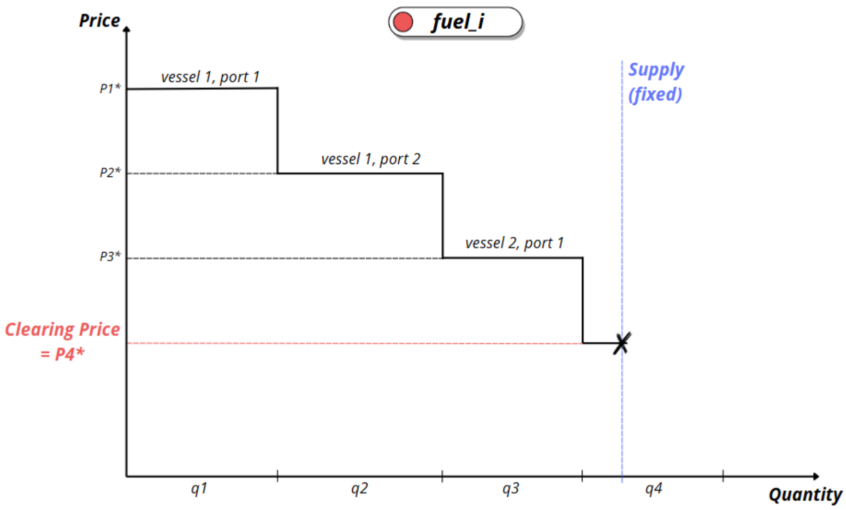


Figure 3.1: Staircase demand curve representation in NavigaTE's global market setting. Each step reflects a vessel-port bid for fuel `fuel_i`, ordered by price. The market-clearing price ($P4^*$) is set where aggregate demand equals fixed supply ($q4$).

At each iteration, the allocation model is solved under the current set of port-fuel prices, determining which vessel demands are met. If imbalances remain, such as excess demand at a port or underutilised capacity, the prices π_{pf} are incrementally adjusted. Ports experiencing persistent over-demand see their prices rise, thereby discouraging further allocation, while under-demanded ports may maintain or reduce their prices. This feedback loop continues until no vessel can improve its allocation given the prevailing price signals and all supplies are fully utilised or declared infeasible due to constraints.

The clearing mechanism thus produces a partial market equilibrium in which:

- All fuel supply is allocated (within feasibility and capacity limits).
- No vessel can obtain more fuel at a lower marginal cost.
- Prices reflect the scarcity and urgency of allocation at each location.

This approach offers a distinct advantage by aligning incentives on both sides of the market. From the supplier's perspective, the staircase mechanism ensures that fuel is sold at the highest feasible prices, thereby maximising revenue while guaranteeing full clearance of available supply. Simultaneously, for vessels as buyers, fuel is only acquired at or below their implicit willingness to pay, ensuring that no allocation is inefficient or economically unjustified. This dual-optimality, clearing the market while respecting the marginal valuation of each actor, represents a key strength of the mechanism, balancing efficiency and individual rationality without imposing centralised fairness constraints. As a result, the system reaches a state where supply meets demand through price signals alone, embodying a decentralised yet optimal distribution of scarce maritime energy resources.

3.3 System Flowchart

3.3.1 NavigaTE's Flowchart

This section aims to provide the reader with a visual roadmap helps to follow how data, decisions, and results circulate and how algorithms are structured inside NavigaTE.

In Figure 3.2, the green block on the left represents the full NavigaTE package. The grey block in the centre denotes the Bunker sub-package, while the darker shaded grey box inside points to the actual Python file `BunkerAlgorithm.py`. The blue stack on the right breaks that file into its main function blocks.

These two right-hand blocks: the Bunker folder and, within it, `BunkerAlgorithm.py`, are the only parts of NavigaTE that have been revised to incorporate the market-pricing logic presented in Chapter 5; all other modules remain unchanged and serve solely as data providers and result collectors.

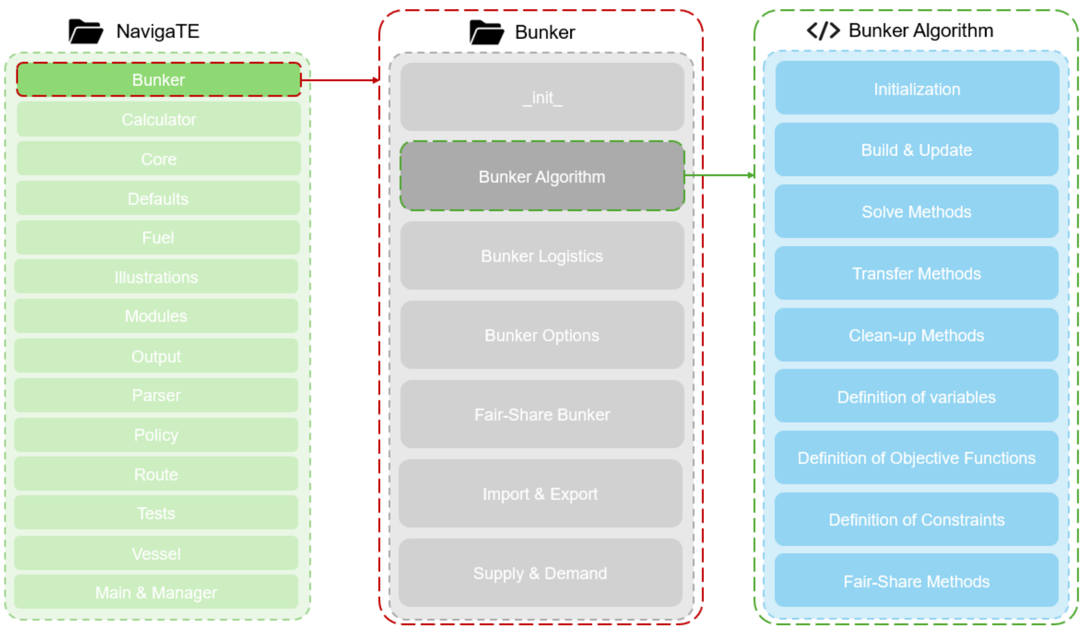


Figure 3.2: Overview of the NavigaTE architecture with emphasis on the modified `BunkerAlgorithm.py`, the only module updated to include market price coordination logic.

3.3.2 Bunker Algorithm's Flowchart

The following three diagrams summarise the operational logic of NavigaTE's bunkering module and highlight the extensions developed in this thesis. First Figure 3.3 represents the overall bunker algorithm flowchart. Figures 3.4 and 3.5 take a deep dive into the bunker algorithm's flowchart. First Figure3.4 takes a deeper look into the Fair Share algorithm and how it works, and second, Figure 3.5 is a visualisation of the Market Clearing mechanism in the Navigate overview.

A simple colour legend is used throughout the charts. Grey boxes represent legacy steps that were left unchanged; blue boxes mark the components added or modified in this research; a red dashed frame encloses the outer loop, which repeats until a market-clearing price is achieved; a green dashed frame encloses the inner (bisection) loop, where the provisional price is updated and each vessel's LP is re-optimised.

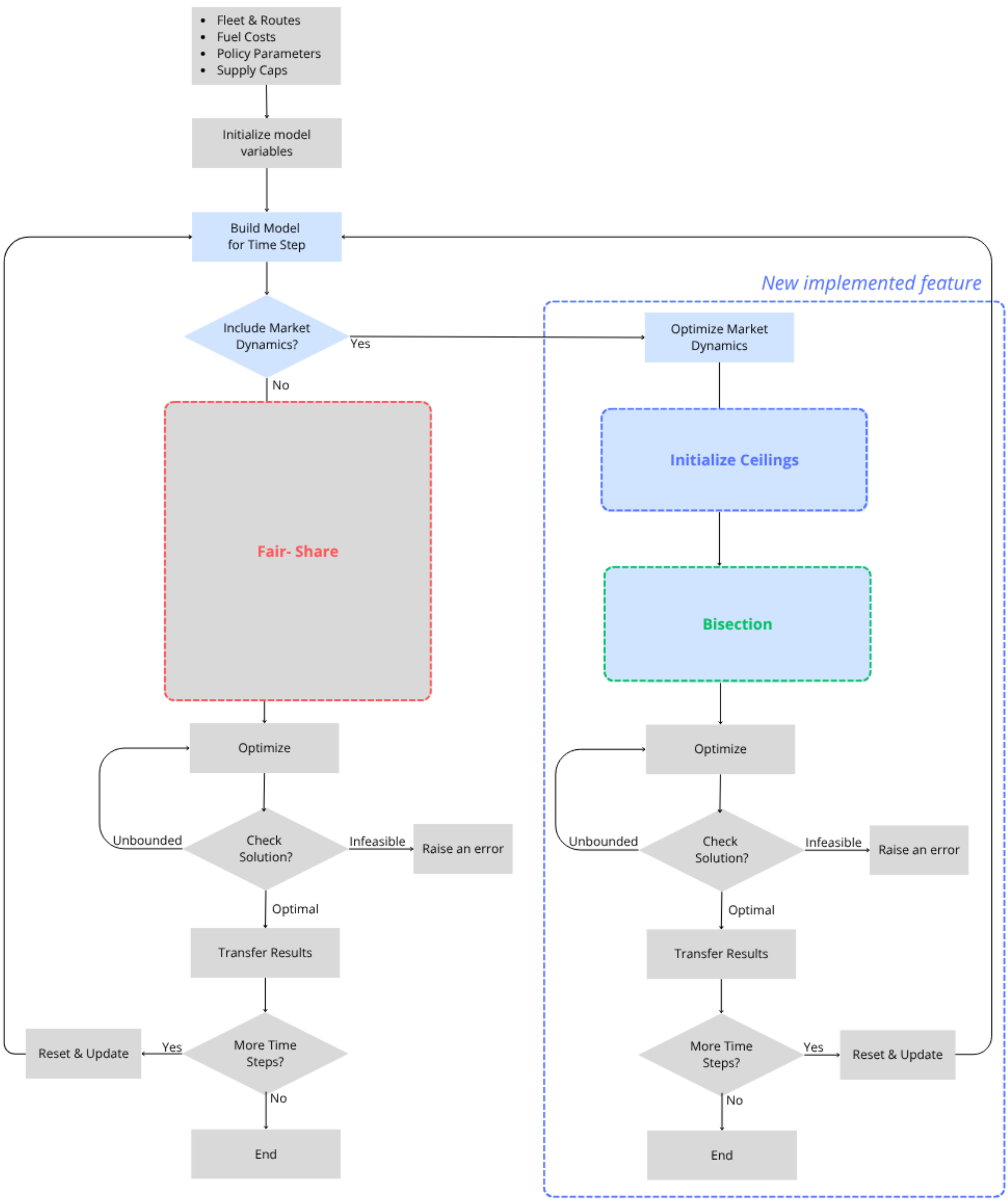


Figure 3.3: Flowchart of NavigaTE's Bunker Algorithm which highlights the modified and involved areas for the market pricing feature on a high level

Fair-Share Flowchart

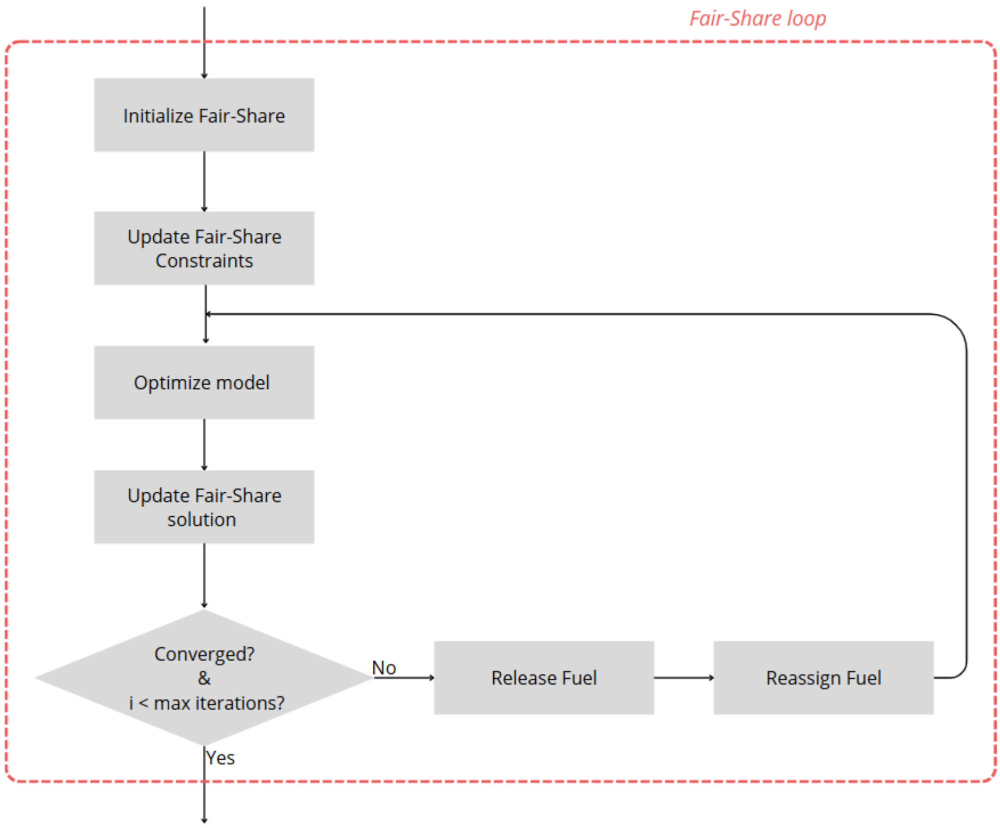


Figure 3.4: Detailed view of the Fair-Share allocation in NavigaTE, illustrating how the model iteratively updates constraints and reassigns fuel until convergence.

Market-Clearing Flowchart

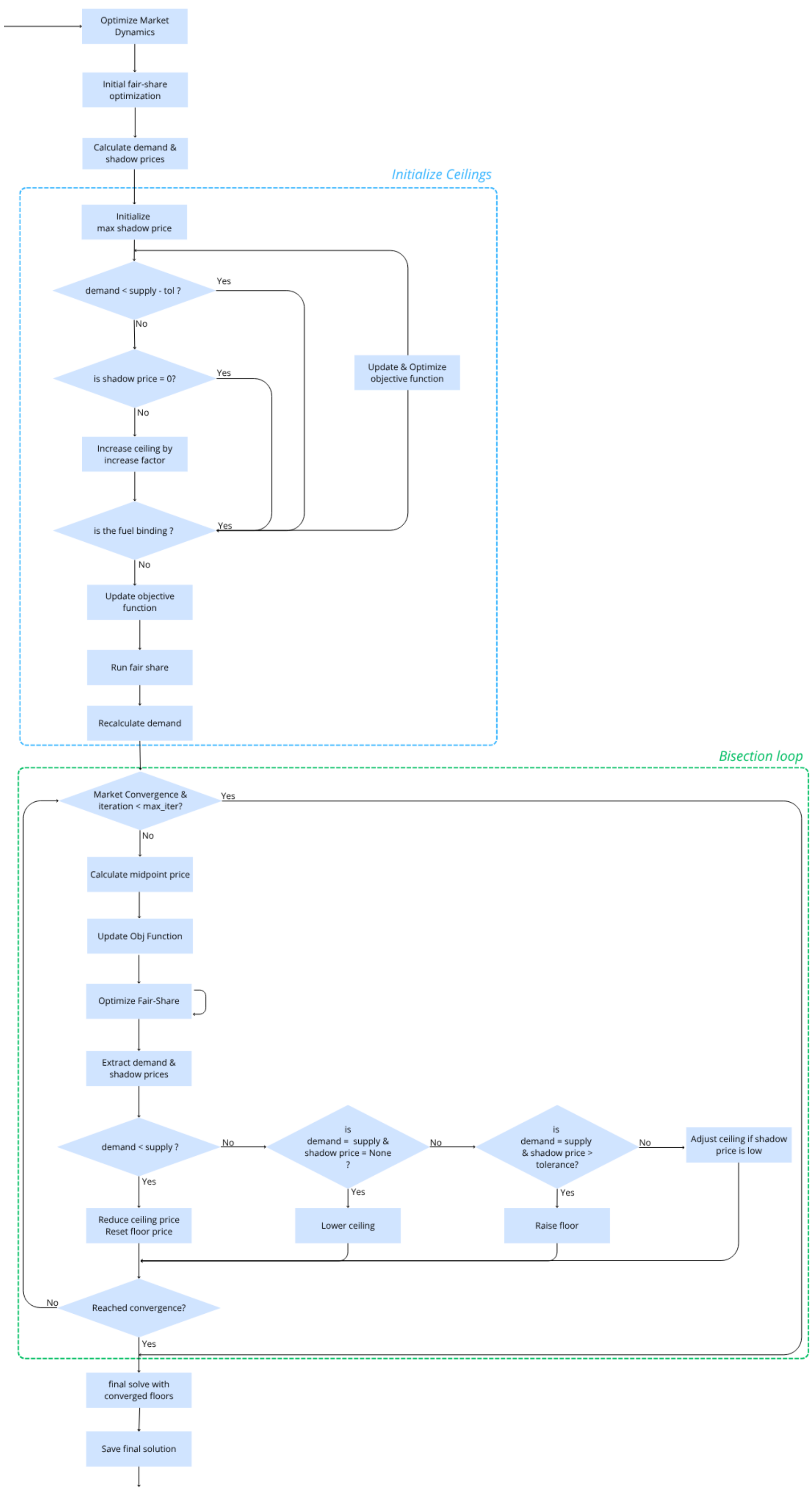


Figure 3.5: Structure of the Market Dynamics module in NavigaTE, highlighting the ceiling initialisation and the iterative bisection loop used to reach market price equilibrium.

3.4 Configuration File Structure

The NavigaTE modelling framework is structured around a set of configuration files that, together with the Python back end, fully define and execute simulation scenarios. The process is initiated through a main file with the `.NAV` extension, which is run via the command line using `navigate <filename>.NAV`. This file acts as the entry point and includes a sequence of `.inc` files containing the simulation parameters.

The `.inc` configuration files define the core model assumptions: vessel characteristics, technology availability, regulatory timelines, fuel properties, and other relevant inputs. These files control how the simulation evolves over time, enabling full transparency and flexibility in scenario design.

Upon execution, a `.PRT` file is generated, which provides logs, warnings, and summary information about the run. This output helps users validate model performance and troubleshoot potential issues during scenario development.

4 Methodology

This chapter describes the integration of the new market pricing mechanism into NavigaTE and explains how the model was used to carry out simulations focused on policy analysis. It begins with a presentation of the main modelling assumptions, then moves on to explain the preparation of the data and the steps involved in implementing the algorithm, ending with a discussion of transparency considerations and the limitations of the model.

4.1 Modelling Data Assumptions

4.1.1 Development-stage assumptions

The test environment is built using a structured set of configuration files that define the initial conditions, operational rules, and temporal dynamics of the simulated maritime fuel system. In total, 38 configuration files, listed in Appendix D, support the simulation, although only the most relevant ones are discussed in this section. These files handle the availability of fuels, regulatory parameters, market structure, and vessel technology interactions.

To verify the correct functioning of the model, a controlled test scenario is implemented using artificial input data provided by the Maersk Mc-Kinney Møller Center for Zero Carbon Shipping. The purpose of this phase is purely technical: ensure that the model correctly matches fuel demand and supply with the generation of a price, that the linear programming sub-problems reach valid optima, and that the outer price adjustment loop converges as expected. Fuel supply caps are simplified and held constant across types, but vessel bunkering remains constrained by the network structure, meaning vessels can only refuel at permitted ports. These deliberately abstracted conditions provide a stable testing ground for the model's core mechanics, without the added complexity of realistic operational data.

4.1.2 Simulation-stage assumptions

The final simulation stage relies on a real-world base case provided by the Maersk Mc-Kinney Møller Center for Zero Carbon Shipping. The input data are the result of internal modelling efforts, parameter calibrations, and discretisations based on IMO publications, literature review, and knowledge from partner companies and internal experts at the Center. The population of interest is the global merchant fleet (international and domestic) and the set of regions (Africa, Americas, Asia, Europe and Middle East) with significant bunkering activity. Vessels are grouped into twenty segments based on the type of commodity transported (e.g., bulk carriers, tankers, container ships) and vessel size. Within each segment, further discretisation captures the range of technical configurations, defined by engine technology and corresponding fuel compatibility.

The total amount of input files to model the final simulation is over 1.200, but only the relevant files are explained.

Fuels - Supply

The fuel supply space includes conventional and alternative fuels, grouped into five families:

- **Oil-based fuels**: e.g. LSFO.
- **Methane variants**: Including fossil LNG and bio-methane.
- **Methanol**: Bio and E-methanol.
- **Amonia**: Electro and Blue amonia.
- **Other emerging fuels**.

Each fuel type is assigned a production cost, emission factor, and energy density, and supply limits vary by port and year according to infrastructure assumptions.

Vessels - Demand

The global merchant fleet is modelled using 20 representative vessel classes that span the major shipping segments. These include:

- **Bulk carriers**: Capesize, Panamax, Handy.
- **Containers**: 3,500 TEU, 8,000 TEU, 15,000 TEU.
- **Cruise ships**: 25k GT, 100k GT, 175k GT.
- **Tankers**: 35k DWT, 100k DWT, 300k DWT.
- **Other types**: Ferries, gas carriers, general cargo, offshore, RORO 4000, RORO 7000, tugs, and other.

Each class reflects a typical operational profile and size category, and includes multiple main engine technology options corresponding to different fuel types. Most vessels are assumed to operate with dual-fuel engines with different tanks, combining a conventional oil-based fuel with one alternative fuel, typically ammonia, methane, or methanol, regardless of production pathway.

Fuel demand is generated as part of the optimisation process, where each vessel determines its preferred fuel mix based on cost, compliance with emissions regulations, and the availability of different fuel options. This formulation allows the model to capture realistic behavioural responses across a variety of vessel types and simulation conditions.

Levies

Levies are implemented as additive costs applied at the time of bunkering. They are defined per port and fuel type and reflect the carbon content of each fuel. They expressed mathematically as:

$$\text{Levy}_{p,F} = \sum_{L \in \mathcal{L}_p} \xi_p^L \cdot \text{EC}_{L,F}^{p,\text{ref}}$$

where ξ_p^L is the levy rate, measured in cost per unit mass of emissions, applied to levy L at port p, and $\text{EC}_{L,F}^{p,\text{ref}}$ is the reference emissions coefficient for fuel F under that levy. These levies are incorporated directly into the LP's objective function as part of the cost term, influencing bunkering decisions by adjusting the relative attractiveness of each fuel.

The levies apply to a range of greenhouse gases, including carbon dioxide, methane, and nitrous oxide, and are implemented according to scenarios guided by the IMO. Within the model, their function is to encourage the use of fuels with lower emissions by reducing the cost competitiveness of fuels with higher emissions. In practice, the levies influence the shape of the demand curve by incorporating environmental costs into the economic decision process.

Regulations

Emissions regulations are introduced to enforce greenhouse gas intensity limits within the maritime system. These constraints can lead to either penalties or financial rewards, depending on whether a vessel complies with its assigned emissions threshold. Each regulation is defined by several attributes, including its jurisdictional coverage, which distinguishes emissions based on where they occur: *intra* emissions take place entirely within the regulated area, *inter* emissions arise from outbound voyages starting within the jurisdiction, and *extra* emissions occur entirely outside the regulated region.

In practice, the implementation of these regulations follows a Marginal Abatement Cost Curve (MACC) logic. Each vessel is assigned a maximum allowable emission intensity based on IMO targets. If this limit is exceeded, a penalty is applied up to a predefined ceiling price. Shipowners may then decide whether it is economically more efficient to switch fuels or pay the penalty, depending on marginal abatement costs.

The model includes two distinct compliance schemes:

- **Flexible compliance** permits trading of surplus fuel allowances between ships. This market mechanism allows more efficient vessels to sell excess credits to less efficient ones, lowering the system-wide cost of compliance.
- **Individual compliance** enforces emissions limits at the ship level. Vessels must meet their assigned targets independently, leading to higher marginal abatement pressures for older or less efficient ships.

4.2 Research Strategy and Study Design

The thesis follows a *quantitative, simulation-based* strategy in which each scenario functions as an experiment on a virtual fleet. The design is best described as *exploratory–descriptive*: the intention is to observe how price formation and bunkering choices evolve once market feedback is allowed, rather than to test a single null hypothesis.

4.3 Tools Utilised

The development, implementation, and execution of the fuel pricing module and scenario simulations relies on a variety of software tools, each serving a specific role in the research workflow. The following list summarises the main tools and platforms employed throughout this thesis:

- **Python**: The primary programming language used in the development of the pricing algorithm and in running the NavigaTE model. All simulations were executed using Python version 3.12. Key libraries include:
  - `Pandas`, `NumPy`: for data handling and numerical manipulation.
  - `Matplotlib`: for plot generation and visualisation.
  - `Gurobipy`: interface to the Gurobi solver, used for linear programming optimisation.
  - `os`, `sys`: for file and environment management.
  - `NavigaTE`: the modular simulation framework under development, within which this project was conducted.
- **GitHub**: Used for version control and collaborative development. The full NavigaTE codebase is hosted in a private GitHub repository, allowing systematic tracking of contributions and updates.
- **Visual Studio Code**: Code editor used for algorithm design and code development. GitHub Copilot was used during prototyping to streamline function writing and syntax generation.
- **PyCharm**: The main integrated development environment (IDE) used to execute and debug the full simulation pipeline. PyCharm enables efficient execution of the NavigaTE model without requiring repeated reinstallation or manual launching via PowerShell.
- **Notepad**: A simple text editor employed to modify and manage configuration files (`.inc` and `.nav`).

Together, these tools provided a robust environment for iterative development, performance monitoring, and scenario execution, while maintaining full flexibility for future updates or extensions to the model.

4.4 Outputs and Analysis Techniques

This section presents simulation outputs and the experimental strategy used to assess how endogenous price formation influences fuel choice and system dynamics, compared to conventional cost-based optimisation still common in maritime decarbonisation models.

This analysis makes *two main academic contributions*. First, *analytically*, it examines how market prices evolve under varying regulatory and structural conditions, generating dynamic price signals that better reflect fuel scarcity, competitiveness, and sustainability than fixed cost assumptions. Second, *mathematically*, it assesses the value of introducing pricing mechanisms that respond to system conditions in maritime energy models. Since most existing frameworks rely solely on static costs, the study quantifies how results change when shadow prices are used, and evaluates whether this added complexity leads to improvements that are relevant for future decision-making.

To do so, the model is run sixteen times, covering a 4×4 grid of market types and policy regimes. Each run corresponds to a combination of one market configuration and one regulatory environment. The market configurations include:

1. **Cost-only baseline**: Prices are fixed and correspond to base fuel costs. The new dynamic market logic is not applied.

2. **Global market**: A unified price is applied to each fuel, equal across all ports and vessel types.

3. **Local market**: Each port establishes its own price for each fuel, independent of other regions.

4. **Emerging market**: A scenario simulating an emerging market with heterogeneous prices across vessels and ports, based on fixed costs, regulations, and fair-share allocation, without endogenous price formation.

For each of these four market types, the model is tested under four regulatory configurations: `No regulations`, `Regulations with Flexibility`, `Regulations without Flexibility` and `Levy`. All these different market types and scenarios are explained in detail in Chapter 6.

All runs use a modified `basecase.nav` scenario limited to international routes, focusing fuel use and regulatory exposure in key regions to improve interpretability.

4.4.1 Outputs Analysed

From each simulation run, the following key outputs are extracted:

- **Final fuel prices**: In both global and local market configurations, fuel prices are extracted at the global level and by port. In the emerging market configuration, prices are reported as a weighted average across vessels.

- **Fuel volumes**: Total quantities of fuel bunkered, disaggregated by fuel type and by port.

- **Convergence behaviour**: Number of iterations and linear program solves required to meet convergence criteria. This metric is used to evaluate the efficiency of the algorithm.

- **Dual values and shadow prices**: Used to confirm that price signals emerge only in cases where markets are constrained.

- **Emissions and regulation compliance**: Total emissions produced, along with any resulting penalties or credit transactions under regulatory schemes.
- **System costs**: Overall system expenditure, including baseline fuel costs, levies, and penalties related to regulatory compliance.
- **Runtime and computational load**: Total runtime of each simulation, providing insight into the scalability of the model and identifying opportunities for performance improvement.

These outputs are stored in the form of structured spreadsheets and visual reports for each of the sixteen model runs. Comparative analysis across the different combinations of market conditions and policy settings allows the effects of dynamic pricing to be studied, highlights behavioural changes in fuel selection, and evaluates the robustness of the model under different regulatory environments.

Particular attention is given to the interaction between internally generated prices, emissions levies, and emissions caps. The analysis considers how these interactions influence convergence behaviour and whether the inclusion of greater model complexity leads to meaningful changes in economic signals and fuel distribution patterns. These findings contribute to both the validation of the modelling approach and its relevance for informing policy.

4.5 Ethical Considerations and Transparency

This study involves no personal or sensitive data. All input sources are either open-access, publicly available, or used under valid licenses granted by institutional partners, notably the Maersk Mc-Kinney Møller Center for Zero Carbon Shipping. No confidential information or commercially sensitive algorithms are exposed in the analysis, and no human subjects are involved.

All code developed for this project has been version-controlled and documented. The project uses modular and auditable configuration files for scenario definition, fuel availability, and regulation logic. The structure ensures that experiments are replicable and that key modelling choices can be clearly traced.

This section does not attempt to justify the economic conclusions of the model but acknowledges that its correct functioning depends on a series of technical and design assumptions. These are explicitly referenced in the interpretation of results.

Chapter 7 revisit these assumptions to assess their quantitative impact on model performance and outputs. There, we explore how the outputs of this methodology - from both controlled test cases and applied scenarios - are influenced by model design, including the price mechanisms and assumptions laid out here.

4.6 Challenges Encountered, Limitations & Solutions

The development and integration of a dynamic market-pricing system into NavigaTE involved multiple technical and conceptual difficulties. This section summarises these along with the main assumptions and simplifications that may influence the model's validity.

4.6.1 Technical and Structural Challenges

- **Code integration**: The original structure of NavigaTE was not designed for dynamic price formation. A new bisection loop and modular LP framework were implemented to manage price updates, equilibrium detection, and shadow price extraction.
- **Performance tuning**: Early price update mechanisms failed to converge reliably. A switch was made to an external bisection loop, with warm-starts and carefully defined convergence tolerances to ensure computational efficiency and numerical stability.

- **Debugging and versioning**: As the model evolved, several interdependencies between fuel types, regulations, and vessel-port links required continuous testing and staged debugging. Modularisation of configuration files helped isolate bugs and improved the traceability of logic errors.

4.6.2 Conceptual Modelling Limitations

- **Demand-driven supply with external adjustment**: Fuel supply responds to demand but is not optimised within the linear programming model itself. Instead, fuel availability is fixed within each time step and provided as an external input, but can vary across time steps based on scenario assumptions. This setup allows supply to respond to long-term demand trends without being dynamically adjusted during price iteration.

- **Forward-looking investment under uncertainty**: Investment and bunkering decisions are made at each time-step based on current expectations of the future. While these expectations guide choices, actual future conditions often diverge, capturing real-world uncertainty and decision-making dynamics.

- **Linear programming and assumed efficiency**: LP methods implicitly assume that actors make optimal decisions, which may be unrealistic in a fragmented and competitive shipping market. While the alternative, equal scaling or agent-based approaches, would reduce this assumption, LP remains the established benchmark method for constrained optimisation problems.

- **Fleet aggregation**: Vessels are grouped into representative classes by size and type. While sufficient for system-wide trends, this may obscure the behaviour of specialised vessel types or extreme cases.

- **Emerging Market simplification**: In the Emerging Market configuration, the model does not use dynamic price discovery. Instead, a static fair-share allocation is used, assigning bunker quantities based on vessel-port-fuel cost rankings. No price convergence is attempted. This simplification ensures compatibility with the NavigaTE framework but means the price signals in this scenario are not endogenously generated.

4.6.3 Design Adjustments and Technical Solutions

Several adjustments were implemented to ensure model consistency and improve computational performance:

- Parameters were calibrated to maintain consistency across technologies, levies, and regulations prior to running scenarios.

- A bisection algorithm was introduced to replace earlier update methods, improving convergence stability in the market-clearing process.

- Performance metrics such as runtime, iteration counts, and solver calls were logged to support the efficiency analysis in Chapter 7.

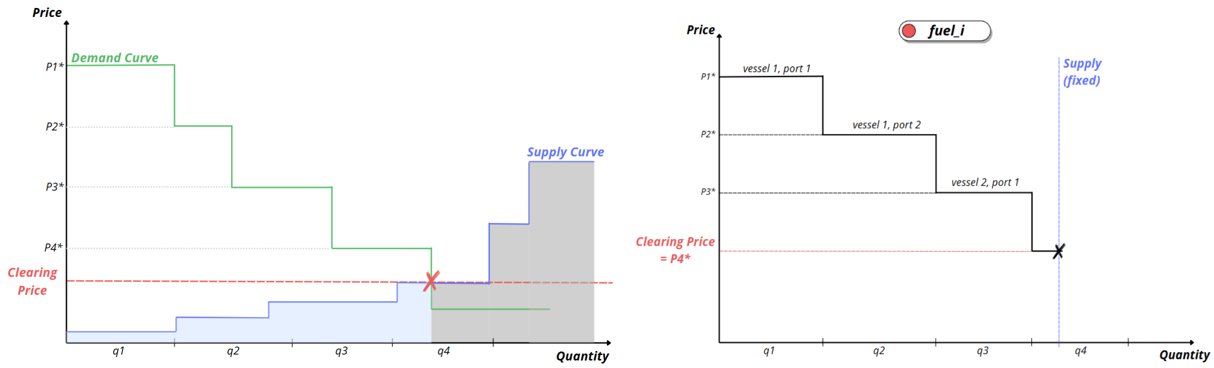
5 Market-Based Fuel Pricing Module

5.1 Module Overview

This section presents the design and implementation of the new fuel allocation module developed within the NavigaTE framework, which applies market-based coordination principles inspired by classical energy market theory and linear programming theory. The module follows a logic similar to a Walrasian market equilibrium, where fuel is allocated among vessels and ports based on an iterative process of price formation and supply-demand balancing.

At the core of this module is a price adjustment process that gradually increases the marginal price at each port and fuel combination until demand matches the available supply. This clearing mechanism works like a staircase: vessel-port-fuel combinations are ranked based on their marginal value, and fuel is sequentially allocated to those with the highest valuation until no supply remains. Unlike approaches that rely on declared willingness to pay, this valuation is calculated internally by the model's optimisation structure and continuously updates based on evolving demand and supply conditions.

Figure 5.1 illustrates this concept. The left Figure 5.1a shows the general staircase-clearing principle commonly used in energy markets, while the right Figure 5.1b shows how this logic is applied within NavigaTE's fuel pricing algorithm.



(a) Representation of a generic energy market-clearing mechanism

(b) Stair-case implementation in NavigaTE where demand cannot go over supply

Figure 5.1: Visual comparison between general clearing theory and its implementation in NavigaTE's constrained fuel market

This shift from an equity-based approach to a price-driven allocation marks a conceptual evolution in the model's design, moving from fairness rules to decentralised market coordination. The prices π_{pf} act as market signals: they rise when demand exceeds supply and fall when there is a surplus, naturally directing fuel flows toward the vessels and ports where they create the highest value in each iteration.

The approach is made out of three primary components:

- An *allocation engine* that solves the optimisation model using current price signals.
- A *price updating routine* that adjusts π_{pf} based on over-demanded or under-utilised resources.
- A *convergence controller* that monitors allocation changes and stops iterations once approximate market-clearing is achieved.

The setup keeps full compatibility with the original fair-share method, making it easy to switch between approaches focused on fairness and those that follow market signals. This kind of flexibility matters, especially when testing different policies, since users may want to compare outcomes where fairness takes priority versus those that focus more on economic efficiency under different conditions.

The rest of this section first explains how the fair-share system works (Section 5.1.1), then moves on to how the model handles market-clearing (Section 5.1.2), and concludes with a description of the iterative coordination process used to reach equilibrium (Section 5.1.3). This module is central for later analysis, including how fuels are distributed in competitive settings, where bottlenecks may appear, and how the system responds to changes in pricing.

5.1.1 Simplified Concept of the Approach

To make the logic behind the market-clearing algorithm accessible to a broader audience, a simplified example is presented. This toy model mimics the key structure of the NavigaTE bunker pricing mechanism but strips it down to its essential components.

Problem Setup

Assume a fleet consists of two vessels that consume fuel with three types of fuels available:

- **Fuel 1** (b_1): moderately priced, with a limited supply capacity (c_1).
- **Fuel 2** (b_2): more expensive but also constrained (c_2).
- **Unconstrained Fuel** (b_{unc}): highly priced but available in unlimited quantity.

The objective is to **minimise the total fuel cost**, represented by the following linear program:

$$\begin{aligned} \text{Minimise} \quad & 50b_1 + 100b_2 + 200b_{\text{unc}} \\ \text{Subject to:} \quad & b_1 \leq c_1 \quad (100) \\ & b_2 \leq c_2 \quad (100) \\ & b_1 + b_2 + b_{\text{unc}} = D \quad (500) \end{aligned}$$

Here, $D = 500$ is the total demand, and each fuel has a per-unit cost: $p_1 = 50$, $p_2 = 100$, and $p_{\text{unc}} = 200$. The aim is to allocate fuel to minimise cost while respecting supply constraints.

Solution

Solving this system provides the following allocation:

$$b_1 = 100, \quad b_2 = 100, \quad b_{\text{unc}} = 300$$

The constrained (*cheaper*) fuels are consumed fully first, and the remaining demand is met using the more expensive unconstrained fuel.

The **shadow prices** (*dual values*) indicate the marginal value of relaxing each constraint. These dual values π_1 and π_2 are obtained by solving the primal LP and reading the dual variables associated with the capacity constraints $b_1 \leq c_1$ and $b_2 \leq c_2$; in any LP solver these correspond to the Lagrange multipliers that quantify the cost saving of relaxing the constraint by one unit. In this case:

$$\pi_1 = -150 \quad \text{(for constraint on } b_1\text{)}, \quad \pi_2 = -100 \quad \text{(for } b_2\text{)}$$

This means that if we could increase the capacity of fuel 1 by one unit, the total cost would decrease by \$150, highlighting the economic value of that constraint.

Impact of Changing Capacities

A new scenario where fuel 2 becomes more available is simulated:

$$c_1 = 100, \quad c_2 = 450$$

Re-solving the model:

$$b_1 = 100, \quad b_2 = 400, \quad b_{\text{unc}} = 0$$

Here, the system avoids the expensive fuel altogether. The shadow prices also shift:

$$\pi_1 = -50, \quad \pi_2 = 0$$

Fuel 1 remains valuable, but relaxing Fuel 2's constraint has no further cost benefit, it is no longer binding. In simple terms, since there is extra availability (or slack) of Fuel 2, it becomes the reference point for price competition. Not everyone is willing to pay a high price for it, so it cannot command a premium. As a result, the *"price to beat"* in the market is set by Fuel 2 rather than a more expensive option like Fuel 3.

To support this example, a Python implementation using Gurobi is included in Appendix A.1.

5.1.2 Proof-of-Concept Prototype: First Working Model

Building on the two fuel, two vessel example introduced in Section 5.1.1, a compact but complete proof of concept model is developed to simulate dynamic price formation within a realistic maritime fuel market context. This minimal viable product is constructed to capture system behaviour across multiple years under supply constraints, emissions penalties, and iterative price adjustments. The prototype extends the problem dimensionality to include several fuel types, year by year supply variation, emissions thresholds, and price updates informed by dual values.

The prototype covers a ten year period from 2025 to 2034 and includes four representative fuels: biodiesel, ethanol, hydrogen, and conventional diesel. These fuels compete under production limits that vary annually, along with a gradually tightening global CO_2eq emissions budget. After each linear programming step, the dual values associated with the capacity constraints are interpreted as willingness to pay markups. These markups are incorporated into the objective function, and the model is re-solved iteratively until the remaining gap between total demand and the applicable supply cap falls below a tolerance of 10^{-3} t.

The model reveals three main observations. First, the price adjustment loop guided by dual values consistently reaches convergence in fewer than ten iterations, indicating numerical stability. Second, positive premiums are observed only when supply or emissions constraints are active, confirming the economic interpretation of the dual values. Third, removing price updates and relying on fixed costs increases total system expenditure by approximately ten percent, demonstrating that market signals improve the efficiency of fuel allocation compared to a basic merit order approach.

The full source code of this prototype is reproduced in Appendix B.1. Its successful performance supplied both empirical confidence and practical parameter choices for the final implementation.

5.1.3 Iterative Algorithm to Reach Equilibrium

To match supply and demand in a way that reflects market behaviour, the model uses an iterative process to adjust the fuel price premiums π_{pf}. The idea is simple: if the premium is too high, demand falls short of supply; if it is too low, demand exceeds what is available. The goal is to find a level of π_{pf} for each port and fuel that balances the market.

This is done using a bisection method. For each fuel and location, the algorithm starts with a price range, between a floor, usually based on production and regulatory costs, and a ceiling, where demand becomes negligible. In each step, it sets π_{pf} to the midpoint, solves the fair-share allocation, and checks the result. Based on whether supply is met or not, the range is updated. This continues until convergence.

The logic distinguishes between three basic outcomes: (a) when demand is lower than supply, the premium is likely too high; (b) when demand matches supply but the shadow price is zero, buyers are indifferent and the price can be reduced; and (c) when demand matches supply and the shadow price is positive, the premium is too low and should be raised.

Since fuel types can substitute for one another, changes in one π_{pf} can shift demand across the system. For this reason, the process may need to reset some values to ensure the algorithm converges globally.

This method keeps the pricing structure flexible and grounded in vessel-level decisions. Each ship optimises its behaviour based on current fuel costs, leading to a decentralised outcome where market balance is achieved through coordination. The result is a set of π_{pf} values that reflect both system constraints and buyer willingness to pay, allowing fuel prices to emerge naturally from the simulation process. This process can be visually seen in the algorithm flowchart displayed in Figure 3.5.

5.1.4 Integrated Bunkering Coordination Logic

NavigaTE's fuel allocation system is built in three steps: a Fair-Share allocation, a market-clearing adjustment, and an outer price update loop. These layers work together to simulate how limited fuel supply gets distributed across the fleet in response to both operational needs and market behaviour.

At the base, the Fair-Share method handles equity. It takes available fuel and spreads it proportionally across vessel–port combinations. This step makes sure all suitable vessels get some access, avoiding early exclusion of lower-priority routes. It also provides a clean starting point, a baseline demand, that the model uses to calculate price signals. This part follows the logic already detailed in Chapter 3.

After that, the market-clearing step comes in. Here, the model looks at the dual values (or shadow prices) from the Fair-Share problem. These values show how much a vessel is willing to pay for extra fuel. Using that, the algorithm reshuffles allocations: it gives fuel first to vessels with the highest marginal value, until the available supply is used up. This creates a ranked, economically grounded distribution, without breaking the fairness logic from before.

The final layer is an iterative price loop, described in Section 5.1.3, which adjusts premiums π_{pf} to align supply and demand. It typically converges in a few iterations, accounting for cross-fuel effects.

Together, these three steps allow NavigaTE to simulate realistic fuel distribution without imposing fixed prices. Fair-Share gives a starting point, market-clearing ranks demand by value, and the price loop finds an outcome that balances supply and demand based on actual willingness to pay.

5.2 Mathematical Formulation and Iterative Convergence

5.2.1 Sets and Indices

$$\begin{aligned} V &: \text{Set of vessels} \\ P &: \text{Set of ports} \\ F &: \text{Set of fuel types} \\ T &: \text{Set of time periods} \\ (v,p,f) &: \text{Tuple denoting a vessel } v \in V, \text{ port } p \in P, \text{ and fuel } f \in F \end{aligned}$$

5.2.2 Decision Variables

Variable	Description
$x_{vpf} \in R_+$	Amount of fuel f bunkered by vessel v at port p
$\pi_{pf} \in R$	Price premium for fuel f at port p
$\delta_{vpf} \in R_+$	Slack variable for fair-share relaxation
$\lambda_{vpf} \in R_+$	Dual variable (shadow price) for fuel constraint

5.2.3 Model Parameters

Parameter	Description
D_v	Demand of vessel v
C_{pf}	Unit production cost of fuel f at port p
R_{pf}	Regulation or carbon tax per unit of fuel f at port p
ϕ_{vpf}	Fair-share ratio of vessel v for fuel f at port p (iteration-dependent)
β_{vpf}	Fuel allocation amount for vessel v, fuel f, port p (iteration-dependent)
S_{pf}	Total supply of fuel f at port p
u_{vpf}	Usage ratio of bunker fuel by vessel v at port p, fuel f
Re_{pf}	Total released fuel ratio at port p, fuel f
LHV_f	Lower Heating Value of fuel f (MJ/ton)
Access_{vpf}	Binary: 1 if vessel v can bunker fuel f at port p, 0 otherwise
Compat_{vf}	Binary: 1 if vessel v is compatible with fuel f, 0 otherwise
ϵ	Convergence tolerance
α	Flexibility penalty coefficient

5.2.4 Objective Function

Without Market Dynamics (Fair-Share Only)

The model seeks to minimise the total cost of fuel allocation, incorporating production costs and emissions-related levies. Fairness is enforced through hard constraints rather than penalties or slack variables. The simplified objective function is:

$$\min_x \sum_{v\in V} \sum_{p\in P} \sum_{f\in F} \left[(C_{pf} + R_{pf}) \cdot x_{vpf} \right] \tag{5.1}$$

This formulation captures the core economic drivers while fairness in allocation is ensured through constraint logic. More complex regulatory costs, such as compliance penalties or caps, are handled separately within the constraint structure, making the model suitable for policy testing under diverse distribution regimes.

With Market Dynamics

When market dynamics are introduced, the objective function is redefined to reflect market-driven behaviour, where allocation is influenced not only by costs and regulation, but also by demand-side pressure. The revised objective is:

$$\min_x \sum_{v\in V} \sum_{p\in P} \sum_{f\in F} \left[(C_{pf} + R_{pf} + \pi_{pf}) \cdot x_{vpf} \right] \tag{5.2}$$

In this formulation, π_{pf} denotes the willingness to pay for fuel type f at port p, reflecting both scarcity and operational urgency through a price signal that adjusts during the iterative solution process. This approach turns the model into a system that responds to market conditions, allocating fuel to vessels with the highest marginal value. In contrast to the fair-share method, it focuses on economic efficiency rather than strict equity, using price signals to guide allocation while continuing to respect capacity limits and feasibility conditions.

This shift from a fairness based to a market driven objective reflects a change in modelling priorities, moving from centrally regulated coordination toward decentralised economic optimisation. It provides a framework for analysing how vessels compete for limited fuel resources under allocation mechanisms guided by price signals.

5.2.5 Model Constraints

At each time step, the model solves an optimisation problem that incorporates technical, operational, and market constraints. These define how fuel is distributed across vessels while respecting compatibility, availability, and capacity limits. After computing the optimal allocation for a given year, key outcomes, such as vessel retrofits, fuel production, and technology choices, are passed to the next period. This sequential structure captures the influence of earlier decisions on future conditions, allowing the model to reflect how investments and regulations affect the system over time.

Demand Satisfaction

$$\sum_{p \in P} \sum_{f \in F} \text{LHV}_f \cdot x_{vpf} = D_v, \quad \forall v \in V \tag{5.3}$$

This constraint ensures that each vessel's total energy demand D_v is satisfied by the fuels it bunks across all ports. Fuel quantities x_{vpf}, measured in tons, are converted to energy using the fuel's lower heating value LHV_f, allowing different fuel types to contribute to a vessel's energy needs.

Fair-Share Allocation

The fair-share allocation is implemented in two stages. In the first iteration, each vessel is assigned a proportional share of the available fuel at a given port, based on equal access principles. This is enforced as a hard upper bound:

$$x_{vpf} \leq FS_{vpf}, \quad \forall v \in V, p \in P, f \in F \tag{5.4}$$

where FS_{vpf} denotes the fair-share allocation of fuel f at port p for vessel v. This ensures that no vessel exceeds its initial allocation based on equity.

In subsequent iterations, vessels that do not utilise their full allocation release unused fuel, which becomes available to others. To support this redistribution, the fair-share constraint is relaxed by introducing a slack variable δ_{vpf}:

$$x_{vpf} \leq FS_{vpf} + \delta_{vpf}, \quad \forall v \in V, p \in P, f \in F \tag{5.5}$$

The slack δ_{vpf} is bounded and penalised in the objective function to preserve fairness while enabling more efficient allocation. This iterative logic allows the algorithm to refine the distribution based on vessel-level demand signals while respecting the original equity rule in the first round.

Vessel-Port-Fuel Access Feasibility

$$x_{vpf} = 0 \quad \text{if Access}_{vpf} = 0 \tag{5.6}$$

This constraint enforces accessibility feasibility, ensuring that a vessel can only bunker a specific fuel at a port if it is technically or operationally possible. If access is denied (i.e., Access$_{vpf}$ = 0), then no bunkering can occur in that port for that fuel.

Fuel Compatibility Constraint

$$x_{vpf} = 0 \quad \text{if Compat}_{vf} = 0 \tag{5.7}$$

This constraint enforces technical compatibility between vessels and fuels. If a vessel cannot safely or effectively operate using a particular fuel (i.e., Compat$_{vf}$ = 0), it is prohibited from bunkering that fuel at any port, regardless of availability or demand.

Non-Negativity

$$x_{vpf}, \delta_{vpf} \geq 0, \quad \forall v \in V, p \in P, f \in F \tag{5.8}$$

This constraint ensures that both the fuel bunkering amounts x_{vpf} and the fair-share relaxation terms δ_{vpf} remain non-negative. In other words, vessels cannot receive negative fuel quantities, and any deviation from the fair-share allocation must also be zero or positive.

5.2.6 Fair-Share Fuel Allocation

Initialisation

Each vessel v is assigned an initial fair-share ratio $\phi_{vpf}^{(0)} \in [0, 1]$ for fuel f at port p. The total available supply of fuel f at port p is S_{pf}. The initial fuel allocation to vessel v is:

$$\beta_{vpf}^{(0)} = \phi_{vpf}^{(0)} \times S_{pf} \tag{5.9}$$

Released Fuel Calculation

At iteration t, the usage ratio of vessel v is:

$$u_{vpf}^{(t)} = \frac{x_{vpf}^{(t-1)}}{\beta_{vpf}^{(t-1)}} \tag{5.10}$$

The updated fair-share ratio and total released fuel ratio are:

$$\phi_{vpf}^{(t)} = \phi_{vpf}^{(t-1)} \times u_{vpf}^{(t)} \tag{5.11}$$

$$Re_{pf}^{(t)} = \sum_{v \in V} \left(\phi_{vpf}^{(t-1)} - \phi_{vpf}^{(t)} \right) \tag{5.12}$$

Fair-Share Update Rule

The allocation $\beta_{vpf}^{(t)}$ is updated by redistributing released fuel:

$$\beta_{vpf}^{(t)} = \begin{cases} \dfrac{\phi_{vpf}^{(0)}}{1 - Re_{pf}^{(t)}} \times S_{pf}, & \text{if } 1 - Re_{pf}^{(t)} > \epsilon \\ S_{pf}, & \text{otherwise} \end{cases} \tag{5.13}$$

For vessels that released surplus:

$$\beta_{vpf}^{(t)} = x_{vpf}^{(t-1)} \tag{5.14}$$

Convergence Criterion
The iteration converges when the change in bunker decisions satisfies:

$$\Delta x^{(t)} = \left| x_{vpf}^{(t)} - x_{vpf}^{(t-1)} \right| \tag{5.15}$$

$$\Delta x^{(t)} < \epsilon \tag{5.16}$$

The algorithm terminates when the maximum change in bunkering decisions between iterations falls below a threshold, indicating stability.

5.2.7 Market Convergence (Outer Bisection Loop)

Although not part of the LP model directly, market premiums π_{pf} are adjusted through a bisection process until convergence is achieved:

$$\left| \sum_{v \in V} x_{vpf} - S_{pf} \right| \leq \epsilon, \quad \forall p, f \tag{5.17}$$

$$\lambda_{vpf} \approx 0 \quad (\text{marginal buyer is indifferent}) \tag{5.18}$$

The premiums π_{pf} are updated using:

- If demand $<$ supply: decrease ceiling on π_{pf}
- If shadow price $\lambda_{vpf} > \epsilon$: increase floor on π_{pf}
- Repeat until convergence

5.3 Code Implementation

The implementation follows the mathematical structure of the linear programming model described in Section 5.2. It incorporates both the fair-share constraints, introduced in Sections 5.2.5 to 5.2.6, and the dynamic adjustment of price premiums, which is handled through a non monotonic bisection process. The code is developed with a clear and modular structure to support future improvements, such as the inclusion of non linear cost functions or long term planning across multiple years. A complete description of the implementation is available in Appendix C.

5.3.1 Initialising Prices and Model Data

When the model is initialised, it performs a preliminary solve to observe which fuel markets are constrained and to extract dual values (shadow prices) for those constraints. For each binding market, an initial price ceiling is set by multiplying the maximum observed shadow price by a pre-defined increase factor, ensuring that the ceiling covers the possible equilibrium range. If the resulting price is still insufficient to balance supply and demand, the ceiling is iteratively increased until the market clears. This ensures that the bisection algorithm starts from a feasible and sufficiently wide search interval. The lower bound is always set to zero.

5.3.2 Iterative Bisection Routine

The main iterative loop uses a midpoint update approach. At each step, the midpoint of the current price interval is calculated and applied to the vessel level cost coefficients in the objective function. The optimisation problem is then resolved, with only the objective function being updated while the constraints remain unchanged. After each solve, the total fuel demand is compared to the available supply at the port, and the shadow prices are retrieved. If demand exceeds supply or the shadow price is positive, indicating that the constraint is active and binding, the lower bound of the price interval is increased. If demand is below supply or the shadow price is zero, the upper bound is reduced. The visual representation of this in Navigate can be found in Chapter 3.

5.4 Test Environment and Scenario Setup

This section covers the text environment information regarding the model setup along with the involvmenet of each one of the scenarios developed.

5.4.1 Assumptions and Input Data

Market Setup and Pricing Parameters: The file `test_bunker_options` specifies the market structure type (`GLOBAL`, `LOCAL`, or `EMERGING`), the maximum number of iterations permitted in the price adjustment loop, and the tolerance threshold for clearing the market. Convergence is achieved when the difference between supply and demand falls below ten units.

Fuel Availability Over Time: The file `test_fuel_availability` sets out the timeline for when different fuel types become available in the model. Initially, conventional fuels such as low sulphur fuel oil, liquefied natural gas, FAME, and biomethane are included. In 2025, a selection of electrofuels and biofuels is added, followed by synthetic options like diesel from direct air capture in 2030. Some fuels may be phased out by 2040, reflecting the evolving maturity of technologies and the readiness of markets.

Fleet Access and Fuel Bans: The file `test_ban_vessels` defines when different vessel types are permitted to use specific fuels or retrofitting technologies. For example, tug vessels are allowed to adopt methane in 2026 and methanol in 2030, while a complete ban on fuel oil is introduced in 2032 and lifted in 2042. These rules are used to simulate realistic delays in adoption and cycles of regulatory enforcement.

Emission Levies: Carbon pricing is modelled using `test_levies` and `test_levies_activate`, which define a well-to-wake CO_2 equivalent levy. The levy applies in selected regions (Asia, Europe, and the Middle East) and evolves in steps: baseline rates from 2028–2031, doubling by 2032, and tripling from 2038 onward.

Regulation Activation: The files `test_regulations` and `test_regulations_activate` define the timing of global limits on greenhouse gas intensity and regional standards, such as a fuel requirement specific to the European Union. These regulations are introduced gradually to assess system compliance and to evaluate their impact on market behaviour.

Simulation Horizon and Forecast Inputs: The scenario runs annually from the base year to 2050. The file `test_time_steps_yearly` defines the simulation timeline. Forecast files provide assumptions for cost trends, fuel price evolution, and levy escalation.

Output Selection and Reporting: The `test_reports` file identifies which results are exported, including fuel prices, demand allocations, emissions, and vessel-level metrics. Outputs are available in both graphical and tabular formats to support analysis and validation.

Additional Supporting Data: Auxiliary files describe the static properties of ports, vessels, and fuels, as well as dynamic factors like technology uptake, regional dependencies, and transport links. These include:

- `test_ports`, `test_vessels`, and `test_fuels`,
- `test_technology_uptake_initial`, `test_technology_availability`,
- `test_regions`, `test_canals`, and `test_transports`.

Together, these configuration files create a flexible and modular framework for testing the market-clearing algorithm and analysing how it responds to different policy choices and the introduction of alternative fuels over time.

5.4.2 Test Results and Convergence Behaviour

This test environment is designed to validate the correct functioning of the market-clearing algorithm across a range of controlled scenarios. By varying fuel types, vessels, and regulatory settings over time, the tests assess whether the bisection logic used for adjusting fuel prices converges reliably and performs consistently. Key outputs, including prices and allocation patterns, are evaluated through graphical and tabular results generated during the simulations.

Output Overview

The simulation produces a wide set of outputs in both visual and spreadsheet formats, covering fuel supply and demand, emissions, energy use, costs, fleet activity, and compliance metrics. For validation of the market-clearing logic, three main output types are used:

- **Fuel Supply and Demand Plots:** They help verify that prices are only introduced when the market is tight and supply equals demand.
  - `fuel_supply_demand.png`
  - `fuel_supply_demand_expectation.png`
  - `fuel_type_supply_demand.png`
- **Excel Reports:** The file `test_comprehensive_market_dynamic.xlsx` includes final price values for each fuel and port at every time step. These are cross-referenced with the plots to confirm whether prices appear only under binding conditions.
- **Market Price Behaviour:** Prices are checked to ensure they only emerge when the market is constrained. When slack conditions exist, prices remain at base levels. Prices are also examined to confirm they follow logical trends and remain economically reasonable.

Beyond these technical validations, the simulation also provides insights into the broader evolution of the maritime system, including emissions, technology shifts, cost trends, and responses to regulatory pressures. Although these broader metrics are not the primary focus in this thesis, they help validate that the introduction of dynamic pricing shifts behaviour in expected ways, further supporting the credibility of the algorithm.

Output of the Test Simulation

This section talks about the key plots used to validate the algorithm for each of the three market configurations in the test environment. For simplicity, the focus has been set on results from the port of Middle East. All plots discussed in this section are available in Appendix F.

Global Market: In this setting, all ports and regions share a common market price for each fuel. Figure F.1 shows supply and demand curves confirming that prices only emerge when the market clears within the defined threshold.

Local Market: Each port has its own market price for a fuel, which is consistent across vessels within that port. Figure F.2 confirms that prices only appear under constrained conditions.

Emerging Market: In this setup, prices vary not only across ports, but also across vessels for the same fuel. This reflects a more fragmented structure where vessel-specific contracts are allowed. Figure F.3 confirms that the algorithm continues to assign prices only under constrained conditions, with values now differentiated by vessel. In this market, the fair-share algorithm is only used, with no market-clearing routine. As a result, prices reflect individual vessel preferences and constraints, rather than a unified market mechanism.

6 Scenario Design and Simulation Setup

This chapter outlines the design of the simulation scenarios and describes how they are integrated and executed within the NavigaTE modelling environment. Following the implementation of a new market-based pricing mechanism, the next step is to evaluate how the system behaves under a range of economic and regulatory conditions. The aim is double: to assess the mathematical performance of the new price formation routine and to explore the economic and policy implications of price-based fuel allocation.

Sixteen scenarios combine four market configurations: cost-only baseline, which represents the model prior to introducing market-based pricing; global; local; and emerging pricing, paired with four regulatory frameworks: no regulation, carbon levies, regulations with flexible compliance that allow trading, and regulations with strict individual compliance. This setup allows for a systematic comparison of how different combinations of regulatory instruments and pricing mechanisms influence key model outcomes, including price formation, fuel allocation, and overall system emissions.

This chapter is divided into three sections. The first defines each scenario in detail and outlines the assumptions that inform their design. The second describes how the scenarios are implemented within the NavigaTE environment, including adjustments to input data and parameter values. The final section presents the validation approach used to confirm the correct operation of the market clearing mechanism under each configuration. This includes a technical assessment of convergence behaviour, computational performance, and robustness, along with consistency checks on key output variables.

The results and discussions presented in the following Chapters 7 and 8 will draw directly from the scenarios presented in this section.

6.1 Scenario Definitions and Assumptions

This section introduces the design of the sixteen scenarios developed in this thesis, structured as a 4×4 matrix combining four market configurations with four regulatory frameworks. This setup directly supports both main research objectives introduced in Chapter 2: analysing the informational value of price signals, and testing the added value of explicit price modelling compared to traditional cost-minimisation approaches.

Each scenario simulates both international and domestic vessel operations between major ports, starting from a consistent base case. Only the market configuration and policy parameters are varied across runs. This controlled setup enables direct comparison of how different pricing mechanisms and regulatory schemes influence model outcomes. A detailed overview of this structure is provided in Appendix E.

A cost-driven reference case where fuels are chosen based on production costs and penalties, with fair-share allocation and no market pricing. This setup reflects the approach commonly used in many existing maritime energy models, and matches the original version of the NavigaTE framework prior to the pricing extensions developed in this thesis.

Additionally, the three types of market configurations are also simulated: global, local, and emerging. In the global setting, a single price is formed for each fuel type across all ports, representing an idealised and fully integrated market. In the local configuration, prices are determined independently at each port, introducing spatial differences in fuel allocation. The emerging market reflects a fragmented context where fuel is allocated using vessel specific costs without activating the price formation routine. Further explanation of these market types is provided in Chapters 2.2 and 4.4.

6.1.1 Policy Settings

No Regulations: All emissions constraints are disabled, creating a neutral setting where fuel choices are determined purely by cost or market conditions. This configuration provides a reference case to isolate the effects of the pricing mechanisms without interference from environmental regulations.

Levy-Based Emissions Cost: Levies are applied at the point of bunkering and increase with the carbon intensity of each fuel. Defined by port and fuel type, they raise the effective cost of high emission fuels and encourage a shift toward cleaner options. In the model, levies are introduced directly into the objective function of the optimisation problem.

Regulations with Flexibility (Trading): Emission intensity targets are imposed at the fleet level, but flexibility is allowed. Vessels that over comply may "sell" excess reductions, while those that under comply pay a penalty. This forms a simplified emissions trading scheme and encourages cost-efficient compliance across the fleet.

Regulations without Flexibility (No Trading): Intensity targets are imposed individually on each vessel. No trading is allowed, and penalties apply strictly per ship if targets are exceeded. This configuration reflects a rigid policy regime, forcing stricter abatement and often resulting in sharper fuel switching.

6.1.2 Configuration Files and System Logic

Scenario implementation in NavigaTE is managed through a modular set of configuration files with the `.inc` extension, which serve as the main interface between the user and the simulation logic. Instead of hard coding parameters, structural assumptions, policy settings, and fuel constraints are defined in editable text files, allowing users to modify scenarios flexibly without changing the underlying code.

Each file controls a specific dimension of the simulation:

- `bunker_options.inc`: This file defines the market structure used for price computation. By adjusting a flag named `IncludeMarketDynamic`, the user can switch between the four main configurations analysed in this thesis. When the flag is set to off, the scenario corresponds to `COST_ONLY`. When enabled, the `MarketType` parameter can be specified as `GLOBAL`, `LOCAL`, or `EMERGING`. The same file also sets the convergence tolerance, the maximum number of iterations for the pricing loop, and the solver configuration.

- `levy.inc`: This file defines a global emissions levy aligned with IMO guidelines. The levy imposes a fixed carbon cost (300 USD per tonne of CO_2eq) on international vessels starting in 2027, covering all greenhouse gases including methane and its level remains constant after its introduction. The levy is applied based on a well-to-wake (WTW) framework and is implemented in conjunction with regional schemes such as the EU ETS and FuelEU Maritime.

- `regulations.inc`: This file defines an emissions regulation based on fuel intensity, aligned with the IMO's Goal-based Fuel Standard. It specifies a marginal abatement cost of 380 USD per tonne of CO_2eq for vessels that exceed an emissions intensity threshold. This threshold becomes more strict over time, decreasing linearly from 2028 to 2050 to achieve a 95% reduction from 2025 levels. The policy can be applied either at the vessel level, without trading, or across the fleet, with trading allowed, as defined by the `SchemeType` attribute. These settings are implemented through the `.NAV` scenario file.

- `report.inc`: This file activates output logging for computational performance. It generates reports such as `performance_statistics.xlsx`, recording key metrics like model size, solve time, and the number of iterations across solver types (LP, fair-share, and price update loops).

- `cii.inc`: This file defines the CII regulation, which applies to international shipping under the jurisdiction of the IMO. It is used for reporting rather than enforcement. The file includes a timeline of annual reduction targets, beginning in 2019 and becoming progressively more strict each year until 2030. The regulation accounts for Well-to-Tank (WTT) emissions and supports the tracking of compliance trends throughout the simulation period.

- `eu_ets.inc`: Defines the structure of the *European Union Emissions Trading Scheme*. It includes three main forecast variables: the penalty price per tonne of CO_2 equivalent, the implementation phase toward full coverage, and the inclusion of methane and nitrous oxide emissions. These elements evolve over time, with costs increasing substantially between 2025 and 2050. The gradual expansion of coverage and the addition of further greenhouse gases account for the rising regulatory cost observed in the later years of the simulation.

- `fuel_eu.inc`: This file defines the structure and penalty mechanism of the *FuelEU Maritime* regulation. The policy sets an intensity based limit on WTW emissions and calculates penalties according to the extent of deviation from the target emission intensity. The target becomes increasingly strict between 2025 and 2050 and is differentiated for intra European and international voyages. This regulation plays a central role in shaping fuel mix decisions and compliance behaviour throughout the simulation.

- `default_fleet_domestic.inc`: Defines the fleet structure and route assignments for the domestic market. It generates domestic variants of each vessel type and assigns them to national routes. The file specifies how many vessels operate within national boundaries and includes forecasts for domestic fleet expansion based on the share of vessels not deployed internationally. This setup enables the analysis of policy impacts on voyages limited to domestic operations.

- `default_fleet_international.inc`: Similar to the domestic configuration, this file generates dedicated vessel and route combinations for international transport. It allocates the internationally assigned fleet and links it to global trade routes, enabling the simulation to capture differences between domestic and cross border operations.

- `default_technology_available.inc`: Defines when specific technologies become available to each fleet segment. In this case, the file governs the entry of chemical absorption technologies. Initially, these are unavailable to any vessel group. From January 1, 2030, the technology becomes accessible to bulk carriers, containers, tankers, gas carriers, and roro vessels. This staged introduction supports realistic modelling of technological readiness and adoption timing in the simulation.

The remaining `.inc` files in NavigaTE contain default settings that define each simulation's structure, including regulatory timelines, technology constraints, cost assumptions, and vessel characteristics. Although these files are beyond the scope of the market pricing analysis, they enable flexible and transparent scenario design by shaping how system conditions evolve over time.

6.1.3 Model Execution Pipeline

Each simulation run in NavigaTE follows a structured workflow consisting of three stages: data preprocessing, optimisation, and post processing. These stages are implemented as modular

Python scripts. The process adapts dynamically to the configuration files loaded at runtime, enabling the same core engine to simulate a wide range of market structures and policy settings.

The first stage involves reading and processing all configuration files associated with the selected scenario. These files define model behaviour by specifying regulatory frameworks, fuel availability, levy schedules, and pricing settings. Based on this information, the model initialises vessel level demand matrices and port level fuel supply capacities for the simulation year under consideration.

The key component of the execution is the optimisation stage, where fuel allocation decisions are solved using a linear program. The exact flow depends on the selected market structure:

- For `GLOBAL` and `LOCAL` market configurations, the price convergence routine is activated. This process applies a bisection algorithm to identify the equilibrium price premiums (λ_{pf}) for each port and fuel type. In each iteration, the linear programme is rebuilt with updated cost coefficients that reflect the current price estimates. The model is solved using Gurobi, and the dual values from the port fuel supply constraints are extracted as economic signals to adjust the premium bounds. The routine continues until the difference between demand and supply falls within the specified convergence tolerance.
- In the `EMERGING` and `COST_ONLY` scenarios no iterative market-based price discovery occurs. Instead, multiple LPs are solved per time step through the fair-share convergence method, with costs either fixed (`COST_ONLY`) or adjusted for regulations (`EMERGING`). Marginal cost outputs are interpreted as prices but are not shaped by market interaction.

Following optimisation, the model transitions into the post processing stage, where output files are generated and stored for subsequent analysis. Each run produces a consistent set of files:

- `basecase_performance_statistics.xlsx`: A detailed log of computational performance, including solve times, number of LPs created, number of fair-share and market dynamics iterations, and solver diagnostics.
- `basecase_report_default.xlsx`: A scenario summary report with key outputs such as fuel consumption by type and region, vessel energy use, emissions intensities, regulatory compliance costs, and total expenditures.
- *Fuel price plots*: For each fuel type, a time series chart tracks the evolution of computed prices alongside static production costs, providing insights into scarcity, policy effects, and demand shifts.
- *Fuel supply-demand plots*: Stacked bar charts illustrate fuel production and consumption across ports and globally, highlighting market balance, temporal trends, and potential bottlenecks.

6.1.4 Time Horizon and Temporal Setup

All scenarios in this study are simulated over the period from 2025 to 2050, using a fixed annual time resolution. This temporal structure is implemented through the main scenario file `basecase.nav`. Within this file, the `SIMULATION FT` block includes the directive `IMPORT DefaultTimeStepsYearly`, which loads a predefined `.inc` configuration specifying yearly time steps. This ensures that the simulation progresses in discrete, one year intervals, aligning all system events, such as levy activation, regulation enforcement, and technology availability, with the correct point in time.

This structure guarantees that scenario dynamics evolve in a coherent way, as each year's policy and supply assumptions are applied precisely when scheduled. Levies, regulations, fuels and technologies are introduced or restricted at specific milestones throughout the time horizon.

The model assumes investment and bunkering decisions at each time step are based on current expectations of future conditions. While these expectations guide decision-making, the actual future may diverge, capturing a more realistic representation of decision making under uncertainty. This structure balances analytical clarity with behavioural plausibility in modelling system level transitions.

Finally, the use of annual time steps balances model resolution and computational efficiency. It is detailed enough to capture long term shifts in fleet composition, fuel switching, and compliance behaviour, while remaining computationally manageable across the 16 scenario simulations.

6.1.5 Units

This subsection introduces the main variables used throughout the model outputs and results chapter. Each variable is defined together with its interpretation and measurement unit:

- `BunkerMass`: demand, in t / year (tons of fuel per year).
- `BunkerSupplyMass`: supply, in t / year (tons of fuel per year).
- `BunkerPrice`: cost of fuels, in USD / GJ (US dollars per GJ of fuel).
- `BunkerFinalPrice`: price of fuels, in USD / GJ (US dollars per GJ of fuel).
- `FuelExpenses`: fuel production expenses, in USD / year.
- `FuelRelatedExpenses`: fuel, levy, and fuel conversion expenses, in USD / year.
- `FuelConversionExpenses`: fuel conversion expenses, in USD / year.
- `VesselExpenses`: expenses for purchasing new vessels, in USD / year.
- `VesselRelatedExpenses`: vessel and vessel technology expenses, in USD / year.
- `LevyExpenses`: levy expenses, in USD / year.
- `RegulationExpenses`: regulation expenses, in USD / year.
- `Expenses`: sum of Fuel Related, Vessel Related, and Regulation Expenses, in USD / year.
- `TotalEquivalentEmissions`: total absolute emissions, in t CO_2eq / year (tons of CO_2 equivalent per year).
- `TotalIntensityEquivalentEmissions`: total emissions intensity, in g CO_2eq / MJ (grams of CO_2 equivalent per megajoule of energy used).

These variables create the foundation of the model outputs and are key to interpreting the simulation results in the next chapter. When reviewing scenarios, differences in these values will reflect the effects of market typology, policy design, and technological readiness.

6.2 Validation and Testing - Cross-Scenario Comparison

To verify the internal consistency of the model across different configurations, a systematic comparison is conducted over all 16 scenario runs. The analysis ensures that model outcomes respond in logical and traceable ways to changes in primary assumptions. This section aims to explain the metrics used for the scenario comparison:

- **Total system expenses:** Across all scenarios, total expenses related to fuels and vessels evolve in line with model expectations. Scenarios with regulation or levies show higher total expenses due to penalties or carbon costs. These values are extracted from `basecase_report_default.xlsx` and validated for each run.

- **Emissions trajectories:** CO_2-equivalent emissions follow consistent patterns. In unregulated scenarios, emissions remain relatively flat or increase slightly. In regulated scenarios, the model achieves declining emissions profiles, consistent with the tightening intensity targets.
- **Fuel mix evolution:** The composition of fuels shifts appropriately depending on scenario conditions. When regulations are active, fuel switching toward low or zero emission options increases. When only levies are in place, the switch is more gradual. In the `COST_ONLY` scenarios, fuel choice remains driven primarily by production cost and availability.
- **Price activation logic:** Dynamic market prices only appear in scenarios where the market module is enabled (`GLOBAL`, `LOCAL`, `EMERGING`). Within these, prices emerge only when fuel constraints are binding, as verified through the price-cost plots discussed earlier. In `COST_ONLY` runs, no market prices are produced, as expected.
- **Convergence diagnostics:** For scenarios with market pricing enabled, the solver reaches convergence within reasonable time and iteration bounds. Fair-share iterations and market dynamic iterations appear only in the appropriate scenarios, confirming selective activation of the relevant algorithmic logic.

To ensure internal consistency and verify that all 16 scenario configurations function as intended, a structured cross validation was conducted. Table E.1 in Appendix E summarises key dimensions from each model run.

These consistency checks are not intended to assess policy effectiveness or economic outcomes. Instead, they confirm that the simulation responds coherently to changes in input settings, ensuring stable configuration logic, correct activation of algorithms, and consistent outputs across all combinations of market structures and policy frameworks. This form of structural validation complements the checks on convergence and supply demand balance, providing a reliable foundation for the scenario based analysis presented in Chapter 7.

7 Results & Analysis

Following the scenario description, this chapter presents the outcomes of all the 16 simulation scenarios. It is divided into four main sections, each covering one regulatory setup: `No Regulation`, `Regulation with Flexibility`, `Regulation without Flexibility`, and `Levy-Based Regulation`.

Within each section, results are structured in three parts. The first part, *Performance Analytics*, analyses the computational performance of the model across scenarios. It covers total runtime, model size, iteration counts, and solver effort required for each regulatory and market setting. This helps to quantify the computational burden associated with more complex policy designs and pricing mechanisms.

The second part, *Market Dynamics*, summarises the aggregated outcomes for each market configuration (`Cost-Only`, `Global`, `Local`, and `Emerging`). It focuses on total cost, market price levels, fuel demand, and fuel supply, allowing us to observe how market design shapes price formation and allocation across fuels and ports.

The third part, *Emissions and Expenses*, reviews system-wide emissions, the adoption of low-carbon fuels, and overall cost structure. This includes the breakdown of vessel costs, fuel costs, and costs related to emissions, providing a clear picture of how compliance costs evolve under each policy scenario and whether decarbonisation goals are achieved. It is important to note that the main indicator that is used in the emissions analysis is the Well-to-Wake (WTW), composed of the sum of well-to-tank (WTT), measuring upstream emissions, and tank-to-wake (TTW) emissions, that measures the downstream emissions.

Special attention is given to the `Regulation with Flexibility` scenario, as it uniquely explores both the official IMO GFS with a remedial cost of 380 USD per tonne of CO_2 equivalent and a more ambitious variant at 1,200 USD. While the 380 USD case reflects current policy, it proved insufficient to drive full compliance, fossil fuels remained economically viable. In contrast, the 1,200 USD version achieved full compliance by 2050 and revealed a transition from a demand-constrained system (continued fossil use) to a supply-constrained one, where limited clean fuel production became the main bottleneck. This stronger price signal expanded the marginal abatement cost curve and enabled broader uptake of low-carbon fuels, including biofuels, blue fuels, and e-fuels. The price-adjusting mechanism also played a greater role, reallocating scarce fuels to vessels with the highest willingness to pay. Given these dynamics, the 1,200 USD penalty was extended to the `Levy` and `Regulation with No Flexibility` scenarios to maintain comparability and realistic decarbonisation pressure.

After presenting the individual results of each regulatory scenario, the chapter closes with a cross-scenario comparison. This final section brings together the key findings across all policies, analysing *Performance Analytics*, *Market Dynamics*, and *Emissions and Expenses*. The goal is to clearly illustrate the trade-offs between different regulatory approaches and provide a solid basis for the broader discussion developed in the following Chapter 8.

7.1 No Regulation Scenario

In the `No Regulation` scenario, the system operates without any policy constraints. This serves as a baseline to observe how the shipping sector would naturally behave if decisions were driven purely by market forces, where fuel choices and technology adoption depend only on operating costs and fuel availability.

7.1.1 Performance Analytics

Figure 7.1: Runtime evolution in seconds from 2025 to 2050 across the four market configurations in the `No Regulation` scenario.

As illustrated in Figure 7.1, simulation runtimes decreases over time, evidenced by the gradient of the runtime curves tapering off in later years. This trend is due to the model's nested time-stepping structure, which performs approximately $\frac{n_t^2}{2}$ linear programs, where n_t is the total number of time steps. The majority of these solves occur in the early stages of the simulation, as each new year requires fewer nested solves than the initial years. Consequently, although the system becomes more complex over time, the computational effort per year declines.

Among the four market structures, the `Local` market takes the longest to solve, exceeding 5,200 seconds by 2050. This reflects the additional computational effort required when prices are cleared separately at each port, resulting in more iterations and solver calls. The `Global` market follows a similar trend but remains slightly faster, as prices are coordinated centrally rather than independently. The difference highlights the extra complexity of decentralised price setting. Meanwhile, both `Cost-Only` and `Emerging` configurations are much faster to compute. A full disaggregated vision of these metrics, can be found in Appendix L.

7.1.2 Market Dynamics

The table in Appendix M summarises the key market indicators for the `No Regulation` scenario, comparing total system costs, market prices, total supply and total demand across the four market configurations. `Cost-Only` case yields zero prices, since fuel allocation is performed purely based on production costs. Once market dynamics are introduced in the `Global`, `Local`, and `Emerging` configurations, actual price signals emerge as the model balances supply and demand at each time step. These price signals generally lead to higher price levels compared to the simple cost-based allocation, reflecting supply limitations and competition for available fuels. Among these market configurations, the `Local` Market displays the highest prices because these are determined independently at each port. This localised pricing creates more variability across regions driving prices above the levels observed in more centralised or coordinated market structures.

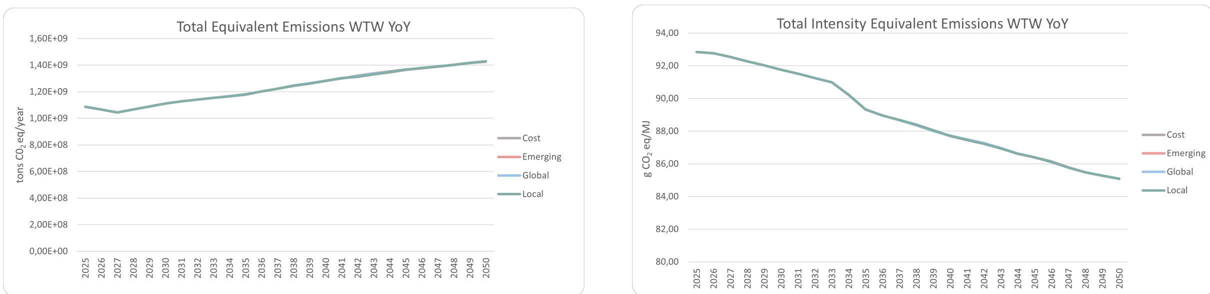
As shown in Appendix G, total demand remains stable across the four configurations. The apparent gap between demand and supply arises because unconstrained fuels such as `LNG` and `LSFO` dominate bunker consumption but are not captured in the aggregated supply figures, as their production is not limited within the model.

Across all configurations, fossil fuels remain dominant due to their lower production costs and practically unconstrained availability within the model. In the `Cost-Only` case, allocation is strictly cost-driven, resulting in `LSFO` and `LNG` fully covering almost the entire demand. Biofuels such as `FAME` and `Bio-oil (Pyrolysis)` only enter the mix marginally, limited by their relatively small available supply capacity. No pricing mechanism exists in this setup, so the allocation strictly follows production cost hierarchies.

When price coordination is introduced in the `Global`, `Local`, and `Emerging` configurations, biofuels gain slightly more market share as vessels adjust willingness to pay in response to price signals. These pricing mechanisms allow some substitution towards biofuels when market conditions justify higher costs. However, the price premium required to trigger significant biofuel uptake remains high, which limits their expansion. In the `Local` configuration, geographically changing prices result in slightly more biofuel use in certain ports facing localised supply shortages. The `Emerging` model allows for more gradual shifts at the vessel level, but fossil fuels remain the dominant energy source throughout the simulation period in all scenarios.

Complete regional results and full supply-demand and price-cost plots for all locations are provided in Appendix G.2 (`Cost-Only`), G.2.3 (`Global`), G.2.4 (`Local`), and G.2.2 (`Emerging`).

7.1.3 Emissions and Expenses



(a) Total Equivalent Emissions WTW (in tons CO_{2eq}/year).

(b) Total Intensity Equivalent Emissions WTW (in g CO_{2eq}/MJ).

Figure 7.2: Global WTW emissions across the four different market typologies for the `No Regulation` setup

In the absence of regulatory constraints, the overall emissions across all market types remain very close, this is due to the increase in demand. Since fuel allocation is mainly driven by production cost and technical feasibility, fossil fuels dominate across the board, leading to similar WTW emission totals regardless of market structure. In the equivalent WTW emissions it can be seen that from 2028 the emissions take a shift and start increasing steadily through the years, this is because the absence of regulatory constraints allows vessels to continue relying on high emission fuels as demand grows, and no policy mechanisms are in place to redirect investments toward cleaner alternatives. But, when looking at intensity metrics (g of CO_2/MJ used of fuel) they follow a different pattern. From year 2025 they tend to decrease, due to the works of decarbonisation in the year 2032, there is a jump in the decrease, probably due to the early integration of low-carbon fuels, gradual technology optimisation and fleet renewal, which reduces emissions per unit of energy from 93 g of CO_2/MJ to 85 g of CO_2/MJ.

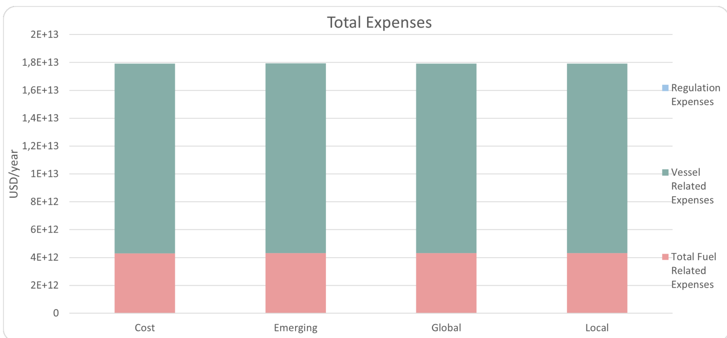


Figure 7.3: Stacked expenses in USD (y-axis) across the four market configurations (x-axis) in the `No Regulation` scenario.

The expense structure across all markets remains almost identical, seen in detail in Table N.1. Since there are no penalties or regulatory charges applied, regulation related costs are zero. The vessel related expenses are the largest contributor to total system costs, reflecting fleet turnover and investment requirements. Fuel related expenses stay stable across markets, with minor differences caused by small shifts in fuel allocation depending on the market pricing coordination applied.

7.2 Regulation with Flexibility

The `Regulation with Flexibility` scenario is particularly important as it represents the most realistic depiction of current regulatory trends in maritime decarbonisation. In this section, both the officially announced IMO remedial unit GFS of 380 USD per tonne of CO_2 equivalent and a higher alternative penalty of 1,200 USD are explored.

Initial model tests confirmed that the IMO remedial unit GFS of 380 USD alone does not sufficiently discourage the use of fossil fuels, allowing high-emission fuels to remain economically competitive. By contrast, the 1,200 USD penalty triggers a stronger shift in market behaviour. Under this higher carbon price, the system moves from being primarily demand-constrained, where fuel users simply choose the cheapest available options, to becoming supply-constrained, where the limited availability of low-carbon fuels becomes the key limiting factor. This leads to greater uptake of biofuels, stronger differentiation in fuel allocation, and higher utilisation of price coordination mechanisms across the various market configurations.

7.2.1 IMO Regulation Value - 380 USD

Performance Analytics

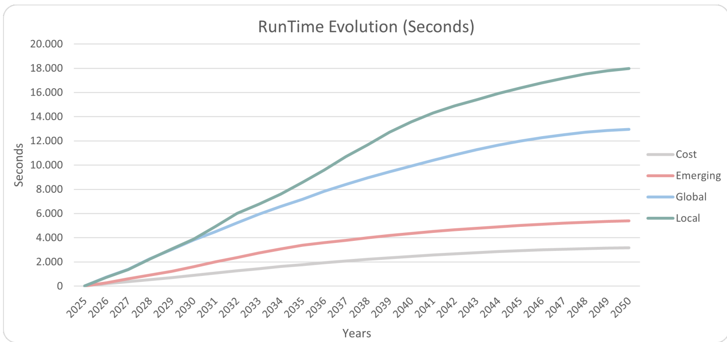


Figure 7.4: Runtime evolution in seconds from 2025 to 2050 across the four market configurations in the `Regulation with Flexibility` under the IMO remedial unit GFS of 380 USD scenario.

The introduction of flexible regulation under the IMO GFS of 380 USD already increases computational complexity compared to the `No Regulation` scenario. As shown in Figure 7.4, all market configurations experience longer runtimes due to the need for allowance trading logic, iterative market clearing, and dynamic price adjustments. While the system remains numerically stable, additional layers of coordination are required to balance emissions between compliant and non-compliant vessels, introducing extra iterations into the model.

The `Cost-Only` configuration is now the fastest to compute, as no price coordination nor trading takes place; fuel allocation continues to follow simple cost minimisation. The runtime increases only slightly relative to the unregulated case due to the presence of additional regulatory constraints being checked at each solve.

The `Emerging` configuration remains relatively efficient but shows longer solve times than the `Cost-Only` case. This is due to more frequent fair-share iterations. These are likely triggered by new fuel prices that affect decisions elsewhere in the model, which then leads to more complex linear problems solved in later time steps.

Computational effort is highest in the Global and Local configurations. In Global, the price algorithm operates at the fleet level, increasing fair share iterations and market updates, though coordination across ports helps keep solution times manageable. In Local, prices are cleared independently at each port, leading to a larger number of iterations. This disaggregated approach results in a runtime that nearly triples compared to the Cost Only configuration by 2050.

The solver performance data in Table L.3 highlights the computational impact of introducing price coordination and market clearing. Iteration counts increase significantly, particularly in the Local market, which records over 11,000 market dynamic iterations and 51,000 fair share iterations. This is driven by the decentralised price determination process at the port level. In contrast, Global requires fewer iterations (6,500 and 28,000 respectively), while Cost-Only and Emerging remain much lower (1,400). Despite this, the model remains computationally feasible under flexible regulation. All numeric results can be seen in Appendix L.

Market Dynamics

The table in Appendix M provides an aggregated overview of market behaviour under the Regulation with Flexibility scenario with the IMO GFS of 380 USD. As in previous sections, results are presented across the four market structures.

Overall, introducing flexible regulation triggers a modest diversification of the fuel mix, though fossil fuels remain dominant. As observed in Appendix H.2, LSFO demand steadily declines across all markets, while LNG follows a bimodal trend, peaking around 2035 before temporarily declining and then increasing again toward 2050. This reflects the system's progressive but still limited shift toward alternative fuels under the current IMO pricing level.

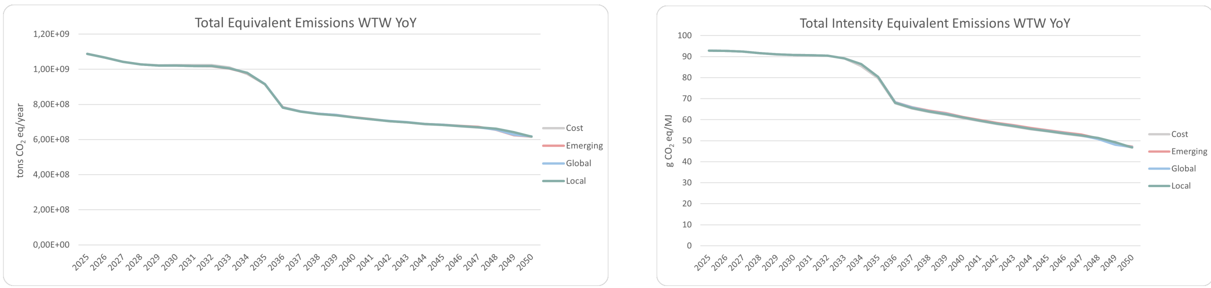
Low and zero carbon fuels such as FAME, Bio-oils, Bio-methane, Bio-methanol, Blue Ammonia, and e-fuels are increasingly introduced into the fuel mix. However, their overall penetration remains limited due to cost competitiveness and compatibility constraints. Some fuels, such as e-Methanol and e-Ammonia, are technically available but remain largely unused, as their prices are still not attractive enough to drive widespread adoption.

The Cost-Only configuration serves as a reference baseline, showing minimal deviation from pure cost-optimal allocations. In the Global Market, despite introducing price coordination, demand patterns remain quite close to the cost-driven allocation, suggesting that at this penalty level, the market price signal alone is not yet sufficient to induce strong behavioural changes.

In contrast, the Local and Emerging markets introduce more regional and vessel-level heterogeneity. Decentralised price signals lead to some variations in fuel selection across locations and time periods, as individual ports and vessels respond differently to local conditions and willingness-to-pay. Nevertheless, while these more granular mechanisms allow some redistribution of fuel allocation, they do not fundamentally shift the system-wide fuel mix under the current IMO GFS. Fossil fuels continue to meet the majority of demand, and supply remains comfortably above consumption across all market setups.

Emissions and Expenses

The introduction of the IMO flexible regulation at 380 USD makes overall emissions shift. Total WTW emissions remain close across all market configurations.



(a) Total Equivalent WTW Emissions (in tons CO_{2eq}/year).

(b) Total Intensity Equivalent WTW Emissions (in g CO_{2eq}/MJ).

Figure 7.5: Global WTW Emission across the four different market typologies in the `Regulation with Flexibility IMO GFS` setup.

For both metrics, Total Equivalent WTW Emissions and Intensity Equivalent emissions there is a decreasing trend in both, with a significant step decrease in the year 2036, which forces a switch away from high emission fuels. Vessels that cannot comply economically begin transitioning to cleaner fuels or rely on emissions trading to avoid penalties, resulting in an abrupt system wide emissions drop. Looking at Intensity Equivalent Emissions, the value decreases from the 93g gCO_2eq/MJ in 2025 to around 45 gCO_2eq/MJ in 2050, achieving lower values than the `No Regulation` scenario.

In terms of total system expenses, all configurations display relatively stable cost structures under the IMO regulation. The `Cost-Only` scenario maintains the lowest overall expenditures, while `Emerging` Market shows slightly higher total expenses due to modestly higher biofuel deployment and more vessel adjustments.

Fuel-related expenses contribute to approximately one quarter of total costs, with vessel-related investments representing the largest share across all configurations. Regulation-related expenses remain relatively small in this IMO case, ranging between 1.19 and 1.22 trillion EUR, indicating that the 380 USD penalty, while non-negligible, does not significantly increase compliance costs under current conditions.

Overall, the relatively minor differences across market types suggest that the IMO 380 USD carbon price still allows the industry to comply mostly through business-as-usual operations, with limited restructuring of the fuel mix and technology adoption. These results are summarised in Table N.

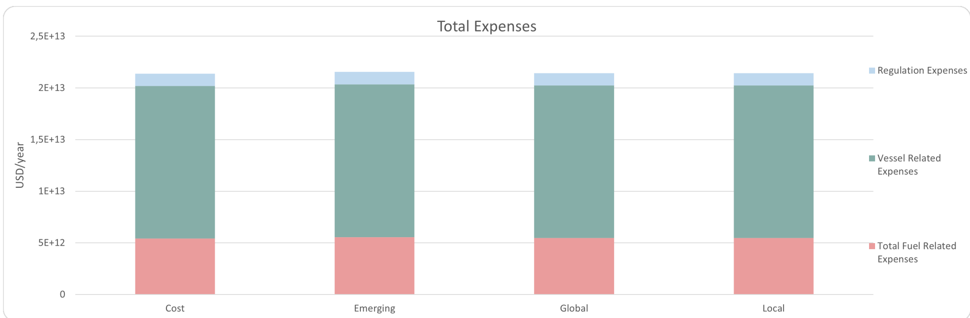


Figure 7.6: Stacked expenses in USD (y-axis) across the four market configurations (x-axis) in the `Regulation with Flexibility` scenario under the IMO remedial unit GFS of 380 USD.

7.2.2 High Penalty Value - 1200 USD

Performance Analytics

When applying the 1200 USD/ton CO_2eq penalty in the `Regulation with Flexibility` scenario, the model exhibits a clear increase in computational effort compared to lower regulation levels. The stronger carbon price forces the system to adjust fuel allocation more drastically, creating increasingly complex market dynamics that directly impact computational performance.

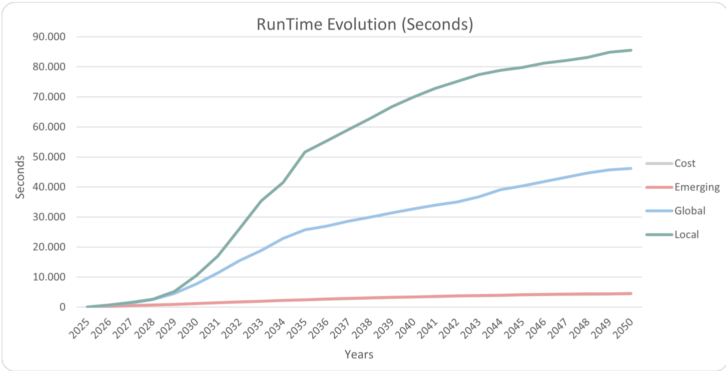


Figure 7.7: Runtime evolution in seconds from 2025 to 2050 across the four market configurations in the `Regulation with Flexibility` under the 1200 USD penalty scenario.

As shown in Figure 7.7, the `Cost-Only` and `Emerging Market` setups remain computationally stable. In contrast, introducing price formation, especially in the `Global` and more so in the `Local Market`, significantly increases solver workload due to repeated market coordination. In decentralised setups like the `Local Market`, regional price adjustments run independently, increasing iterations and extending runtime. All numeric results are detailed in Appendix H.

Overall, stronger carbon pricing drives major shifts in fuel use while increasing market complexity. As fossil fuels lose viability, limited low-carbon fuels must be distributed across diverse vessels and regions, adding negotiation cycles, especially in decentralised settings like the `Local Market`. Despite this, the model remains tractable, showing robustness under ambitious decarbonisation targets.

Market Dynamics

Aggregated results (table in Appendix M) show that system costs remain nearly identical across market configurations under the 1,200 USD penalty, indicating stable total expenditures regardless of pricing flexibility. However, compared to the 380 USD IMO case, both prices and supply increase substantially, signalling a shift from demand-constrained to supply-constrained dynamics. Prices are highest in the `Emerging Market`, followed by `Local` and `Global`, reflecting stronger marginal bidding behaviour in more flexible resale environments. Demand slightly drops in the `Emerging Market`, while `Cost-Only` maintains the highest levels. These differences illustrate how stronger carbon pricing reshapes market interactions and redistributes pricing pressure, warranting further fuel-level analysis.

Across scenarios, the system transitions from demand-driven in `No Regulation` to increasingly supply-constrained under `Regulation with Flexibility` (380 USD) and `Regulation with Flexibility` (1200 USD), with rising prices and expanded low-carbon supply. Under `Reg. No Flex` (1200 USD), demand drops further due to limited fuel substitution options.

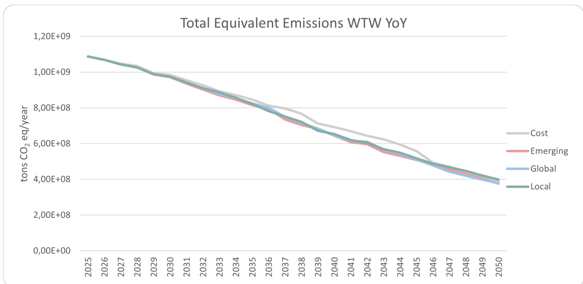
Under the 1,200 USD penalty, demand patterns diverge more across market types as it can be seen in Appendix I. LSFO steadily declines from 10 to 3 EJ/year by 2050 in all scenarios, showing the effectiveness of stronger carbon pricing. LNG, however, follows distinct paths in each market, reflecting sensitivity to local conditions. FAME and Bio-oil (HtL) show stable demand across cases, aside from a brief drop in FAME demand in the Local Market in 2030. Other fuels like e-methanol, blue ammonia, and bio-methane vary more significantly, with uptake shaped by how each market responds to evolving price signals.

With the system now supply-constrained, the pricing algorithm plays a greater role in shaping the fuel mix. The higher penalty shifts the focus from cost minimisation to marginal abatement efficiency, activating a wider range of low- and zero-carbon fuels. Most options are now supplied in substantial volumes, while grey ammonia sees no supply due to its emissions profile. Although supply timing is broadly consistent across scenarios, volumes and ramp-up patterns vary: Global and Emerging Markets show smoother trends, while the Local Market sees sharper shifts, reflecting regional imbalances and fragmented competition.

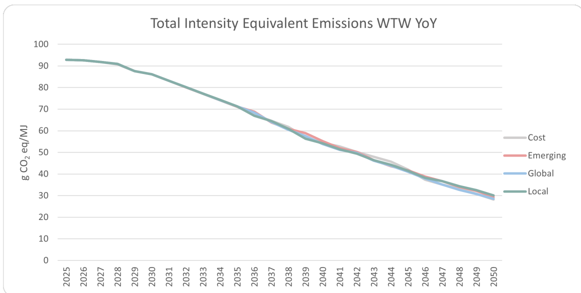
Despite varying supply-demand outcomes, market prices for fuels remain within a similar range across the Global, Local, and Emerging configurations, thanks to the flexibility allowed in fuel resale. The `Global Market` presents the most stable pricing, while the Local Market shows more pronounced spikes, reflecting regional bottlenecks and supply frictions. The `Emerging Market`, in contrast, smooths out these price fluctuations due to its vessel-level aggregation. Importantly, the decoupling of price from pure production cost enables fuels with higher marginal abatement potential to enter the system, even if their base cost is not the lowest. This price differentiation is critical in reallocating fuel supply toward high-value vessels and promotes a more responsive and efficient fuel allocation system, especially under supply-constrained conditions.

Emissions and Expenses

The introduction of a carbon penalty of 1200 USD/tCO_2eq under the `Regulation with Flexibility` scenario results in stronger decarbonisation effects across all market configurations. This higher penalty leads to earlier fuel switching and emissions reductions throughout the simulation.



(a) Total WTW Equivalent Emissions (in tons CO_{2eq}/year).



(b) Total Intensity Equivalent WTW Emissions (in g CO_{2eq}/MJ).

Figure 7.8: Global WTW Emission across the four different market typologies in the `Reg. with Flexibility 1200 USD`

As shown in Figure 7.8a, total WTW emissions decline equally sharp until 2029. After this point, the penalty accelerates stability among market structures, although `Cost Only` continues to produce the highest emissions due to lower fuel prices and higher demand. Figure 7.8b shows that WTW intensity emissions remain relatively stable until 2028, followed by a marked decline and reaching its lowest value of 29 gCO_2eq/MJ. This reflects the shift toward cleaner fuels and more efficient allocation enabled by the flexibility mechanism.

Stronger decarbonisation leads to higher overall system costs, mainly due to increased fuel expenses. Cleaner fuels are more expensive to produce and supply, with the `Emerging Market` showing the highest fuel costs due to greater use of lower-emission alternative fuels. In contrast, the `Cost Only` scenario remains cheapest, as it avoids market pricing and relies on lower-cost fuels, which also drive up demand.

Vessel-related costs rise as well, driven by investments in retrofitting and new ship designs, though these increases are more moderate than those for fuel.

Regulatory expenses vary across markets. In the `Cost Only` case, operators face higher penalties because they do not adjust fuel use. Markets with flexibility, such as `Global`, `Local`, and

Emerging, reduce these costs by shifting to cleaner fuels or using trading mechanisms. Numerical results are provided in Table N.1.

Figure 7.9: Stacked expenses in USD (y-axis) across the four market configurations (x-axis) in the Regulation with Flexibility scenario under the 1200 USD penalty.

7.3 Regulation without Flexibility

7.3.1 Performance Analytics

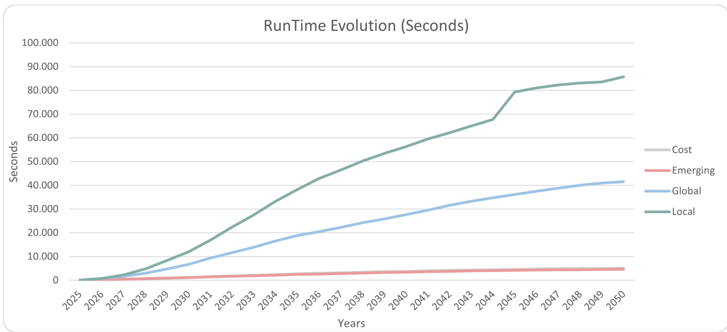


Figure 7.10: Runtime evolution in seconds from 2025 to 2050 across the four market configurations in the Regulation without Flexibility scenario under the 1200 USD penalty.

Under the Regulation without Flexibility scenario with a 1,200 USD/tCO_2eq penalty, all market configurations show a shift toward low carbon fuels and an increase in computational complexity, though the degree of complexity varies notably across market structures.

The Cost Only and Emerging markets remain the simplest from a computational perspective. These rely on direct cost minimisation without iterative price formation, resulting in faster runtimes and fewer solver calls. In contrast, introducing coordinated pricing in the Global and especially Local markets leads to a substantial increase in model complexity. This is due to the iterative mechanisms required to align supply, demand, and willingness to pay under constrained conditions.

The Local Market is the most computationally intensive, reflecting its fully decentralised structure where each port solves its own market independently. The volume of iterations required for price convergence and ceiling adjustments indicates the higher solver load caused by local competition for limited low emission fuels.Interestingly, the Emerging Market maintains low complexity despite the strong regulation.

Histogram plots supporting these outcomes can be found in Appendix H, and all numerical details supporting these observations are provided in L.

7.3.2 Market Dynamics

Under the Regulation without Flexibility scenario with a 1,200 USD penalty, aggregated outcomes remain broadly similar across markets (Table in Appendix M), but some notable contrasts emerge. The `Global` Market now records the second-highest demand after `Cost-Only`, while the `Emerging` Market shows the lowest cost and slightly lower price levels, despite facing the highest price-to-cost gaps in some fuels. These outcomes reflect the inefficiencies introduced by limiting fuel reallocation. Still, all market indicators remain within relatively close ranges, suggesting that flexibility mainly reshapes internal distribution rather than total system behaviour.

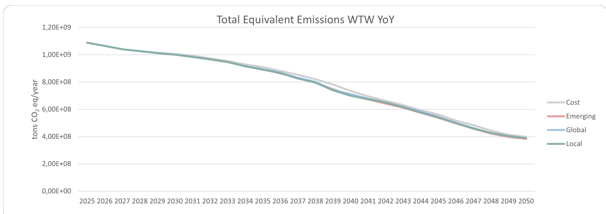
As in the `Regulation with Flexibility` scenario, `LSFO` phases out consistently from 10 EJ/year in 2025 to 3 EJ/year by 2050, confirming the strong effect of the higher penalty across markets (Appendix I). `LNG`, however, shows different demand profiles depending on the market type, reflecting localised responses under supply constraints. For most advanced fuels, the shape of demand over time is similar to the flexible case, but with significant differences in scale. For instance, `e-diesel (PS)` peaks at under 500 PJ/year in the `Cost` Market but reaches up to 1.6 EJ/year in `Global` and `Emerging`. These differences highlight the impact of removing fuel reselling: demand becomes more uneven and tied to individual market constraints.

The supply patterns broadly mirror those in the flexible scenario, but restrictions on resale lead to increased mismatches. Fuels like FAME and both bio-oils are consistently supplied, while others such as e-methanol and bio-methane show much more fragmented deployment. For example, `e-methane (DAC)` has no supply at all in `Emerging`, minimal presence in `Local`, and surplus without demand in `Global`. `Grey ammonia` remains excluded entirely. The inability to reallocate fuels limits responsiveness, resulting in under- or oversupplied fuels depending on market dynamics.

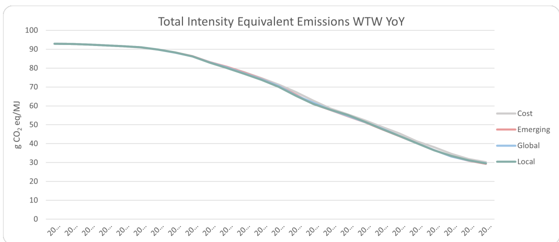
Price signals remain within similar ranges as in the flexibility scenario. `Local` Markets still display the greatest volatility, while Emerging Markets continue to show smoother curves due to vessel-level averaging. As before, `Emerging` also shows more frequent cases where prices exceed production costs, indicating persistent inefficiencies. The absence of reselling further limits the system's ability to reallocate fuels efficiently, constraining the algorithm's capacity to balance marginal abatement across ports and vessels.

7.3.3 Emissions and Expenses

In this section, looking at the absolute WTW emissions in Figure 7.11a, a steady decrease is observed until 2050. Even though cleaner fuels are being used, the overall demand grows but not as much as the previous case. Without flexible compliance options, such as emissions trading, the system cannot fully adapt to keep total emissions from rising.



(a) Total Equivalent WTW Emissions (in tons CO_{2eq}/year).



(b) Total Intensity Equivalent WTW Emissions s (in g CO_{2eq}/MJ).

Figure 7.11: Global WTW Emission across the four different market typologies in the `Regulations with no Flex.` setup.

In contrast, the WTW intensity emissions shown in Figure 7.11b follow a different pattern. If we look at emissions intensity, it declines consistently to 30 gCO_2eq/MJ until 2050. This values is a slightly higher than the regulations with flexibility.

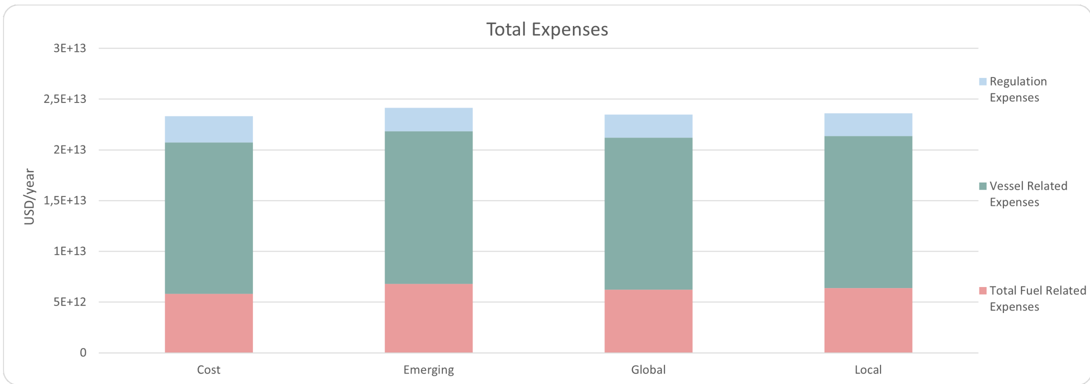


Figure 7.12: Stacked expenses in USD (y-axis) across the four market configurations (x-axis) in the `Regulation without Flexibility` scenario under the 1200 USD penalty.

As shown in Figure 7.12 and Table N.1, applying a strict regulation without flexibility results in high, but relatively stable, total system costs across all market configurations. Fuel-related expenses are highest in the `Emerging Market`, where limited access to international trade pushes the system to rely more on expensive, regionally available low-carbon fuels. In contrast, the `Global` and `Local Market` configurations benefit from better price coordination and broader fuel allocation options, which help slightly reduce overall fuel costs. Vessel related expenses remain fairly similar across all scenarios, as fleet renewal and technological upgrades are mainly driven by the regulatory requirements rather than by market design. Regulation expenses are highest in the `Cost-Only` case, where fossil fuels continue to dominate, resulting in substantial penalty payments. In the other market setups, wider adoption of cleaner fuels helps mitigate these costs, as less emissions translate into lower regulatory charges.

7.4 Levy-Based Regulation

The `Levy-Based Regulation` scenario represents an alternative policy framework where carbon pricing is directly imposed on fuel consumption without setting emission caps or base targets. Instead of complex flexibility mechanisms, this system applies a fixed levy per ton of CO_2 emitted, allowing market participants to adjust their fuel choices purely based on the economic signal provided by the levy.

In this analysis, the levy was set at a value of 800 USD, up from the baseline of 300 USD used in earlier simulations. This parameter is added to the objective value coefficient of the bunker cost of the fuel within the model. It plays an analogous role by increasing the effective cost of carbon-intensive fuels. This higher levy value was selected for two key reasons. First, the initial level of 300 proved insufficient to meaningfully shift demand away from conventional fuels, mirroring the results observed under the IMO GFS of 380 USD/ton CO_2eq. Second, increasing the levy to 800 serves as a midpoint between ineffectiveness and overly aggressive system stress. It strengthens the decarbonisation signal while avoiding the fuel supply bottlenecks and extreme behavioural shifts seen under the more stringent regulation scenario with a 1200 USD penalty. Although the levy mechanism is structurally different from the regulatory penalty, this adjustment follows a similar rationale: testing a more ambitious, yet still feasible, policy intervention.

7.4.1 Performance Analytics

Figure 7.13 displays the runtime evolution across the entire simulation horizon from 2025 to 2050 under the `Levy-Based Regulation` scenario. As observed in previous regulatory setups, model complexity increases substantially when price coordination mechanisms are introduced. The `Cost-Only` configuration remains the fastest to solve, as it relies solely on static cost minimisation with no dynamic pricing loops. The `Local Market` shows the highest computational burden, peaking above 30,000 seconds by the end of the horizon. In this case, each port clears fuel prices independently, resulting in multiple isolated iterations and slower convergence as supply becomes more constrained over time.

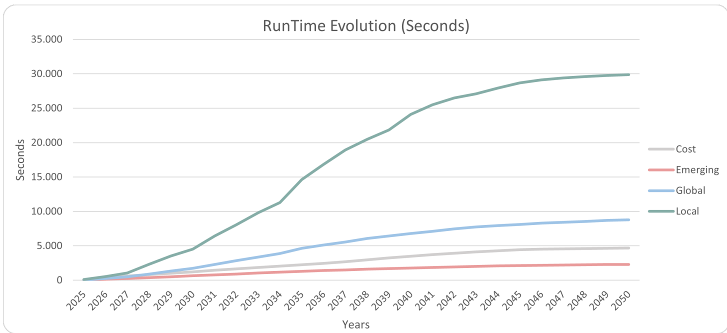


Figure 7.13: Runtime evolution in seconds from 2025 to 2050 across the four market configurations in the `Levy-Based` scenario under a levy of 800 USD.

Table L.1 displays the performance outcomes across the four market configurations. The differences in runtime and solver effort mainly reflect the degree of price coordination required by each structure. In the `Cost-Only` case, where no price discovery is needed, the model solves quickly and with minimal iterations.

As discussed in earlier sections, coordinated pricing mechanisms, particularly in the `Local Market`, significantly increase computational burden due to the complexity of resolving disaggregated fuel prices. In contrast, the `Emerging Market` relies on vessel-level logic, offering a more computationally efficient balance between market responsiveness and tractability.

Overall, although the carbon levy introduces additional layers of complexity, the model remains computationally manageable in all configurations. All results are detailed in Appendix L.

7.4.2 Market Dynamics

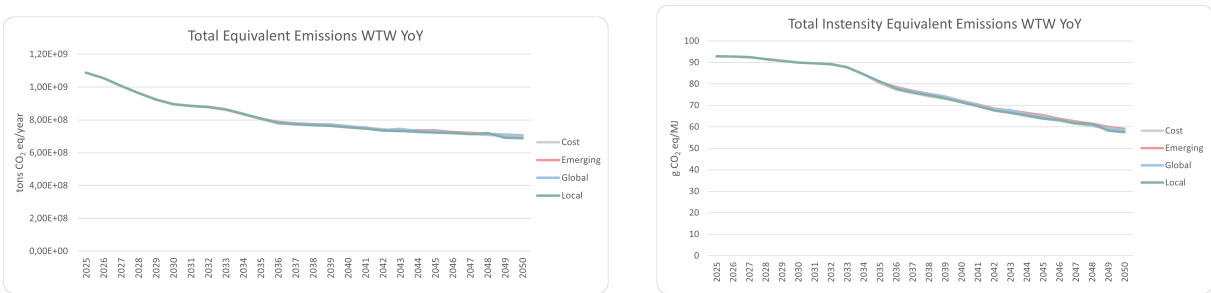
In the `Levies` scenario with a levy level of 800, market-wide differences are more pronounced (Table in Appendix M). The `Global` Market shows the highest costs and prices, driven by its uniform pricing and higher marginal willingness to pay. While `Cost` and `Emerging` Markets maintain lower costs, overall supply and demand are slightly reduced compared to regulatory scenarios. These outcomes suggest that, although levies introduce a strong price signal, the absence of rigid caps allows for less heterogeneity in how markets absorb decarbonisation incentives.

In the Levies scenario with the higher multiplier value, system dynamics resemble the `No Regulation` baseline more closely than the Regulation scenarios, though some deviations appear in specific fuel behaviours. Across all market types, four fuels (LSFO, LNG, FAME, and Bio-oil (Pyr)) remain consistently active, showing supply and demand in all configurations. In contrast, several fuels exhibit no demand at all: Bio-oil (HtL), e-Diesel (PS and DAC), e-Methane (PS and DAC), Bio-methanol, e-Methanol (DAC), and Grey Ammonia, indicating limited competitiveness or unfavourable cost-emissions trade-offs under this levy level.

Among the fuels that show variability, which are e-Methanol (PS), Blue Ammonia, and e-Ammonia, differences emerge in the scale and timing of uptake. For e-Methanol, the `Local` Market displays a more gradual ramp-up in supply until 2050, whereas the other markets reach full supply earlier (by 2044), but demand falls short in the final years. Blue Ammonia shows an inverse pattern, with the `Local` Market again differing from the other three in timing and volume. e-Ammonia sees an earlier uptake (around 2032) in the `Cost` and `Emerging` Markets, while in `Local` and `Global`, growth only begins after 2044, suggesting divergent regional or structural thresholds for economic viability.

In terms of pricing, all three market configurations with computed prices display similar shapes and remain within a tighter value range, especially when compared to the Regulation scenarios. This is a direct consequence of how the price generation algorithm responds under a levy framework. Since levies increase operational costs proportionally to emissions without directly modifying market structure or allocation rules, the pricing mechanism remains closely tied to production costs. In contrast to regulatory penalties that shift marginal abatement priorities and create wider spreads in willingness to pay, the levy approach imposes a uniform cost burden. This limits the emergence of strong price signals and keeps inter-market price differences moderate, reinforcing a selection dynamic based more on cost-efficiency than aggressive decarbonisation incentives.

7.4.3 Emissions and Expenses



(a) Total Equivalent WTW Emissions (in tons CO_{2eq}/year).

(b) Total Intensity Equivalent WTW Emissions s (in g CO_{2eq}/MJ).

Figure 7.14: Global WTW Emission across the four different market typologies in the `Levy-Based` setup.

In terms of emissions, both the total WTW equivalent emissions and the total intensity equivalent WTW emissions show a generally decreasing trend, with a turning point in 2032 where this decrease accentuates, and in 2035 where it becomes less pronounced. In both figures, all market configurations follow very similar trajectories, with only minor differences between them. The values of Intentisity Equivalent WTW Emissions from 93 gCO_2eq/MJ in 2025 to around 58 gCO_2eq/MJ in 2050. This is mainly because the carbon levy encourages an earlier transition to cleaner fuels and reduces the use of high emission options over time.

Figure 7.15: Stacked expenses in USD (y-axis) across the four market configurations (x-axis) in the `Levy-Based` scenario under a levy of 800 USD.

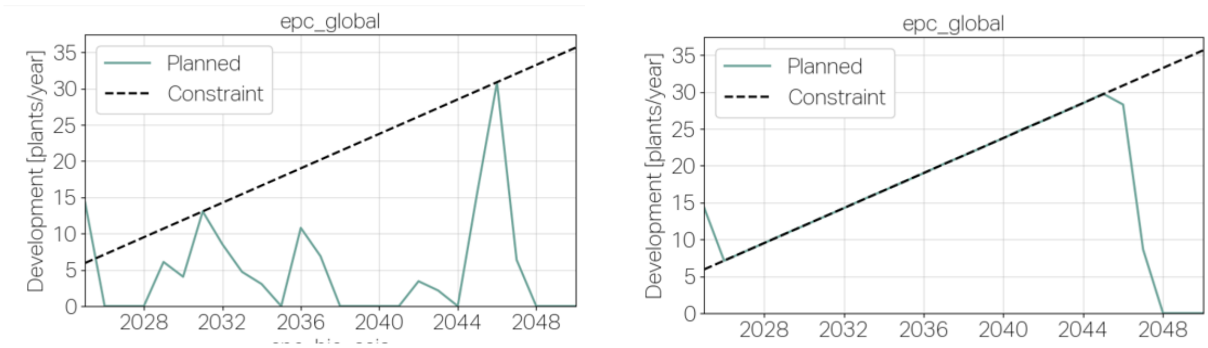
The expenses follow closely the emission and coordination trends. Across all market configurations, both fuel and vessel related expenses remain relatively similar, showing only marginal changes. The `Cost-Only` case reports total fuel-related expenses of approximately 1.41$\times10^{13}$ EUR, while the `Global`, `Local`, and `Emerging Market` scenarios report slightly higher values ranging between 1.43$\times10^{13}$ EUR and 1.44$\times10^{13}$ EUR. This small increase reflects minor shifts in fuel mix and regional allocation but no major structural changes in overall fuel demand. This suggests that, under a flat levy of 800 EUR per tonne CO_2eq, the pricing signal is not strong enough to trigger large-scale structural shifts in the system.

Vessel-related expenses remain nearly constant across all market designs. The minimal differences observed in vessel related expenses suggest that investment decisions in new vessels or retrofits are only slightly influenced by how prices are coordinated across markets. This is because the carbon levy is applied directly through fuel costs, providing a consistent economic signal regardless of the market structure. As a result, the overall investment patterns remain similar across all scenarios. Importantly, there are no regulation expenses in this policy setting, since the levy mechanism replaces direct pricing or penalty schemes with flat levies incorporated directly into market costs. Results are provided in detail in Table N.1 found in Appendix N.

7.5 Cross-Scenario Comparison and Discussion

7.5.1 From Demand Constrained to Supply Constrained

Emissions and Expenses



(a) Producer Development graphs for Regulation with Flexibility at 380 USD IMO GFS.

(b) Producer Development graphs for Regulation with Flexibility at 1200 USD penalty.

Figure 7.16: Producer Development graphs for Regulation with Flexibility in the Global Market showing the built plants vs the maximum physical constraint to build them, showing the difference of a demand-constrained vs a supply constrained market.

A clear distinction in producer behaviour can be observed when comparing the `Global` Market under `Regulation with Flexibility` at penalty levels of 380 USD (Figure 7.16a and 1,200 USD (Figure 7.16b). As shown in the figures, under the lower penalty of 380 USD, the market signal remains too weak to incentivise meaningful investment in new production capacity. Most producers, particularly those supplying advanced biofuels, do not build beyond minimal levels, suggesting that expected returns are insufficient to justify capital deployment.

In contrast, the 1,200 USD penalty creates a much stronger incentive. Here, nearly all producers attempt to scale up rapidly, building towards their respective capacity constraints to meet surging demand for low- and zero-carbon fuels. This behaviour reflects a significant shift from passive participation to aggressive capacity expansion, driven by the higher marginal value of clean fuels under stricter carbon pricing. The observed supply-side response underlines the critical role of regulatory stringency in shaping long-term investment dynamics within decarbonised fuel markets.

As detailed in Appendix F, it is important to note that while total demand remains relatively stable across all market configurations, an apparent gap may be observed between demand and supply. This occurs because unconstrained fuels such as LNG and LSFO continue to dominate a large share of bunker consumption, but their unlimited availability means they are excluded from the aggregated supply figures presented here.

7.5.2 Performance Analytics

The performance results clearly illustrate how different regulatory designs affect both the computational complexity and the solving time of the model. Each scenario introduces different layers of complexity, depending on whether prices need to be coordinated, supply constraints are active, or strict caps are enforced, all of these results are supported in Appendix L.

As shown in Table L.1, the `No Regulation` case remains the fastest and most straightforward, with runtimes between 3,000 and 18,000 seconds across markets. When introducing **Regulation with Flexibility at 380 USD**, the algorithm must iteratively coordinate prices between producers and consumers, leading to longer solve times, especially for the `Global` and `Local` markets. When the penalty rises to **1200 USD**, the problem becomes significantly more complex, as stronger economic incentives drive larger shifts in investments and fuel use. This requires notably more iterations to find equilibrium prices, resulting in runtimes exceeding 46,000 seconds for `Global` and over 85,000 seconds for `Local`.

Table L.2 shows that adding regulations increases the size of the optimisation problem. **Regulation without Flexibility**, which applies strict emission caps without price adjustments, produces the largest models, with almost 2.5 million variables and 1.35 million constraints. In contrast, flexibility-based scenarios keep the model size moderate but require significantly more linear solves to coordinate prices. Again, `Local` markets show the heaviest computational burden due to independent price loops at each port.

Table L.3 highlights the iterative effort required to reach price equilibrium. Flexible regulations, especially at 1200 USD, require over 100,000 fair-share iterations in `Global` and over 180,000 in `Local`. Market dynamic iterations and ceiling iterations also grow as coordination becomes more complex. In contrast, the **Levy-Based** scenario avoids most of this iterative burden, as prices are fixed by design. This keeps both iterations and solving times much lower, while still capturing key regulatory costs.

In summary, the highest computational effort comes from combining price coordination with high penalties, while fixed cap scenarios increase problem size but avoid price iterations. Levy-based mechanisms offer a simpler and more efficient computational solution, although they capture less market interaction.

7.5.3 Market Dynamics Comparison

Following results in Appendix M, peak fuel prices increase with policy stringency, reflecting rising marginal abatement costs and the shifting composition of fuels. In the `No Regulation` scenario, maximum prices remain uniformly low at 14 USD/GJ across all market types, consistent with an environment where fuel selection is driven purely by cost efficiency without emissions constraints.

Under `Regulation with Flexibility (380 USD)`, price signals begin to shape market behaviour more actively. The highest recorded fuel prices reach 45 USD/GJ in both the `Local` and `Emerging` markets, while the `Global Market` peaks slightly lower at 40 USD/GJ. These differences reflect varying degrees of price granularity and allocation efficiency, with more localised or vessel-level coordination leading to stronger marginal bids for clean fuels in specific contexts.

The `Regulation with Flexibility (1200 USD)` scenario marks a significant jump, with all market types registering a peak price of 120 USD/GJ. This convergence indicates a uniform shift toward high-cost abatement fuels as vessels respond to intensified carbon penalties in a fully adaptive market environment.

In the `Regulation without Flexibility` case, where vessels cannot adjust fuel choices dynamically, the system reaches its highest peak prices at 125 USD/GJ across all markets. The lack of flexibility amplifies the cost of compliance for constrained vessels, placing additional pressure on the highest-priced fuels required to meet emissions caps.

Finally, in the `Levies (800)` scenario, price signals are less extreme but still pronounced, with all markets observing peak prices of 85 USD/GJ. The more continuous nature of the levy mechanism moderates price escalation while still encouraging fuel switching, particularly when compared to binary cap-based regulations.

Market typologies significantly influence outcomes. The `Cost-Only` configuration consistently delivers the lowest system costs and avoids greater reliance on fossil fuels, as biofuels remain competitively priced without market premiums. This leads to a smoother, more affordable decarbonisation pathway under pure cost minimisation. In contrast, `Global` Markets exhibit higher fuel prices due to tighter competition, while `Local` Markets tend to trigger stronger supply responses through regional adaptability. `Emerging` Markets show lower overall supply and greater mismatches between prices and system costs, especially under inflexible regulation.

These aggregated outcomes reflect dynamics that are also visible at the disaggregated level when analysing a specific market type across multiple scenarios. For instance, the `Local` Market consistently shows increased supply under strong, flexible regulation, while price levels in the `Global` Market remain elevated across all scenarios. The consistency between system-wide patterns and individual market behaviours reinforces the robustness of the model outcomes.

7.5.4 Emissions and Expenses Comparison

Based on the results presented in the appendix N, both the total emissions of WTW and their intensity tend to decrease over time in all regulatory scenarios. The only exception is the `No Regulation` case, in which total WTW emissions begin to rise steadily after 2026. This is due to increasing transport activity and energy demand, which are not balanced by fuel switching or emissions policies, leading to continued reliance on fossil fuels and no incentives for operational or technological change.

Among all configurations, the scenario that achieves the lowest emission intensity by 2050 is `Regulation with Flexibility` with a carbon penalty of 1200 USD/tCO_2eq. In this case, the `Cost-Only` market structure reaches a minimum value of approximately 28.2 gCO_2 eq/MJ. This outcome derives from two main factors: first, the strictness of the carbon penalty provides a strong economic signal that accelerates the shift toward low-emission fuels; and second, in this market configuration, alternative fuels tend to be cheaper due to the absence of dynamic pricing premiums. This combination supports a deeper decarbonisation process, especially in terms of fuel intensity, despite the fact that total equivalent emissions remain relatively high due to sustained demand levels.

The next best performing scenario is `Regulation without Flexibility`, where emission intensity falls to around 29.3 gCO_2eq/MJ in the `Emerging Market`. This result likely stems from the vessel-level compliance requirement, which forces each actor to adopt cleaner fuels individually, even in the absence of trading. Although this leads to slower optimisation at the system level, it still drives a consistent downward trend in emissions intensity due to regulatory pressure.

At the opposite end of the spectrum, the `No Regulation` scenario results in the highest emission intensity in 2050, with values near 87 gCO_2eq/MJ. This is explained by the complete absence of emissions constraints or pricing mechanisms, which means that the system continues to rely on fossil based fuels with minimal uptake of cleaner alternatives. Consequently, decarbonisation is not incentivised, and total WTW emissions even increase over time, driven purely by rising fuel demand and fleet activity, without any regulatory forces to curb this growth.

Turning to expenses (Table N.1), the regulatory design also has a direct impact on total system costs. Without regulation, the system remains cheapest, as fuel allocation follows the lowest-cost pathway, relying mainly on conventional fuels.

As flexibility is introduced with a moderate penalty (`Regulation with Flexibility 380 USD`), costs increase moderately. Cleaner fuels and minor vessel modifications are introduced, while regulation expenses appear for the first time as compliance mechanisms are activated. When the penalty rises to `Regulation with Flexibility 1200 USD`, stronger decarbonisation measures drive a sharper increase in fuel expenses and vessel investments, reflecting the higher costs associated with producing and using alternative fuels. Interestingly, regulation expenses decrease slightly in this case, as stronger price signals allow the system to comply more efficiently without excessive enforcement costs.

The `Regulation without Flexibility` scenario generates slightly lower fuel and vessel costs compared to `Regulation with Flex 1200 USD`, but regulation costs peak due to the higher administrative and enforcement effort required to maintain strict emission caps without market-based adjustments. Finally, the `Levy-Based` scenario leads to the highest overall expenses. With fixed levies applied directly on fuel consumption and no regulatory flexibility, both fuel and vessel costs climb significantly, resulting in the most expensive decarbonisation pathway.

In summary, regulatory flexibility plays a key role in balancing emission reductions and costs. Policies that combine strong penalties with market flexibility allow the system to adapt more efficiently, spreading costs across cleaner fuels, vessel upgrades, and lower regulatory overhead. In contrast, rigid caps and simple levies lead to higher total costs, as the system lacks mechanisms to dynamically adjust its decarbonisation pathways.

8 Discussion

This chapter outlines several promising avenues for future research and development, reflecting on the model's current capabilities, limitations, and potential enhancements.

8.1 Future Work

8.1.1 Fuel Rerouting and Spatial Market Adjustments

A current limitation of the modelling framework is that fuel produced at one port cannot be rerouted to another, even if the receiving port exhibits higher prices or stronger local demand. This assumption simplifies logistics and supply coordination but misses an important mechanism present in real-world fuel markets, where supply chains adapt to price gradients by reallocating resources across regions. Introducing a mechanism for fuel rerouting would enhance the realism and responsiveness of the market dynamics, especially under flexible pricing schemes. Such an extension could be particularly useful under scenarios where biofuels or synthetic fuels are concentrated in a few production hubs and need to be distributed efficiently across geographically dispersed demand centers.

8.1.2 Algorithmic Enhancements for Price Convergence

While the proposed model provides a solid foundation for simulating market-based decarbonisation, further developments could enhance its performance and scope. From a technical perspective, future work should focus on improving the computational efficiency of the price-discovery algorithm, especially under more complex regulatory designs where runtimes increase substantially.

While the current iterative pricing method based on a modified bisection algorithm has proven robust, it comes with performance trade-offs, especially when the price ceiling must be dynamically adjusted. To reduce simulation time and improve convergence efficiency, future iterations of this model could explore more advanced numerical methods. The Method of Successive Averages (MSA) offers a smoothing mechanism that could reduce oscillations, while Newton-Raphson or quasi-Newton methods may yield faster convergence for well-behaved problem spaces. Hybrid strategies that combine bisection for stability with Newton-based updates for speed could also be explored to balance accuracy and computational performance.

8.1.3 Linking Price Signals to Long-Term Investment Decisions

The current model already incorporates long-term vessel investment decisions that respond to dynamic market price signals. Vessels adapt their fuel technology portfolios based on projected price paths and emissions penalties, enabling strategic fleet evolution over time. However, fuel producers in the model currently base supply-side investment decisions on levelised costs of fuel (LCoF) and the energy supply–demand gap, rather than on market price premiums. A potential extension would be to align producer behavior more closely with market dynamics by incorporating price-based investment logic, allowing for more responsive modeling of fuel infrastructure development under policy and market uncertainty.

8.1.4 Evaluating Policy Strength Through Sensitivity Analysis

The results indicate that the IMO's proposed penalty level of 380 USD/ton CO_2 is insufficient to drive sector-wide compliance with decarbonisation targets by 2050. To provide more actionable insights for policymakers, a deeper sensitivity analysis should be conducted across a range of penalty, levy, and regulatory values. This would enable identification of thresholds beyond which compliance becomes feasible and economically rational. Such analysis could also explore non-linear effects, tipping points, or diminishing returns in policy stringency, helping to inform not only global regulators but also regional authorities seeking to tailor effective carbon pricing strategies.

While highly relevant, this type of in-depth sensitivity study could not be conducted within the time constraints of this thesis and is therefore proposed as a promising area for future research.

8.1.5 Broaden the Model's Coverage

An important avenue for future work involves modelling the interaction between the maritime sector and other fuel-consuming sectors. As carbon penalties increase or fuel prices rise within shipping, there is potential for the sector to become more attractive for fuel suppliers, effectively "stealing" low-carbon fuels from industries such as aviation, heavy industry, or road transport. Conversely, if other sectors are willing to pay higher prices, the shipping industry may find itself outcompeted for scarce decarbonised fuels.

Additionally, expanding the model to incorporate broader geographical coverage, a wider range of fuel technologies, and more detailed fleet characteristics would further strengthen its value for policy design and industry forecasting. These improvements will enable even more robust assessments of future global shipping policies as the sector moves toward full decarbonisation.

9 Conclusion

9.1 Hypothesis Validation

This thesis was guided by two core hypotheses: one addressing the mathematical feasibility of introducing market-based price formation into maritime fuel allocation models, and the other focusing on the analytical insights that these price signals could reveal about system behaviour under decarbonization pathways.

9.1.1 Mathematical Hypothesis Validation

The first hypothesis proposed that it would be possible to model fuel prices directly within an optimization framework, rather than assuming them as exogenous inputs. To test this, the model combined linear programming with a price search mechanism using a bisection algorithm. Since fuel prices were not known in advance, the algorithm iteratively solved the LP for different price levels, progressively narrowing the search interval until supply and demand were balanced. Once equilibrium was reached, the shadow prices from the LP reliably reflected the marginal value of fuel at each market state.

Following the price calculation, fuel was allocated across vessels based on their willingness to pay, which incorporated fuel costs, regulatory penalties, and vessel-specific preferences. The allocation process respected both supply constraints and market behaviour. Through this iterative combination of price search, optimization, and fuel allocation, the model consistently converged to stable solutions across all regulatory and market scenarios. This confirms that market-based pricing can be practically implemented within maritime fuel allocation models, providing a realistic and computationally stable framework for analysing decarbonization policies.

9.1.2 Analytical Hypothesis Validation

The second hypothesis argued that market-based prices would provide deeper insights into how the maritime fuel system reacts to different regulatory designs, compared to traditional cost-minimization models. The simulation results fully confirm this: as price signals emerge under different policy scenarios, they directly influence fuel choices, investment strategies, and vessel retrofitting decisions.

At low penalty levels, such as the IMO's current 380 USD per ton, price signals remain too weak to drive meaningful decarbonization. Fossil fuels continue to dominate, and cleaner fuels see limited adoption. In contrast, when penalties are increased to higher levels like 1200 USD per ton, the economic incentives become strong enough to encourage both fuel switching and substantial investments in clean technologies. These effects are even more visible under supply-constrained conditions, where price formation not only reflects resource scarcity but also serves as a clear signal for long-term investment planning.

In summary, the analytical hypothesis is validated: introducing price formation into the model allows for a richer and more realistic representation of market behaviour, providing valuable insights for the maritime sector and its stakeholders. The results show that prices not only guide current allocations, but also shape long-term decisions, making this approach highly useful for policymakers, shipowners, fuel producers, and investors.

9.2 Main Insights Across Scenarios

The cross-scenario comparison highlights several key conclusions:

- **Decarbonization effectiveness:** Strong price signals are essential. The *Regulation with Flexibility 1200 USD* scenario is the only one capable of triggering substantial fuel switching and significant emission reductions. Lower penalties such as the current IMO 380 USD level do not create enough incentive for large-scale decarbonization.
- **System costs:** While the *No Regulation* scenario remains the least costly, it delivers no decarbonization. The *Regulation with Flexibility 1200 USD* scenario hits a better balance, achieving meaningful emissions reductions while controlling total system costs. In contrast, rigid regulations and levy-based mechanisms lead to higher overall expenses due to their limited market flexibility.
- **Market behaviour:** The fair-share allocation algorithm enables vessels to adjust fuel choices in response to prevailing market signals, reflecting realistic decision-making processes in maritime operations. While all regulatory types influence fuel selection, flexible regulation tends to yield more efficient allocations due to greater adaptability in response to price variations.
- **Computational performance:** While the model performs well, solution times increase significantly under more complex regulatory scenarios, especially with higher penalties and price coordination mechanisms. Future work may explore improved algorithms to accelerate convergence without sacrificing pricing accuracy.

9.3 Thesis Implications

The findings suggest that combining flexible market mechanisms with strong carbon pricing represents the most effective policy pathway for maritime decarbonization. This approach ensures environmental targets are met while allowing the market to adjust investments, fuel choices, and technology adoption efficiently. Such a framework offers valuable signals not only for regulators, but also for shipowners, fuel producers, and technology providers.

Beyond the academic contribution, this modelling approach holds significant importance. First, it offers the maritime sector a much more realistic tool to anticipate how markets will evolve under different policy frameworks. Second, it provides actionable information for global stakeholders, including shipowners, fuel suppliers, policymakers, and financial institutions, to make better investment and operational decisions in the face of regulatory uncertainty. And third, due to its relevance and applicability, this methodology will be directly integrated into the forecasting tools used by the Center to support future scenario analysis and policy discussions at the global level.

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A Mockup of NavigaTE functionality for price convergence

```python
import numpy as np
import pandas as pd
import gurobipy as gp
from gurobipy import GRB

# Create a Gurobi model
model = gp.Model("price_convergence")

# Define variables
b1 = model.addVar(name="b1")
b2 = model.addVar(name="b2")
bunc = model.addVar(name="bunc")

# Define parameters
p1 = 50  # Coefficient for b1
p2 = 100  # Coefficient for b2
punc = 200  # Coefficient for bunc
C1 = 100 # Capacity for b1
C2 = 100 # Capacity for b2
D = 500  # Example demand value

# Set objective function
model.setObjective(b1 * p1 + b2 * p2 + bunc * punc, GRB.MINIMIZE)

# Add constraints
c1 = model.addConstr(b1 <= C1, "c1")
c2 = model.addConstr(b2 <= C2, "c2")
c3 = model.addConstr(b1 + b2 + bunc == D, "c3")

# Optimize the model
model.optimize()

# Get shadow prices (dual values) for the constraints
if model.status == GRB.OPTIMAL:
    print(f"Shadow price for c1 (supply constraint b1): {c1.Pi}")
    print(f"Shadow price for c2 (supply constraint b2): {c2.Pi}")

# Print results
if model.status == GRB.OPTIMAL:
    print(f"Optimal solution found:")
    print(f"b1: {b1.X}")
    print(f"b2: {b2.X}")
    print(f"bunc: {bunc.X}")
    print(f"Objective value: {model.ObjVal}")
else:
    print("No optimal solution found.")

# Retrieve the shadow prices value
shadow_prices = {
    "c1": c1.Pi,
    "c2": c2.Pi,
}

# Print variable values
for f in model.getVars():
    print(f"Variable {f.VarName}: Value = {f.X}")
```

```
#-----Change of constraint capacity---------------
C1_new = 100
C2_new = 450

# Update the model with new capacities
model.remove(c1)
model.remove(c2)
c1_new = model.addConstr(b1 <= C1_new, "c1")
c2_new = model.addConstr(b2 <= C2_new, "c2")
model.update()

# Re-optimize the model
model.optimize()

# Get shadow prices (dual values) for the updated constraints
if model.status == GRB.OPTIMAL:
    print(f"Shadow price for c1 (supply constraint b1): {c1_new.Pi}")
    print(f"Shadow price for c2 (supply constraint b2): {c2_new.Pi}")

# Print results
if model.status == GRB.OPTIMAL:
    print(f"Optimal solution found after updating constraints:")
    print(f"b1: {b1.X}")
    print(f"b2: {b2.X}")
    print(f"bunc: {bunc.X}")
    print(f"Objective value: {model.ObjVal}")
```

Listing A.1: Toy example demonstrating the core concept of shadow prices in linear programming. The model minimizes total cost by allocating demand across three supply options with different costs and capacity constraints. Two scenarios are shown: one with tighter supply constraints and one with relaxed capacity on the second supplier. The resulting shadow prices (dual values) illustrate how the marginal value of relaxing a constraint changes under different conditions.

B Initial MVP for concept proving of duality for NavigaTE

```
import gurobipy as gp
from gurobipy import GRB
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt


# Model parameters
np.random.seed(42)
years = list(np.arange(2025, 2035))  # Convert to list
fuels = ["Biodiesel", "Ethanol", "Hydrogen", "Diesel"]

# Initial supply per fuel (millions of liters)
supply = {fuel: [float(np.random.randint(100, 200)) for _ in years] for fuel in
    fuels}

# Production costs per liter €(\)
initial_production_costs = {"Biodiesel": 1.2, "Ethanol": 0.8, "Hydrogen": 2.5, "
    Diesel": 1.0}

def smooth_cost_curve(initial_cost, peak_year, end_year, peak_factor=1.5):
    years = np.arange(2025, 2035)
    peak_cost = initial_cost * peak_factor
    costs = []
    for year in years:
        if year <= peak_year:
            cost = initial_cost + (peak_cost - initial_cost) * (year - 2025) / (
                peak_year - 2025)
        else:
            cost = peak_cost - (peak_cost - initial_cost) * (year - peak_year) / (
                end_year - peak_year)
        costs.append(cost)
    return costs

# Generates the production costs per year
production_costs = {fuel: smooth_cost_curve(initial_production_costs[fuel], 2028,
    2034) for fuel in fuels}

# Emisions per liter (kg CO2)
emissions = {"Biodiesel": 2.5, "Ethanol": 1.8, "Hydrogen": 0.0, "Diesel": 3.2}

# Total market's demand (million liters per year, constant)
demand = 400

# Emissions threshold and penalty
emission_threshold = 800
penalty = 450

# Parameter to adjust the prices
alpha = 0.05  # Updating prices factor

# To store the results
all_results_with_shadow = []
all_results_without_shadow = []

# Initializes the prices with prduction costs
```

```python
prices = {fuel: production_costs[fuel] for fuel in fuels}
prices_without_shadow = prices.copy()

# Simulation per year
for t in years:
    model = gp.Model(f"Market_Equilibrium_{t}")

    # Decision variables: quantity of sold fuel(b_i)
    b = model.addVars(fuels, lb=0, vtype=GRB.CONTINUOUS, name="b")

    #  Emissions excess variable
    e = model.addVar(lb=0, vtype=GRB.CONTINUOUS, name="e")

    # Constraint of the balance supply-demand
    demand_balance = model.addConstr(gp.quicksum(b[f] for f in fuels) == demand,
        name=f"Demand_Balance")

    # Supply Constraint
    for f in fuels:
        if t > years[0]:  # Ensure t-1 is a valid index
            model.addConstr(b[f] <= supply[f][years.index(t) - 1], name=f"
                Supply_Limit_{f}")

    # Emissions constraint
    model.addConstr(gp.quicksum(emissions[f] * b[f] for f in fuels) -
        emission_threshold <= e, name=f"Emission_Limit")

    # Calculate initial prices based in the production costs of the equivalent year
    prices = {fuel: production_costs[fuel][years.index(t)] * 1.15 for fuel in fuels
        }
    prices_without_shadow = {fuel: production_costs[fuel][years.index(t)] * 1.15
        for fuel in fuels}

    # Objective function: minimize costs + emissions penalty
    model.setObjective(
        gp.quicksum(prices[f] * b[f] for f in fuels) + penalty * e,
        GRB.MINIMIZE
    )

    # Model solver
    model.optimize()

    # Verifies the optimal solution
    if model.Status == GRB.OPTIMAL:
        # Updates prices using shadow prices of the demand balance constraint
        shadow_price = demand_balance.Pi
        for f in fuels:
            prices[f] = prices[f] + shadow_price

        # extracts optimal values and stores them
        results_with_shadow = {"Year": t}
        results_without_shadow = {"Year": t}
        for f in fuels:
            results_with_shadow[f] = b[f].X
            results_with_shadow[f + "_price"] = prices[f]
            results_with_shadow[f + "_shadow_price"] = shadow_price
            results_with_shadow[f + "_supply"] = supply[f][years.index(t)]

            results_without_shadow[f] = b[f].X
            results_without_shadow[f + "_price"] = prices_without_shadow[f]
            results_without_shadow[f + "_supply"] = supply[f][years.index(t)]

        results_with_shadow["penalty"] = e.X
```

```
        results_without_shadow["penalty"] = e.X

        all_results_with_shadow.append(results_with_shadow)
        all_results_without_shadow.append(results_without_shadow)

        # Price evolution based in market equilibrium
        if t > years[0]:
            total_supply_previous = sum(supply[f][years.index(t) - 1] for f in fuels)
            for f in fuels:
                prices[f] = prices[f] + alpha * ((demand / total_supply_previous) - 1) * prices[f]
                prices_without_shadow[f] = prices_without_shadow[f] + alpha * ((demand / total_supply_previous) - 1) * prices_without_shadow[f]

# Creates DataFrames with all results
df_all_results_with_shadow = pd.DataFrame(all_results_with_shadow)
df_all_results_without_shadow = pd.DataFrame(all_results_without_shadow)

# Stores Dataframes in Excel
df_all_results_with_shadow.to_excel("price_dynamics_results_with_shadow.xlsx", index=False)
df_all_results_without_shadow.to_excel("price_dynamics_results_without_shadow.xlsx", index=False)

# Shows the complete DataFrames
print("Results with Shadow Prices:")
print(df_all_results_with_shadow)
print("\nResults without Shadow Prices:")
print(df_all_results_without_shadow)


# Creates a line cgart with the costs and prices of all fuels s
fig, ax1 = plt.subplots(figsize=(14, 8))

# Costs and price graphs
for fuel in fuels:
    ax1.plot(years, [production_costs[fuel][years.index(t)] for t in years], label=f'{fuel} Cost', linestyle='--')
    ax1.plot(df_all_results_with_shadow['Year'], df_all_results_with_shadow[fuel + '_price'], label=f'{fuel} Price with Shadow')
    ax1.plot(df_all_results_without_shadow['Year'], df_all_results_without_shadow[fuel + '_price'], label=f'{fuel} Price without Shadow')

ax1.set_xlabel('Year')
ax1.set_ylabel('Price €()')
ax1.set_title('Cost and Price Dynamics for All Fuels')
ax1.legend()
ax1.grid(True)

# Crates a second line chart for the quantity of sold fuel
ax2 = ax1.twinx()
for fuel in fuels:
    ax2.plot(df_all_results_with_shadow['Year'], df_all_results_with_shadow[fuel], label=f'{fuel} Bunkered Quantity', linestyle=':')

ax2.set_ylabel('Bunkered Quantity (millions of liters)')
ax2.legend(loc='upper left')

plt.savefig('all_fuels_price_and_quantity_dynamics.png')
plt.show()
```

Listing B.1: Illustrative Python implementation of a simplified multi-year, multi-fuel market equilibrium model used to demonstrate the effect of shadow prices on price formation and fuel allocation. The code simulates demand, supply constraints, and emissions limits for four fuels over a decade, solving a cost minimization problem using Gurobi. Shadow prices from the demand constraint are used to dynamically adjust fuel prices, reflecting marginal scarcity and driving convergence. Results with and without shadow price adjustments are compared to highlight their role in guiding economically consistent pricing under constraint-driven market behavior.

C NavigaTE Bunker Pricing Algorithm

C.1 Main Solver Function

```
def solve(self):

    if self._options.include_market_dynamic():

        if self._options.get_market_type() == MarketTypeID.EMERGING:

            # if the market is emerging, each vessel makes individual
            # offtake agreements with individual prices. Hence, the
            # solution is just the fair-share solution but with the
            # shadow-prices added on top as the price premium. These
            # are added later during the transfer of results
            self._optimize_fair_share()

        else:

            # a general price premium must be established across
            # coupled markets requiring an iterative approach
            self._optimize_market_dynamic()

    else:

        # if there is no market dynamics included the
        # model is solved using production costs
        self._optimize_fair_share()
```

Listing C.1: Main solver routine managing price formation across market types in NavigaTE. When market dynamics are disabled, fuel allocation is based solely on production costs via a fair-share solution. For `Emerging` markets, prices are adjusted individually using vessel-specific shadow prices post-optimization. In contrast, `Global` and `Local` markets trigger a coupled optimization loop, solving for market-clearing price premiums across interconnected agents, reflecting coordinated fuel price dynamics.

C.2 Market Dynamics Optimization

```
def _optimize_market_dynamic(self):

    # extract tolerances and maximum iterations
    market_type = self._options.get_market_type()
    max_iter = self._options.get_market_maximum_iterations()
    tol_quantity = self._options.get_market_tolerance_quantity()
    tol_price = self._options.get_market_tolerance_price()

    # define the aggregation key based on market type
    if market_type == MarketTypeID.GLOBAL:
        self._get_market_key = lambda x, y: y
    else:
        self._get_market_key = lambda x, y: (x, y)

    # calculate the cumulative supply of fuels in order to compare against
    self._bunker_supply = self._calculate_cumulative_fuel_supply()

    # initial floor of the shadow price is zero
    floors = {k: 0. for k in self._bunker_supply}

```

```
    # initial ceilings where demand < supply
    ceilings = self._calculate_initial_ceilings()

    converged = False
    iteration = 0
    while not converged and iteration < max_iter:

        middles = {k: (floors[k] + ceilings[k]) / 2. for k in floors}

        self._update_vessel_market_objective(middles)
        self._optimize_fair_share()

        demands = self._calculate_cumulative_fuel_demand()
        shadow_prices_min = self._calculate_minimum_shadow_price()

        for k in floors:

            demand = demands.get(k, 0.)
            supply = self._bunker_supply[k]
            shadow_price_min = shadow_prices_min.get(k, None)

            if demand < supply - tol_quantity:
                ceilings[k] = middles[k]
                floors[k] = 0.
                if floors[k] > ceilings[k]:
                    floors[k] = ceilings[k]
                continue

            if shadow_price_min is None:
                ceilings[k] = middles[k]
                continue

            if shadow_price_min > tol_price:
                floors[k] = middles[k]
            else:
                ceilings[k] = middles[k]

            if floors[k] > ceilings[k]:
                floors[k] = ceilings[k]

        converged = self._check_market_convergence(floors, ceilings)
        iteration += 1

    self._update_vessel_market_objective(floors)
    self._optimize_fair_share()

    self._bunker_fuel_premium = floors
    self._market_dynamic_iterations += iteration
```

Listing C.2: Core market equilibrium algorithm in NavigaTE for simulating price convergence under `Global` and `Local` market dynamics. This iterative bisection method adjusts fuel price premiums between supply floors and demand ceilings, based on vessel responses and shadow price signals. Convergence is determined by fuel-level price and quantity tolerances, ensuring consistent bunker fuel allocation and market-clearing prices across coupled actors.

C.3 Initial Price Ceiling Calculation

```
def _calculate_initial_ceilings(self):
    increase_factor = self._options.get_market_price_ceiling_growth()
    min_ceiling = self._options.get_market_price_ceiling_minimum()
    tol_quantity = self._options.get_market_tolerance_quantity()
```

```python

    self._optimize_fair_share()

    demands = self._calculate_cumulative_fuel_demand()
    shadow_prices_max = self._calculate_maximum_shadow_price()

    iteration = 0
    ceilings = {k: 0.0 for k in self._bunker_supply}

    while True:
        still_binding = set()
        shadow_prices_min = self._calculate_minimum_shadow_price()

        for k in self._bunker_supply:
            demand = demands.get(k, 0.)
            supply = self._bunker_supply[k]
            shadow_price_min = shadow_prices_min.get(k, None)

            if demand < supply - tol_quantity or shadow_price_min is None:
                continue

            if ceilings[k] == 0.0:
                shadow_price_max = shadow_prices_max.get(k, 0.0)
                ceilings[k] = max(min_ceiling, increase_factor * max(
                    shadow_price_max, shadow_price_min))
            else:
                ceilings[k] *= increase_factor

            still_binding.add(k)

        if not still_binding:
            break

        margin_update = {k: ceilings[k] for k in still_binding}
        self._update_vessel_market_objective(margin_update)
        self._optimize_fair_share()
        demands = self._calculate_cumulative_fuel_demand()
        iteration += 1

    self._market_dynamic_ceiling_iterations = iteration
    return ceilings
```

Listing C.3: First outer loop of the market dynamics routine in NavigaTE, responsible for computing initial price ceilings. By iteratively adjusting fuel-specific ceilings based on minimum and maximum observed shadow prices, this routine ensures that subsequent price convergence starts from a feasible upper bound where constraints are no longer binding.

C.4 Market Convergence Check

```python
def _check_market_convergence(self, floors, ceilings):
    return max(abs(ceilings[k] - floors[k]) for k in floors) <= self._options.
        get_market_tolerance_price()
```

Listing C.4: Market convergence check in NavigaTE, ensuring that the difference between fuel-specific price floors and ceilings falls below a predefined tolerance threshold, thereby terminating the iterative market-clearing loop once equilibrium is reached

C.5 Update Vessel Market Objective

```python
def _update_vessel_market_objective(self, shadow_price):
```

```
    for (v, p, f), bunker in self._bunker.items():
        port_name = self._vessels[v].get_route().get_ports()[p].get_name()
        key = (v, port_name, f)
        local_key = (port_name, f)
        market_key = self._get_market_key(port_name, f)

        if market_key not in shadow_price:
            continue

        price = self._bunker_fuel_cost[local_key] + shadow_price[market_key] + self
            ._bunker_levy_cost[key]
        bunker.Obj = price * self._multipliers[v]
```

Listing C.5: Update routine for vessel-specific market objectives in NavigaTE, applying market-clearing shadow prices and regulatory levies to adjust fuel costs used in the optimization, based on port and fuel-level market keys.

C.6 Cumulative Fuel Supply Calculation

```
def _calculate_cumulative_fuel_supply(self):
    tol_quantity = self._options.get_market_tolerance_quantity()
    supplies = {}

    for port_name, port in self._ports.items():
        for f, fuel in self._fuels.items():
            if not port.bunkering_allowed(f):
                continue

            market_key = self._get_market_key(port_name, f)

            if self._scope == BunkerScopeID.EXISTING:
                supply = port.get_expectation().get_existing_bunker_supply(f, self.
                    _idx)
            else:
                supply = port.get_expectation().get_expected_bunker_supply(f, self.
                    _idx)

            if np.isfinite(supply) and supply > tol_quantity:
                supplies.setdefault(market_key, 0.)
                supplies[market_key] += supply

    return supplies
```

Listing C.6: Computation of cumulative fuel supply across ports in NavigaTE, aggregating supply volumes per market region and fuel type based on port-level availability and model scope settings.

C.7 Cumulative Fuel Demand Calculation

```
def _calculate_cumulative_fuel_demand(self):
    tol_sol = self._options.get_solution_tolerance()
    demands = {}

    for (v, p, f), bunker in self._bunker.items():
        port_name = self._vessels[v].get_route().get_ports()[p].get_name()
        key = (v, port_name, f)

        if key not in self._fair_share_fuel:
            continue

```

```
        market_key = self._get_market_key(port_name, f)

        if market_key not in self._bunker_supply:
            continue

        if self._bunker_supply[market_key] < tol_sol:
            continue

        demand = bunker.X * self._multipliers[v]

        if market_key not in demands:
            demands[market_key] = demand
        else:
            demands[market_key] += demand

    return demands
```

Listing C.7: Computation of cumulative fuel demand in NavigaTE, aggregating vessel-level fuel uptake across ports and routes into market-specific demand volumes, aligned with supply and convergence routines.

C.8 Maximum Shadow Price Calculation

```
def _calculate_maximum_shadow_price(self):
    return self._calculate_extremum_shadow_price(max, allow_zero=False)
```

Listing C.8: Compute the maximum shadow price across all market segments by leveraging a general extremum calculation routine, excluding zero values to identify binding constraints with the highest marginal cost.

C.9 Minimum Shadow Price Calculation

```
def _calculate_minimum_shadow_price(self):
    return self._calculate_extremum_shadow_price(min, allow_zero=False)
```

Listing C.9: Calculate the minimum shadow price across all market segments using a general extremum method, excluding zero values to focus on the lowest positive marginal cost indicating binding constraints.

C.10 Extremum Shadow Price Calculation

```
def _calculate_extremum_shadow_price(self, method, allow_zero=False):
    if not ((method is min) or (method is max)):
        raise ValueError("Extremum method must be either 'min' or 'max'.")

    tol_sol = self._options.get_solution_tolerance()
    shadow_prices = self._extract_shadow_prices()
    extremum_shadow_prices = {}

    for (v, port_name, f), shadow_price in shadow_prices.items():
        if (not allow_zero) and (shadow_price < tol_sol):
            continue

        key = self._get_market_key(port_name, f)

        if key not in extremum_shadow_prices:
            extremum_shadow_prices[key] = shadow_price
        else:
```

```
            extremum_shadow_prices[key] = method(extremum_shadow_prices[key],
                shadow_price)

    return extremum_shadow_prices
```

Listing C.10: General method to calculate the extremum (minimum or maximum) shadow price across market segments, optionally excluding values below a solution tolerance to filter out negligible shadow prices. The function aggregates shadow prices by market key and applies the specified extremum method.

C.11 Shadow Price Extraction

```
def _extract_shadow_prices(self):
    tol_sol = self._options.get_solution_tolerance()
    shadow_prices = {}

    for (v, port_name, f), constraint in self._fair_share_fuel.items():
        key = (v, port_name, f)

        if not self._ports[port_name].bunkering_allowed(f):
            continue

        market_key = self._get_market_key(port_name, f)
        if market_key not in self._bunker_supply:
            continue

        if self._bunker_supply[market_key] < tol_sol:
            continue

        shadow_prices[key] = -constraint.Pi / self._multipliers[v]

    return shadow_prices
```

Listing C.11: Extract shadow prices from the fair-share fuel constraints for each vessel, port, and fuel combination. Shadow prices are normalized by vessel multipliers and filtered based on bunkering permission and supply thresholds to ensure only relevant market segments are considered.

D Test Environment Files

The following configuration files are used to construct and execute the test environment:

- `test_alternative_powers`
- `test_ban_vessels`
- `test_bunker_logistics`
- `test_bunker_options`
- `test_bunker_regions`
- `test_canals`
- `test_curves`
- `test_efficiencies`
- `test_feedstocks`
- `test_fleet_inertia`
- `test_fleets`
- `test_forecasts`
- `test_fuel_availability`
- `test_fuel_constraints`
- `test_fuel_conversion`
- `test_fuel_inertia`
- `test_fuels`
- `test_levies`
- `test_levies_activate`
- `test_model_definition`
- `test_plant_readiness`
- `test_plants`
- `test_ports`
- `test_producers`
- `test_regions`
- `test_regulations`
- `test_regulations_activate`
- `test_reports`
- `test_sources`
- `test_speed_management`
- `test_technology_availability`
- `test_technology_uptake_initial`
- `test_technology_uptake_update`
- `test_time_steps_yearly`
- `test_timetables`
- `test_transports`
- `test_uptakes_fleet`
- `test_vessels`

E Modelling Framework

Scenario	Dynamic Pricing	Policy Active	Fuel Mix Response
Cost-Only + No Regulation	No	No	Static
Cost-Only + Levy	No	Yes	Moderate
Cost-Only + Flexible Regulation	No	Yes	High
Cost-Only + Non-Flexible Reg.	No	Yes	High
Global + No Regulation	Yes	No	Price-Sensitive
Global + Levy	Yes	Yes	Price-Sensitive
Global + Flexible Regulation	Yes	Yes	Price- and Policy-Sensitive
Global + Non-Flexible Reg.	Yes	Yes	Policy-Constrained
Local + No Regulation	Yes	No	Price-Sensitive
Local + Levy	Yes	Yes	Levy-Driven
Local + Flexible Regulation	Yes	Yes	Combined Shift
Local + Non-Flexible Reg.	Yes	Yes	Constrained
Emerging + No Regulation	No	No	Cost-Minimal
Emerging + Levy	No	Yes	Levy-Driven
Emerging + Flexible Regulation	No	Yes	Moderate Adjustment
Emerging + Non-Flexible Reg.	No	Yes	Constrained

Table E.1: Summary of active mechanisms across all simulated scenarios, highlighting the presence of dynamic pricing, policy application, and resulting fuel mix behaviour.

F Test Environment Plots

F.1 Global - Middle East Plots

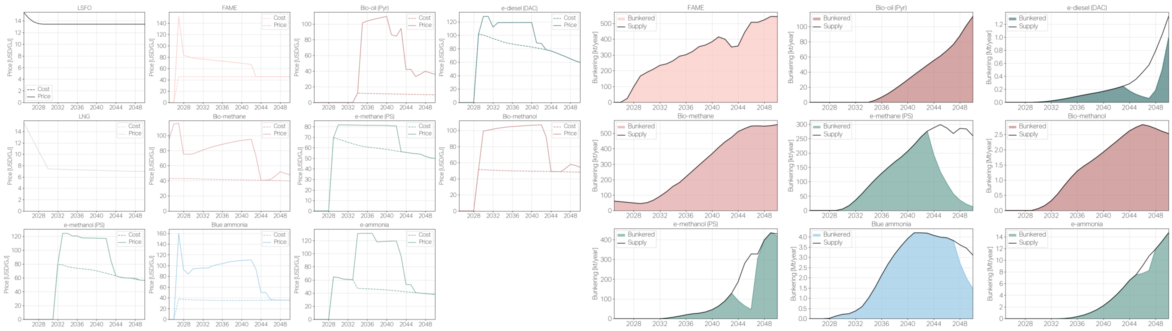


Figure F.1: Bunker fuel supply-demand interaction and price convergence in Middle East ports under Global Market assumptions in the test environment. The left figure presents the price evolution in [USD/GJ] of each fuel type while right figure shows bunker demand versus available supply in [kt/yr] for key alternative fuels.

F.2 Local - Middle East Plots

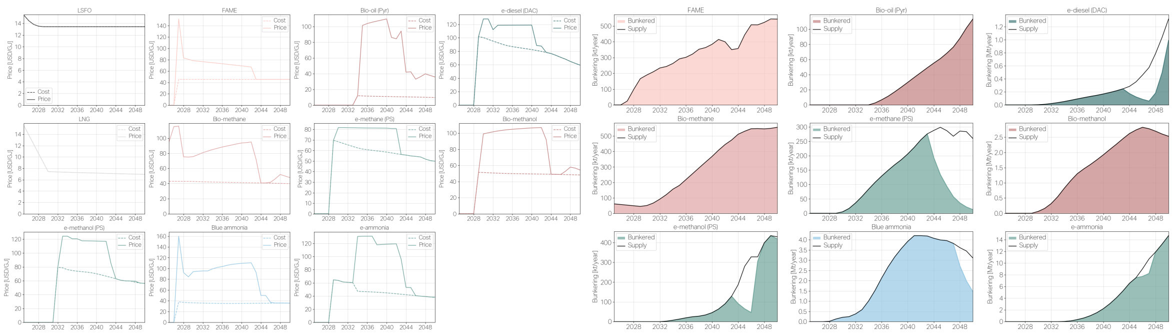


Figure F.2: Bunker fuel supply-demand interaction and price convergence in Middle East ports under Local Market assumptions in the test environment. The left figure presents the price evolution in [USD/GJ] of each fuel type while right figure shows bunker demand versus available supply in [kt/yr] for key alternative fuels..

F.3 Emerging - Middle East Plots

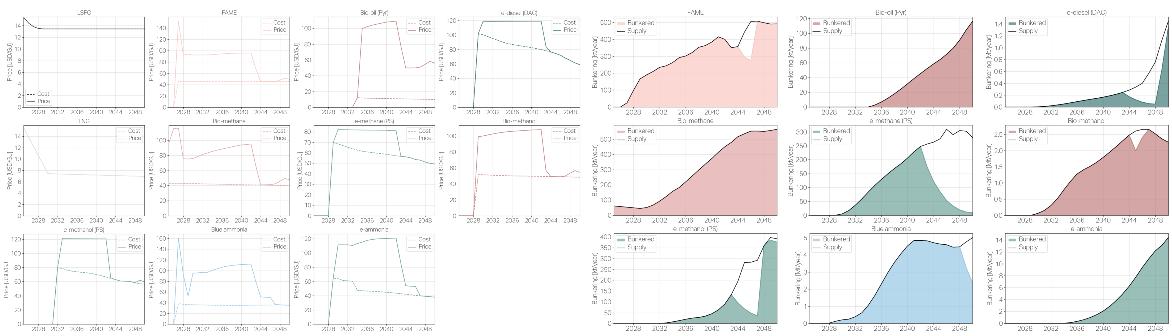
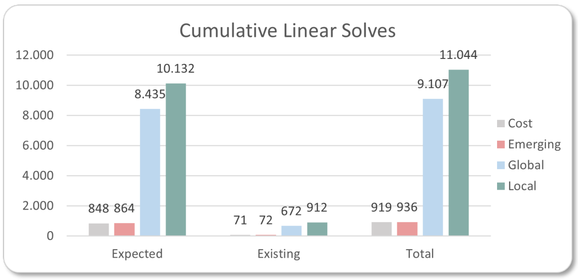


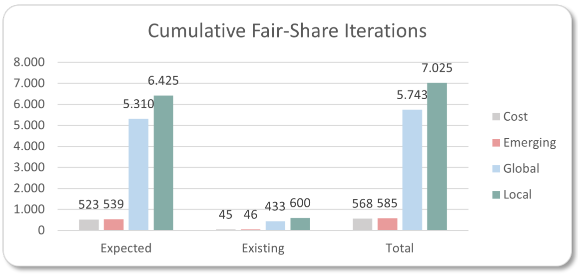
Figure F.3: Bunker fuel supply-demand interaction and price convergence in Middle East ports under Emerging Market assumptions in the test environment. The left figure presents the price evolution in [USD/GJ] of each fuel type while right figure shows bunker demand versus available supply in [kt/yr] for key alternative fuels.

G No Regulation Environment - Results

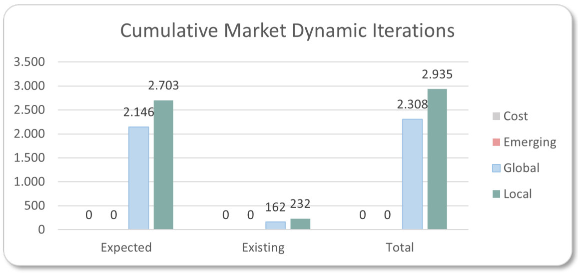
G.1 Performance Analytics



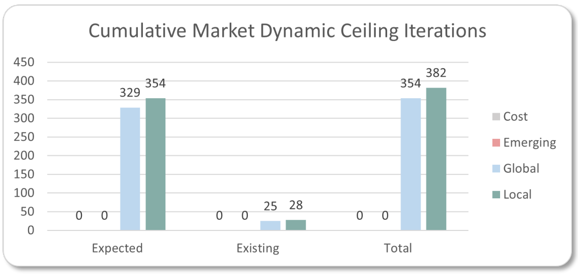
(a) Linear Solves



(b) Fair-Share Iterations



(c) Market Dynamic Iterations



(d) Ceiling Iterations

Figure G.1: Cumulative expected, existing and total solver calls and iteration counts under the `No Regulation` scenario across all model runs.

G.2 Market Dynamics

G.2.1 Fuel Supply and Bunker Prices – Cost-Only

Africa

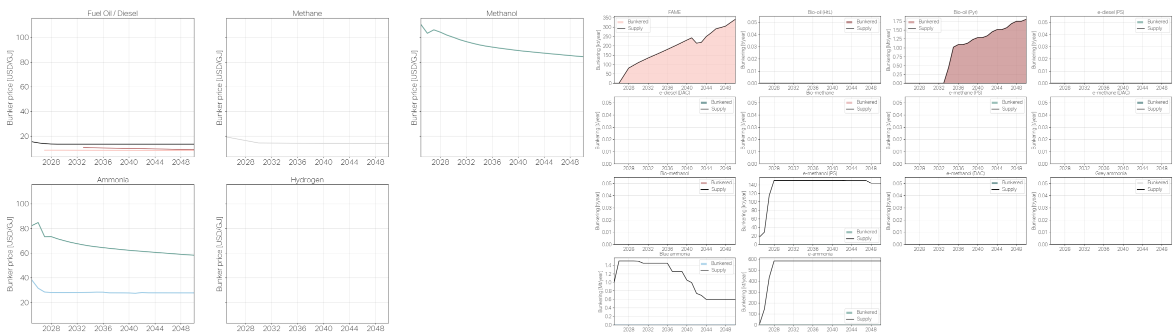


Figure G.2: Bunker fuel cost (left), and fuel supply and demand (right) in African ports.

Americas

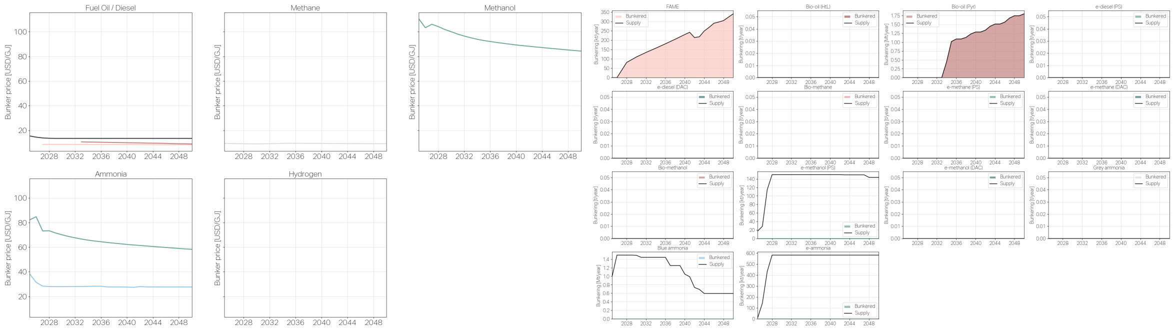


Figure G.3: Bunker fuel cost (left), and fuel supply and demand (right) in American ports.

Asia

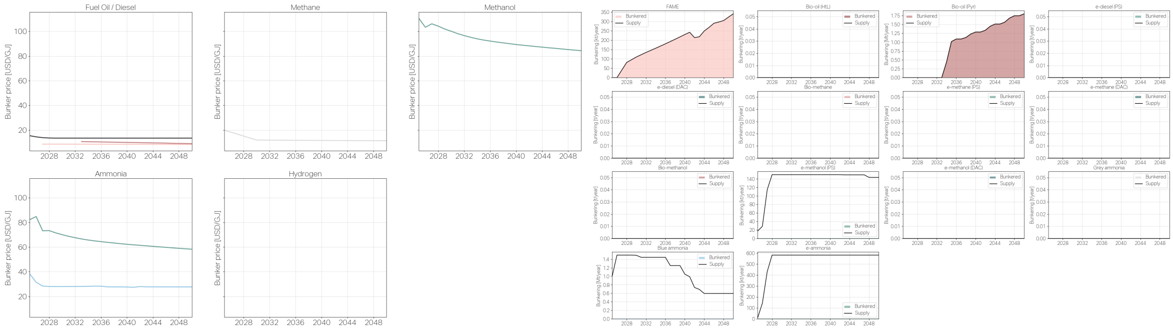


Figure G.4: Bunker fuel cost (left), and fuel supply and demand (right) in Asian ports.

Europe

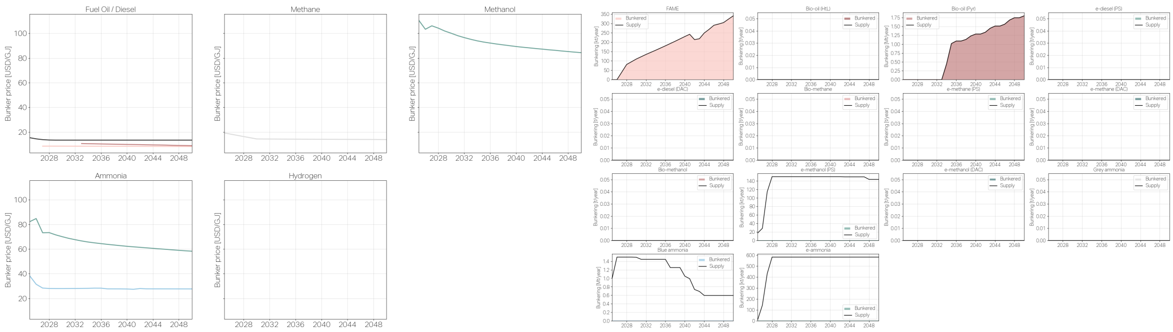


Figure G.5: Bunker fuel cost (left), and fuel supply and demand (right) in European ports.

Middle East

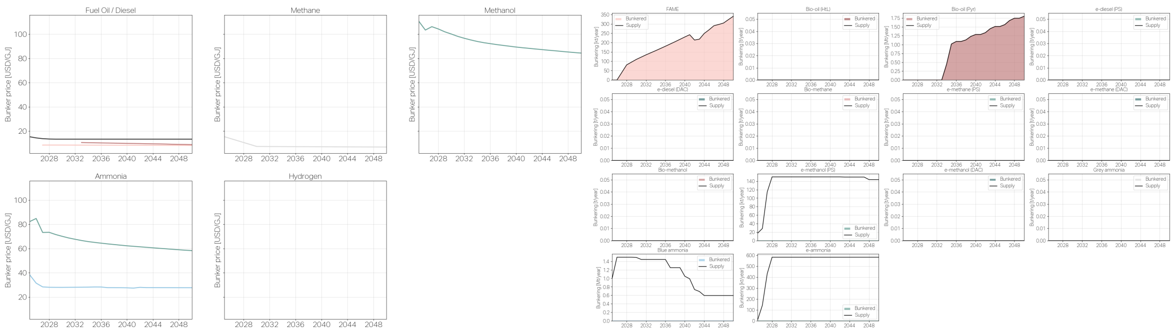


Figure G.6: Bunker fuel cost (left), and fuel supply and demand (right) in Middle Eastern ports.

Global Overview

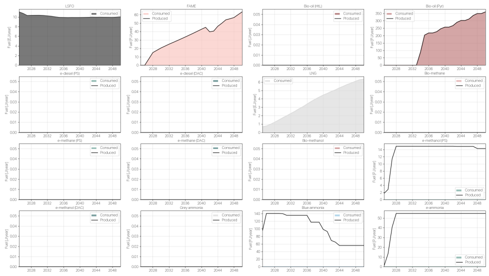


Figure G.7: Global fuel supply and demand overview for the Cost-Only scenario.

G.2.2 Fuel Supply and Bunker Prices – Emerging

Africa

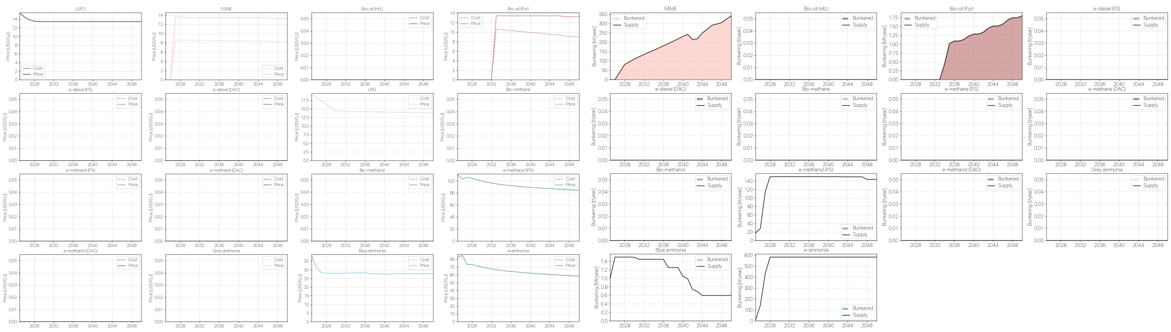


Figure G.8: Market price (left), and fuel supply and demand (right) in African ports under the Emerging configuration.

Americas

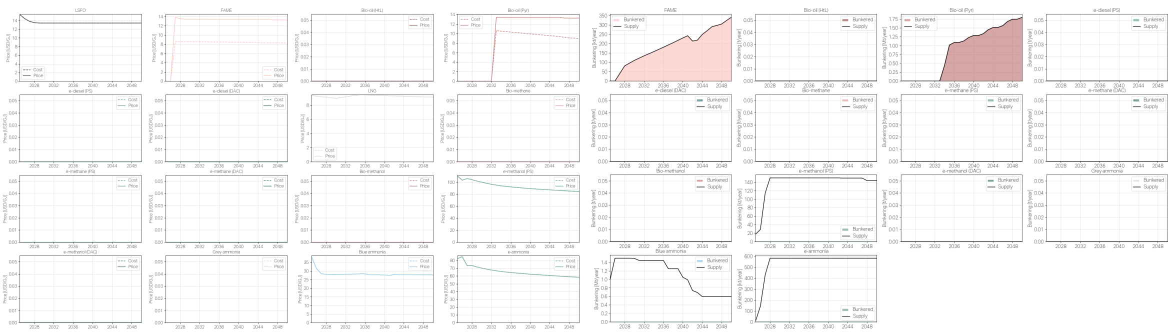


Figure G.9: Market price (left), and fuel supply and demand (right) in American ports under the Emerging configuration.

Asia

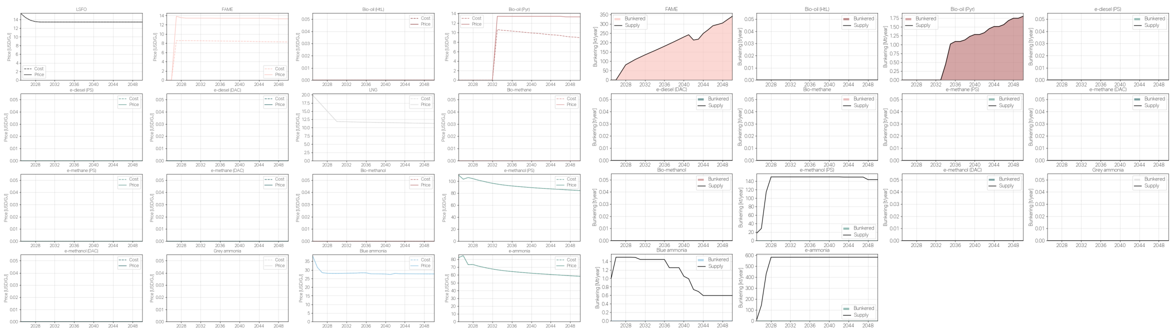


Figure G.10: Market price (left), and fuel supply and demand (right) in Asian ports under the Emerging configuration.

Europe

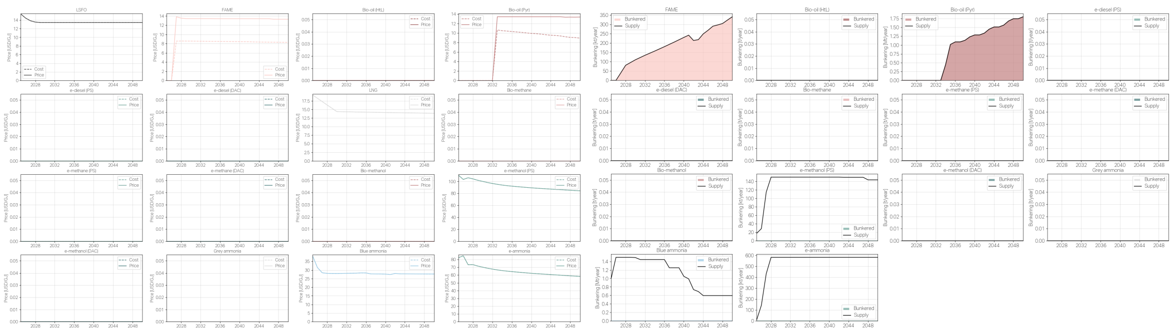


Figure G.11: Market price (left), and fuel supply and demand (right) in European ports under the Emerging configuration.

Middle East

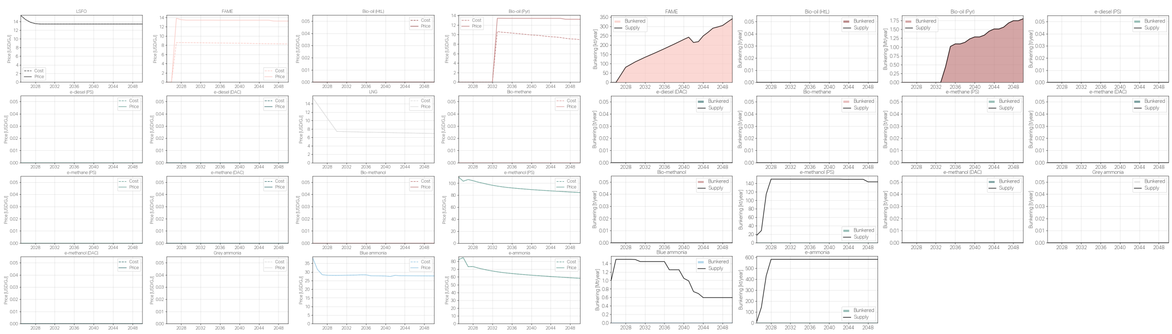


Figure G.12: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Emerging configuration.

Global Overview

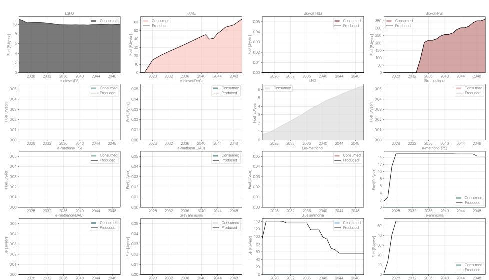


Figure G.13: Global fuel supply and demand overview for the Emerging configuration.

G.2.3 Fuel Supply and Bunker Prices – Global

Africa

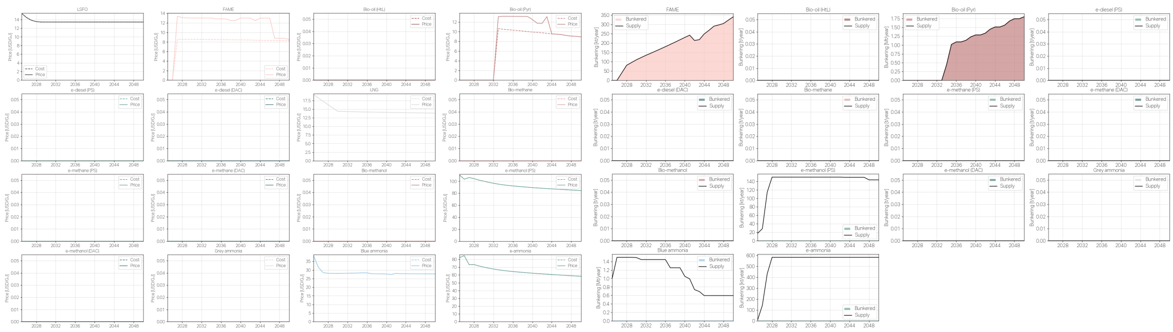


Figure G.14: Market price (left), and fuel supply and demand (right) in African ports under the Global configuration.

Americas

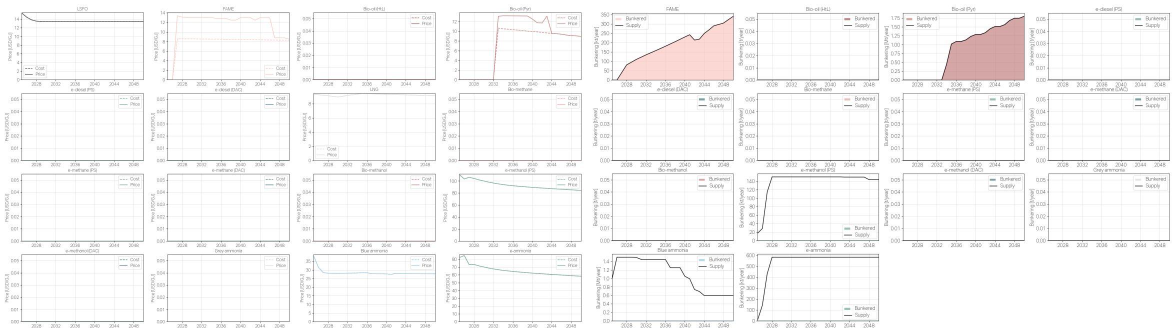


Figure G.15: Market price (left), and fuel supply and demand (right) in American ports under the Global configuration.

Asia

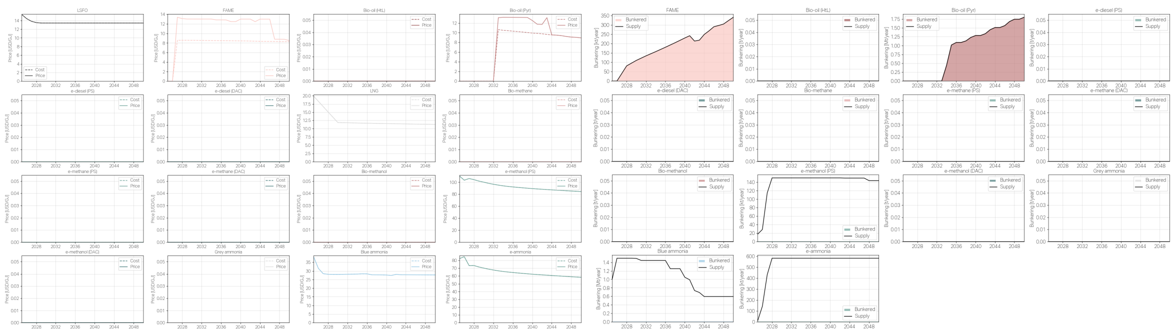


Figure G.16: Market price (left), and fuel supply and demand (right) in Asian ports under the Global configuration.

Europe

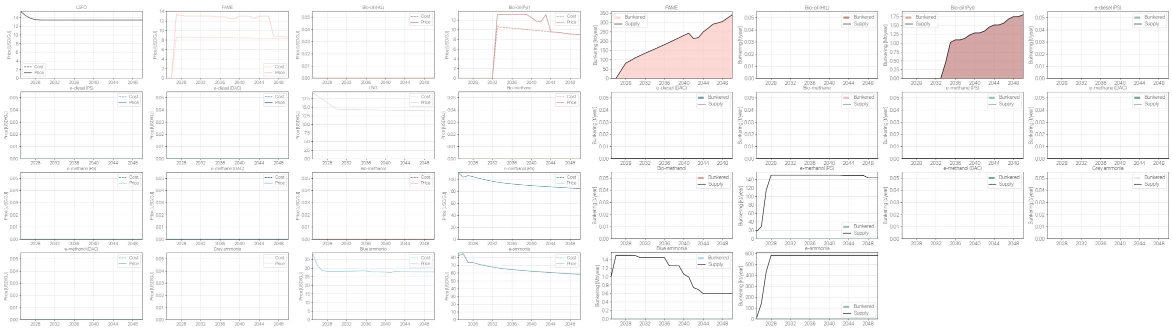


Figure G.17: Market price (left), and fuel supply and demand (right) in European ports under the Global configuration.

Middle East

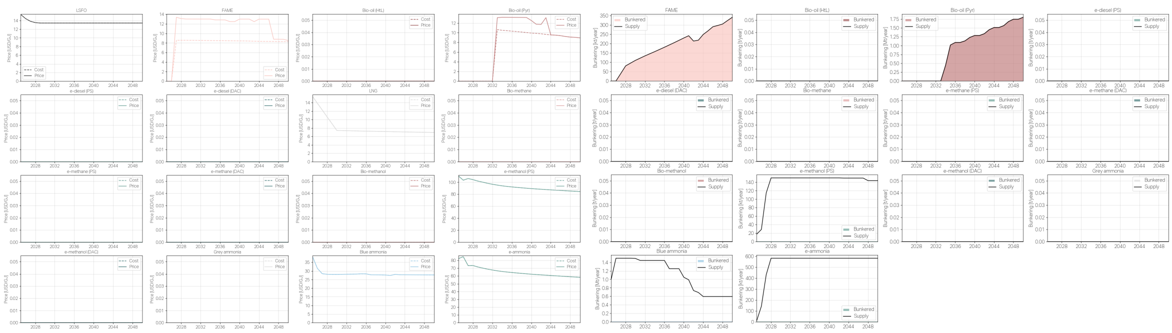


Figure G.18: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Global configuration.

Global Overview

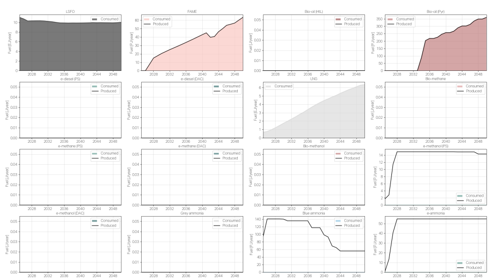


Figure G.19: Global fuel supply and demand overview for the Global configuration.

G.2.4 Fuel Supply and Bunker Prices – Local

Africa

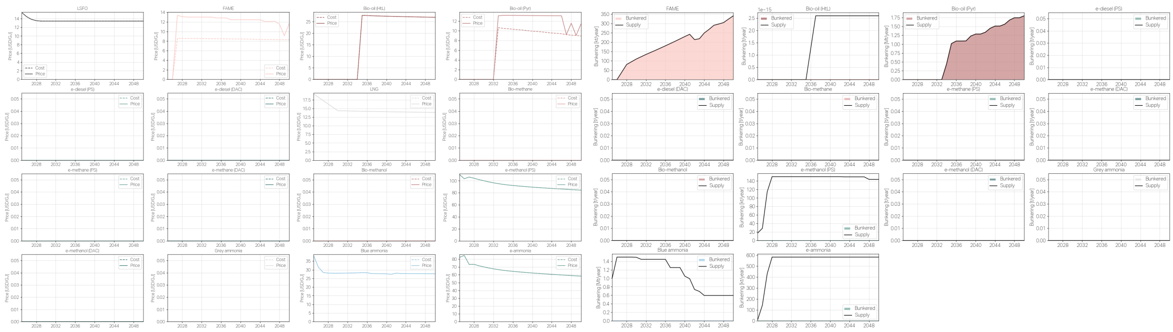


Figure G.20: Market price (left), and fuel supply and demand (right) in African ports under the Local configuration.

Americas

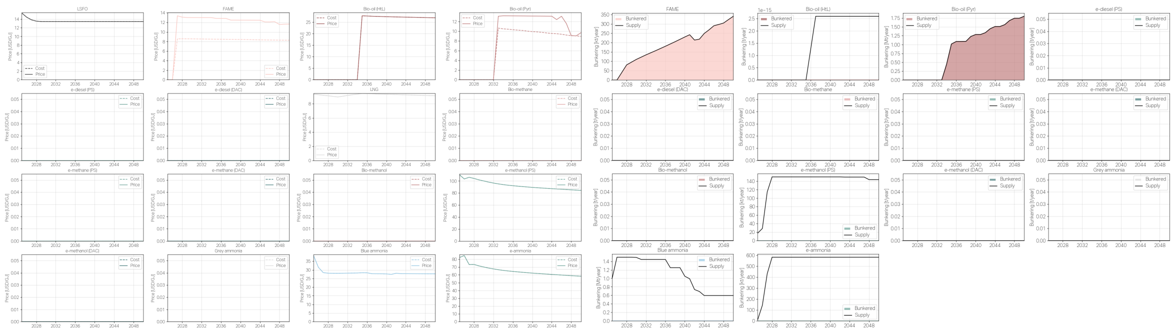


Figure G.21: Market price (left), and fuel supply and demand (right) in American ports under the Local configuration.

Asia

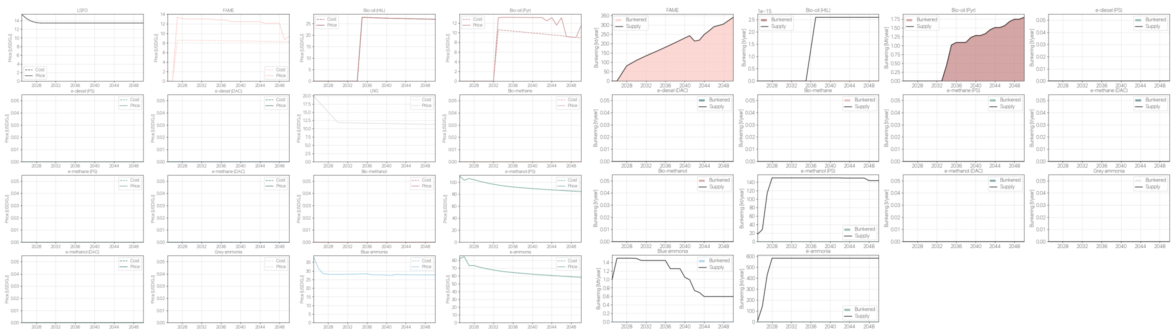


Figure G.22: Market price (left), and fuel supply and demand (right) in Asian ports under the Local configuration.

Europe

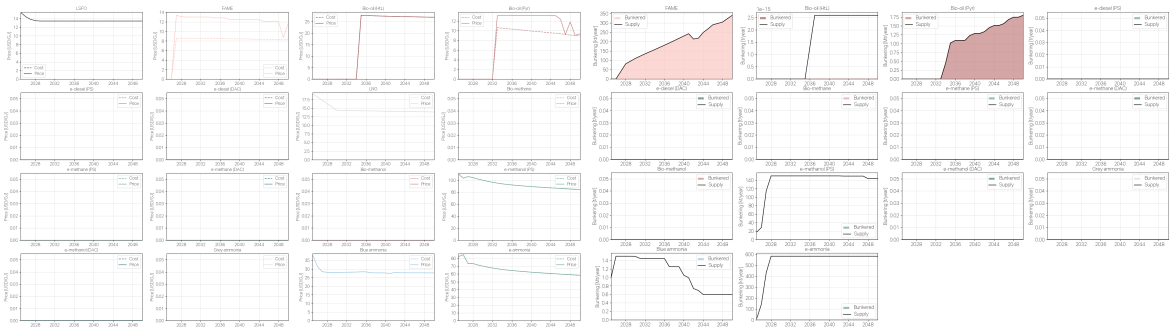


Figure G.23: Market price (left), and fuel supply and demand (right) in European ports under the Local configuration.

Middle East

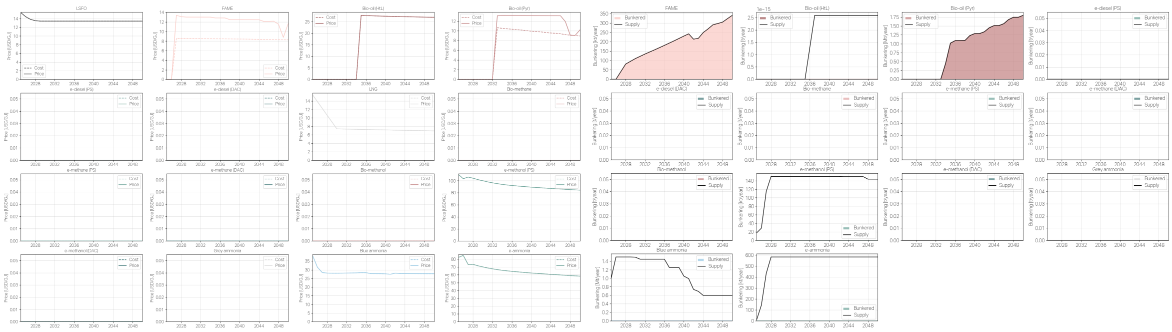


Figure G.24: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Local configuration.

Global Overview

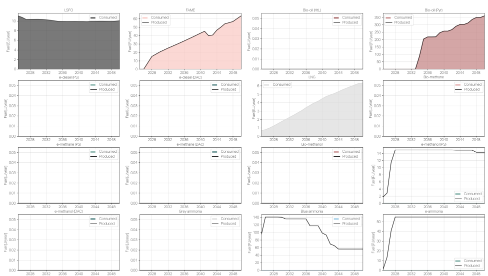
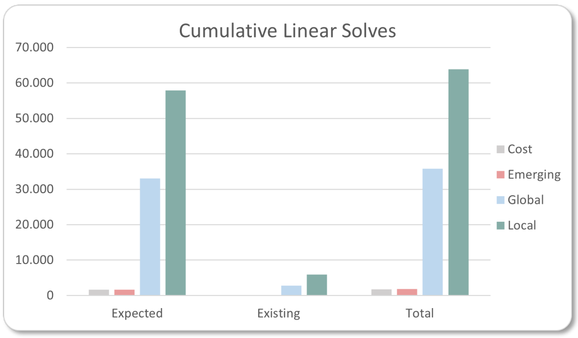


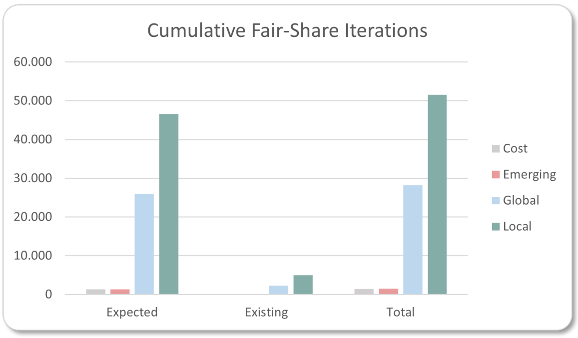
Figure G.25: Global fuel supply and demand overview for the Local configuration.

H Regulation with Flexibility Environment IMO Regulation 380 USD - Results

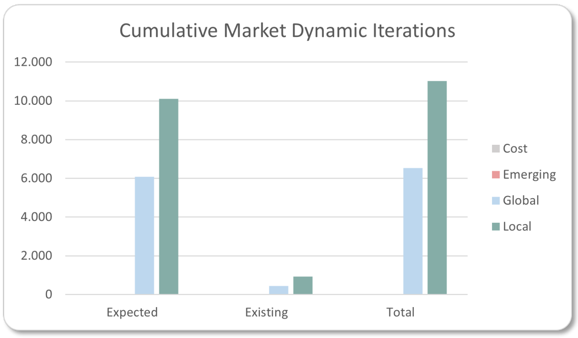
H.1 Performance Analytics



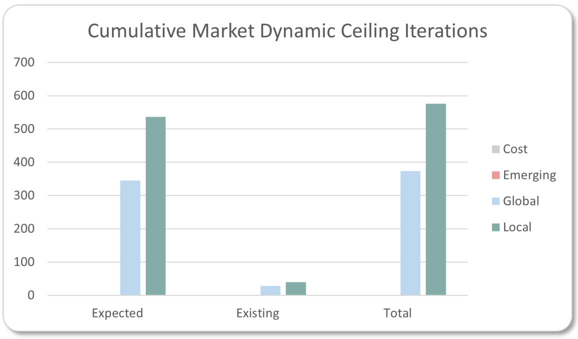
(a) Linear Solves



(b) Fair-Share Iterations



(c) Market Dynamic Iterations



(d) Ceiling Iterations

Figure H.1: Cumulative expected, existing and total solver calls and iteration counts under the `Regulation with Flexibility` (IMO GFS of 380USD) scenario across all model runs.

H.2 Market Dynamics

H.2.1 Fuel Supply and Bunker Prices – Cost-Only, Regulation with Flexibility Africa

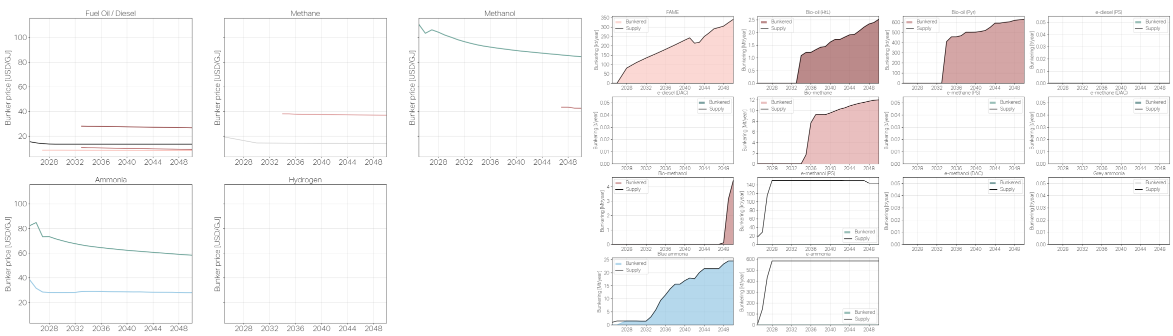


Figure H.2: Bunker fuel cost (left), and fuel supply and demand (right) in African ports.

Americas

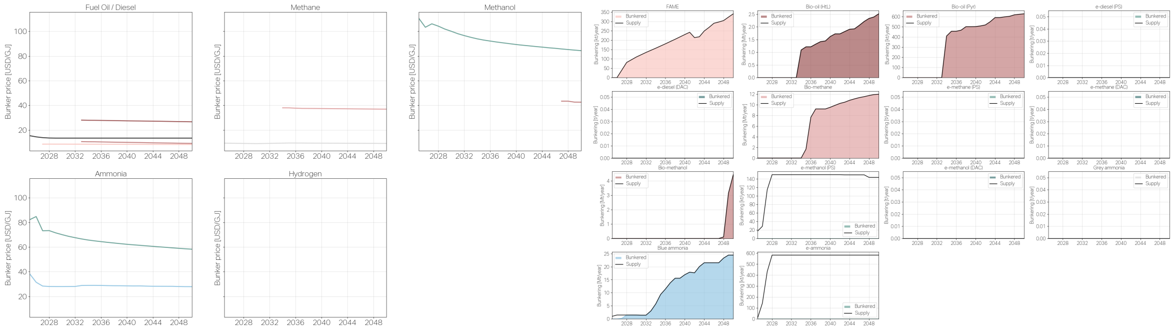


Figure H.3: Bunker fuel cost (left), and fuel supply and demand (right) in American ports.

Asia

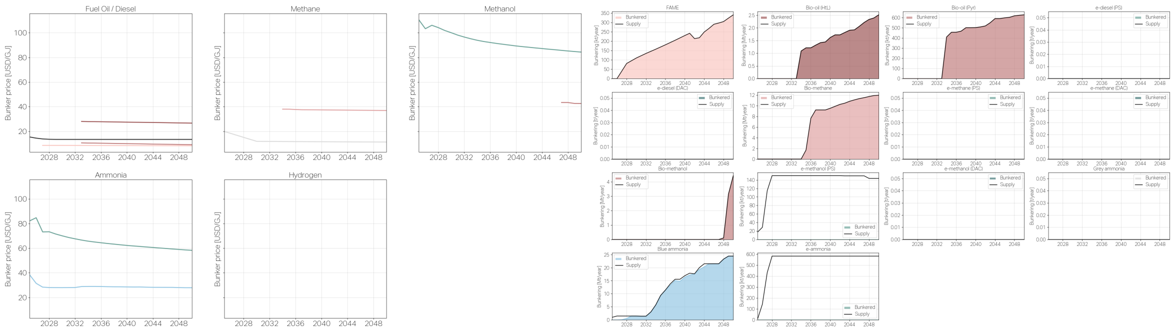


Figure H.4: Bunker fuel cost (left), and fuel supply and demand (right) in Asian ports.

Europe

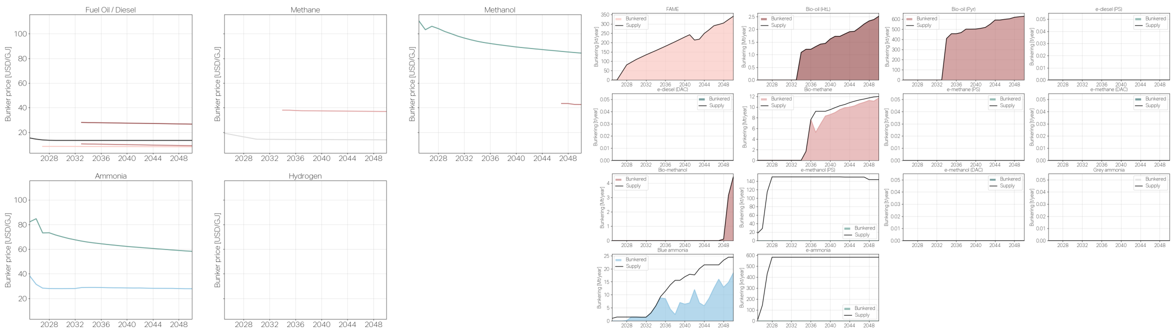


Figure H.5: Bunker price and fuel supply in European ports.

Middle East

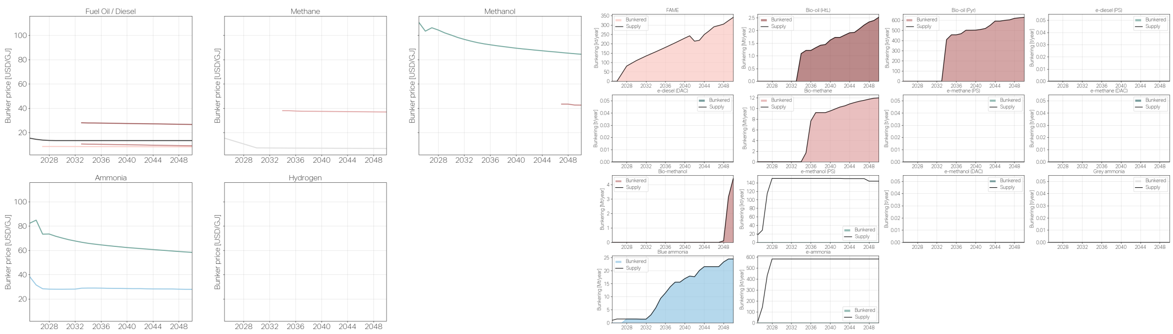


Figure H.6: Bunker fuel cost (left), and fuel supply and demand (right) in Middle Eastern ports.

Global Overview

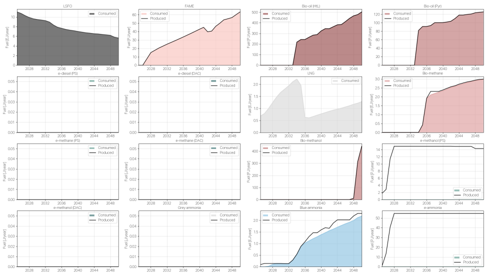


Figure H.7: Global fuel supply and demand overview for the Cost-Only scenario.

H.2.2 Fuel Supply and Bunker Prices – Emerging

Africa

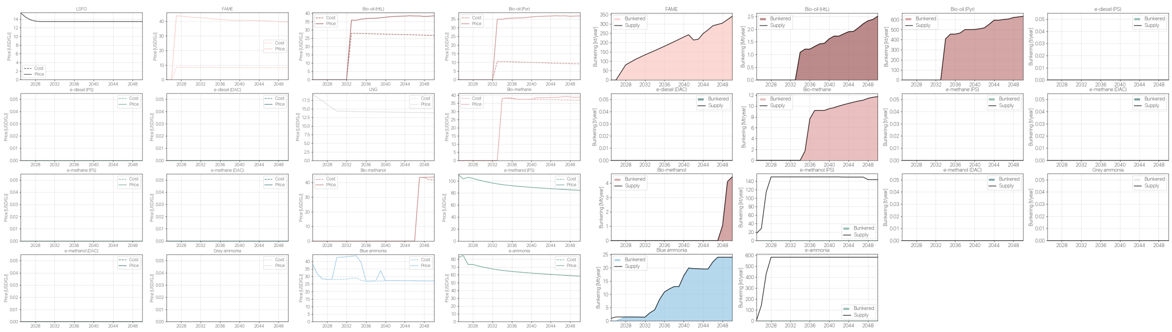


Figure H.8: Market price (left), and fuel supply and demand (right) in African ports under the Emerging configuration.

Americas

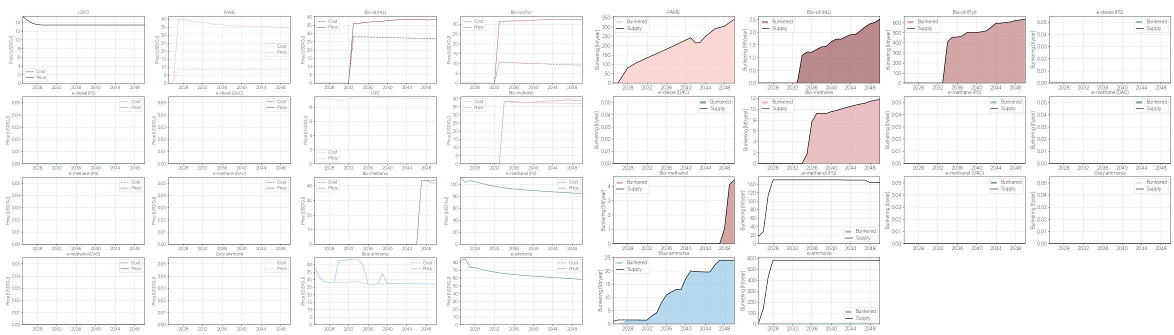


Figure H.9: Market price (left), and fuel supply and demand (right) in American ports under the Emerging configuration.

Asia

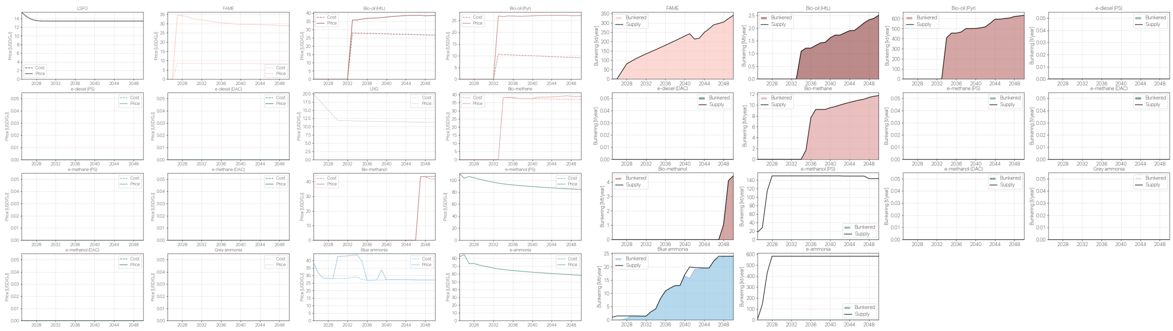


Figure H.10: Market price (left), and fuel supply and demand (right) in Asian ports under the Emerging configuration.

Europe

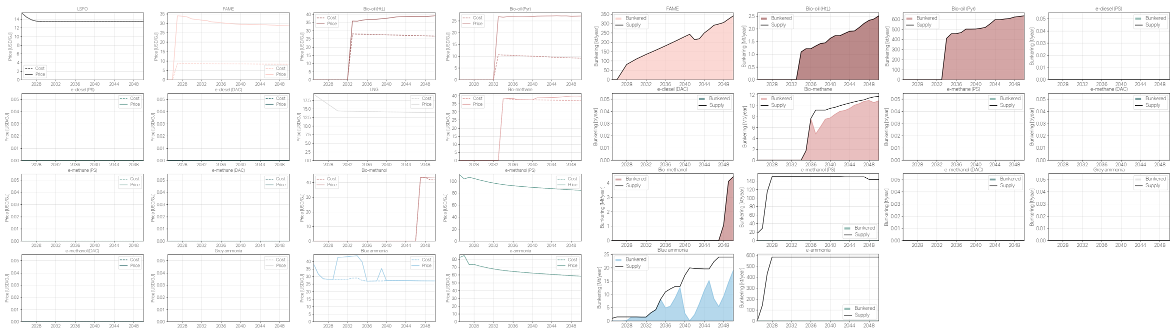


Figure H.11: Market price (left), and fuel supply and demand (right) in European ports under the Emerging configuration.

Middle East

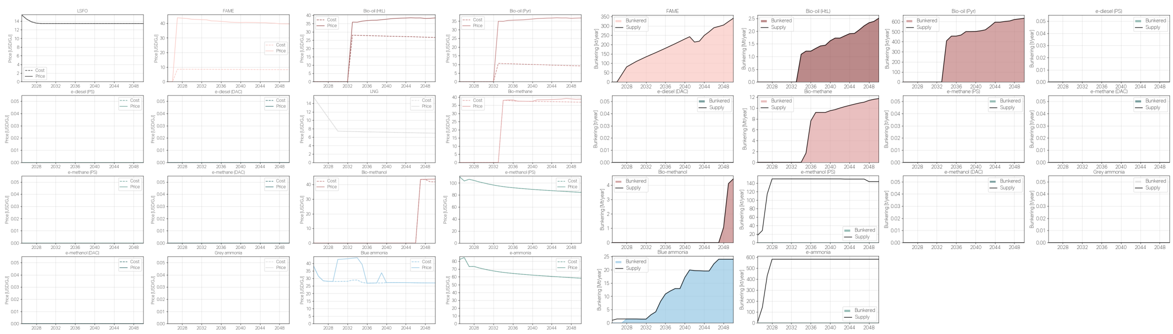


Figure H.12: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Emerging configuration.

Global Overview

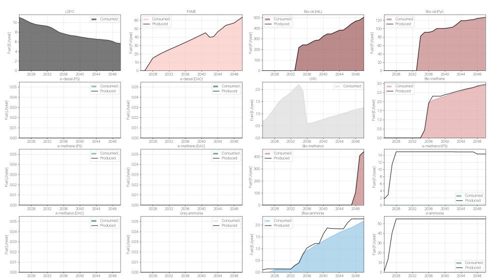


Figure H.13: Global fuel supply and demand overview for the Emerging configuration.

H.2.3 Fuel Supply and Bunker Prices – Global

Africa

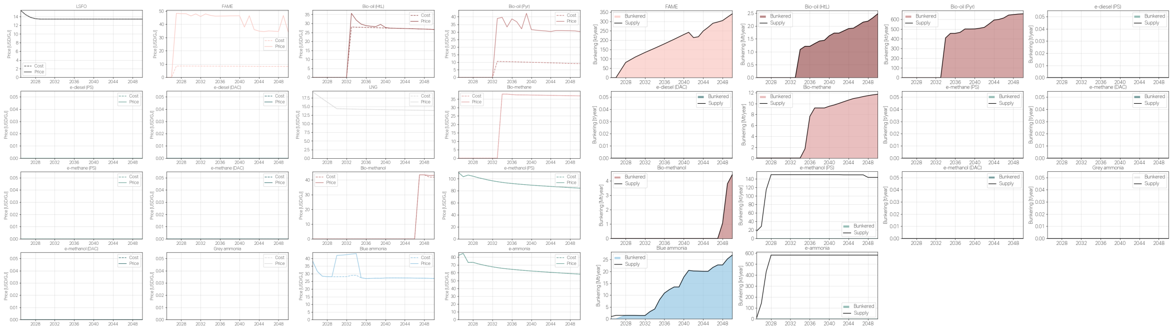


Figure H.14: Market price (left), and fuel supply and demand (right) in African ports under the Global configuration.

Americas

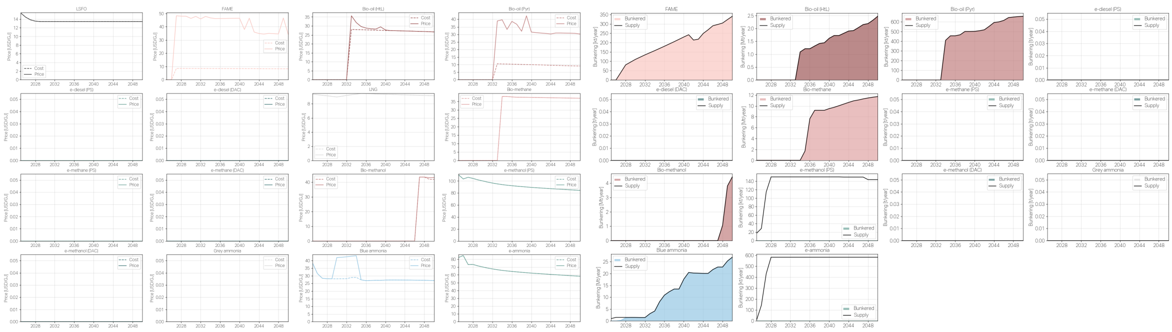


Figure H.15: Market price (left), and fuel supply and demand (right) in American ports under the Global configuration.

Asia

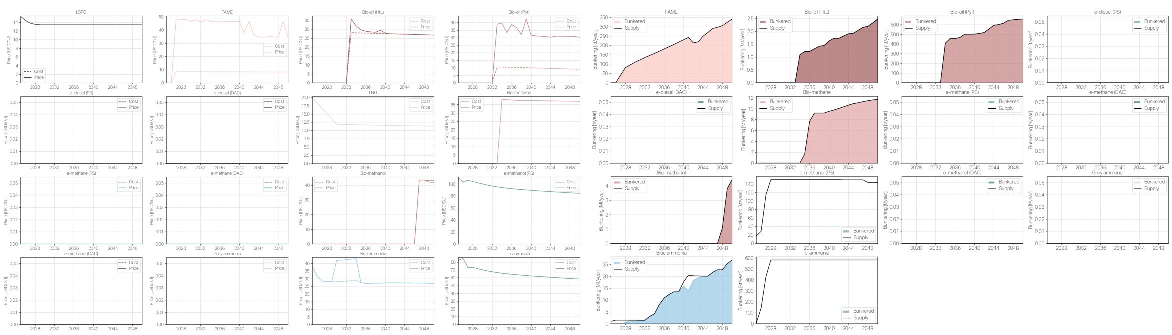


Figure H.16: Market price (left), and fuel supply and demand (right) in Asian ports under the Global configuration.

Europe

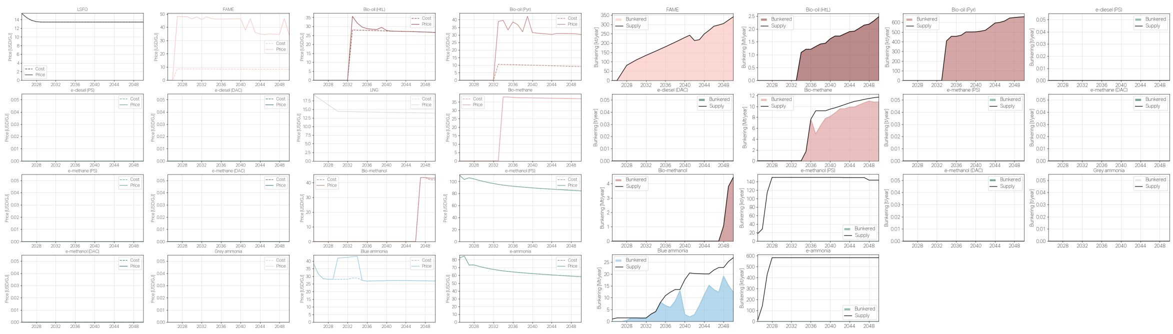


Figure H.17: Market price (left), and fuel supply and demand (right) in European ports under the Global configuration.

Middle East

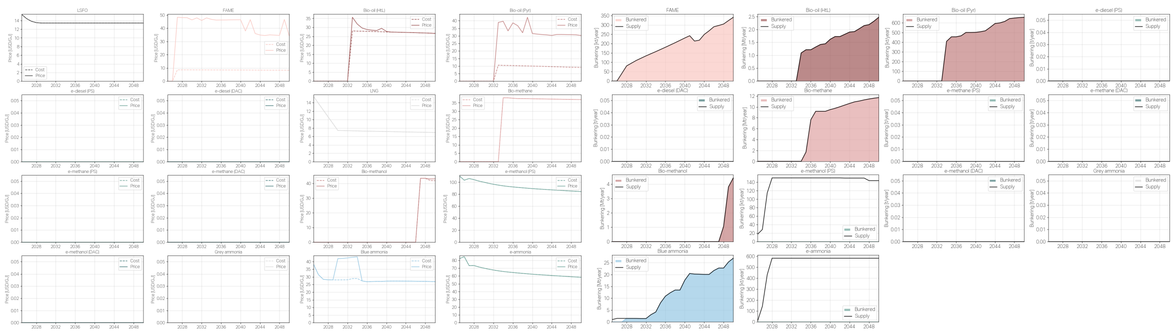


Figure H.18: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Global configuration.

Global Overview

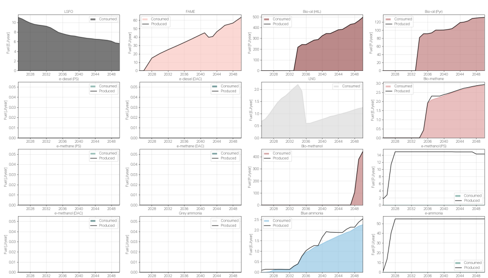


Figure H.19: Global fuel supply and demand overview for the Global configuration.

H.2.4 Fuel Supply and Bunker Prices – Local

Africa

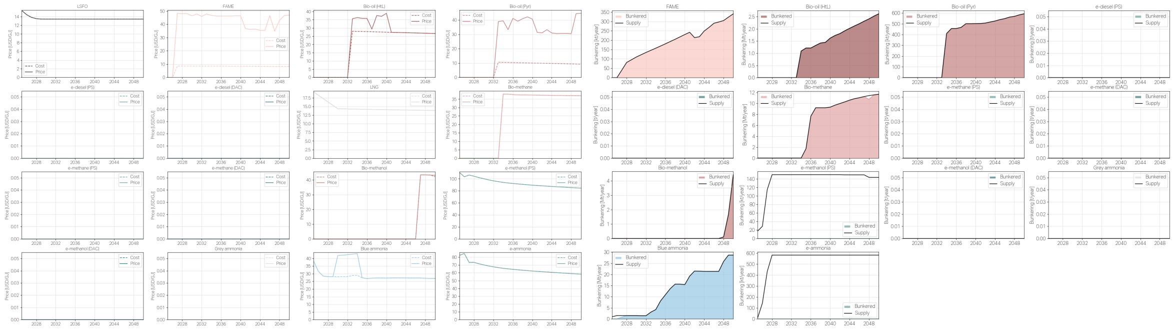


Figure H.20: Market price (left), and fuel supply and demand (right) in African ports under the Local configuration.

Americas

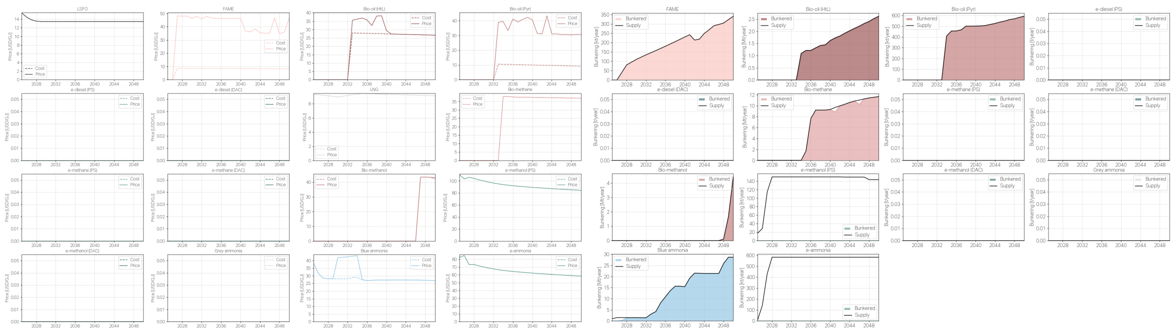


Figure H.21: Market price (left), and fuel supply and demand (right) in American ports under the Local configuration.

Asia

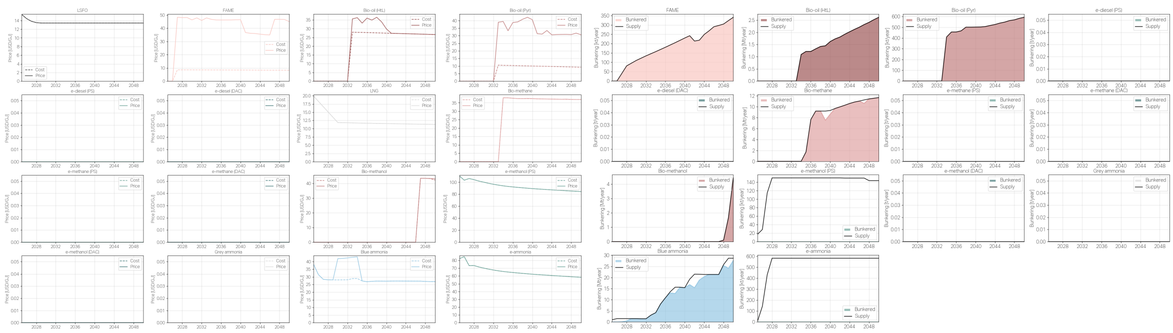


Figure H.22: Market price (left), and fuel supply and demand (right) in Asian ports under the Local configuration.

Europe

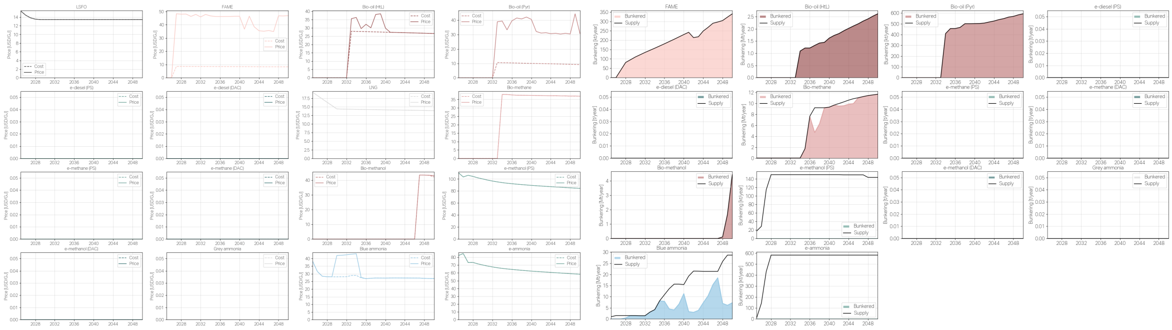


Figure H.23: Market price (left), and fuel supply and demand (right) in European ports under the Local configuration.

Middle East

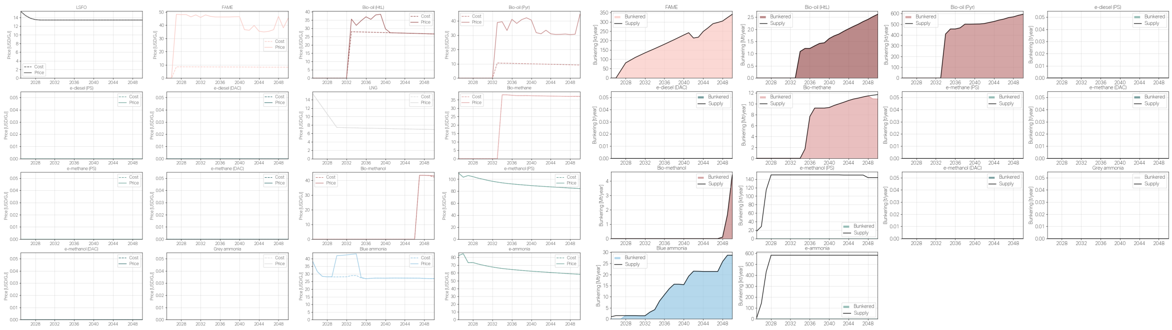


Figure H.24: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Local configuration.

Global Overview

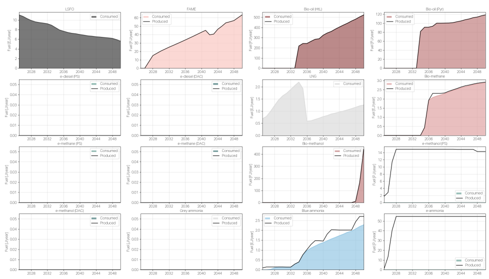
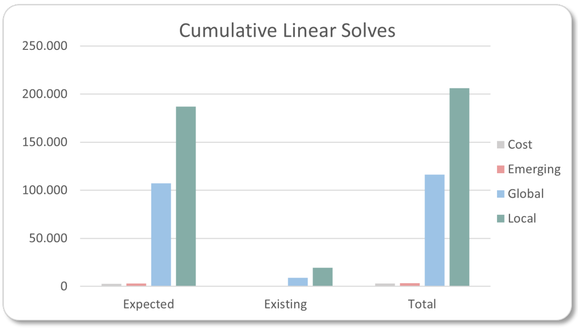


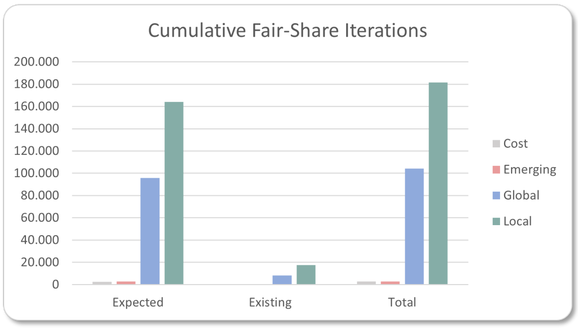
Figure H.25: Global fuel supply and demand overview for the Local configuration.

I Regulation with Flexibility Environment 1200 USD penalty - Results

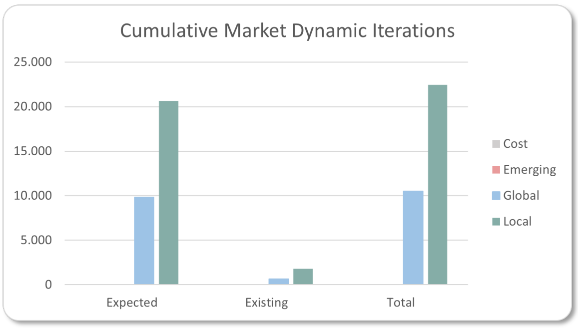
I.1 Performance Analytic



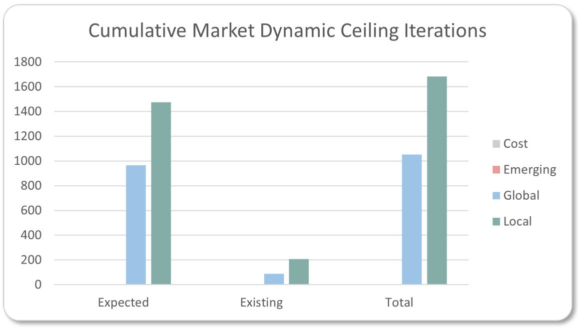
(a) Linear Solves



(b) Fair-Share Iterations



(c) Market Dynamic Iterations



(d) Ceiling Iterations

Figure I.1: Cumulative expected, existing and total solver calls and iteration counts under the `Regulation with Flexibility` (1200USD) scenario across all model runs.

I.2 Market Dynamics

I.2.1 Fuel Supply and Bunker Prices – Cost-Only, Regulation with Flexibility 1200

Africa

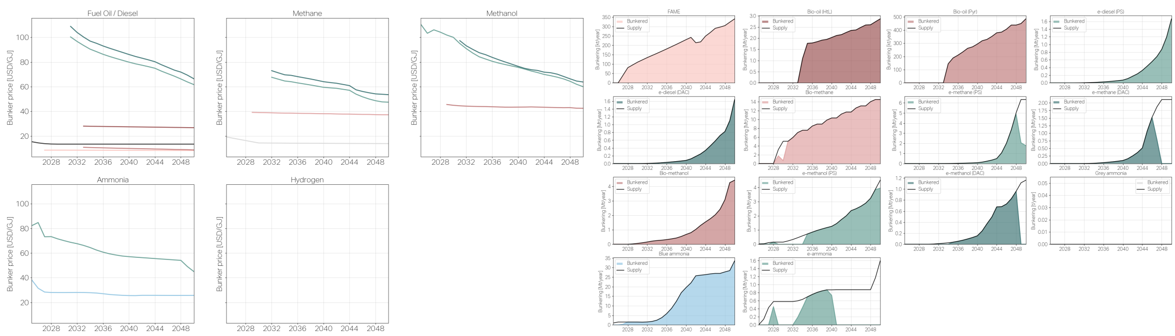


Figure I.2: Bunker fuel cost (left), and fuel supply and demand (right) in African ports.

Americas

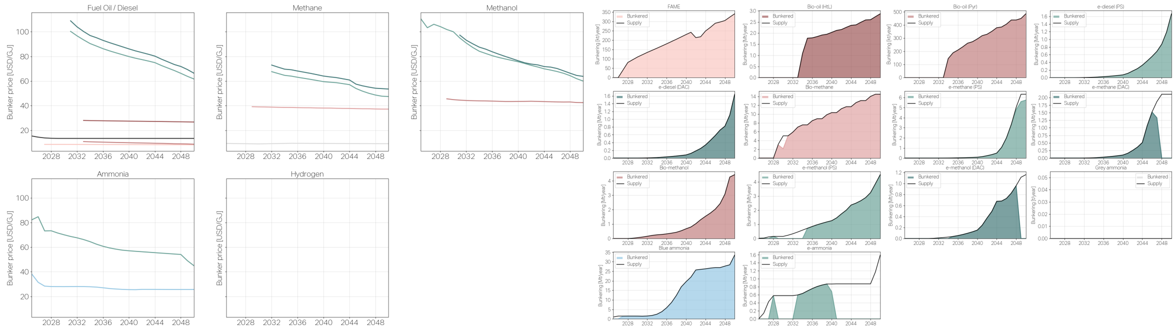


Figure I.3: Bunker fuel cost (left), and fuel supply and demand (right) in American ports.

Asia

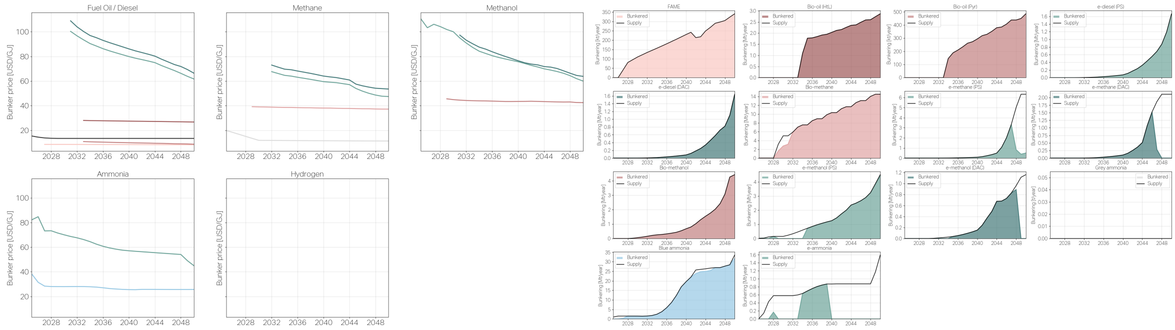


Figure I.4: Bunker fuel cost (left), and fuel supply and demand (right) in Asian ports.

Europe

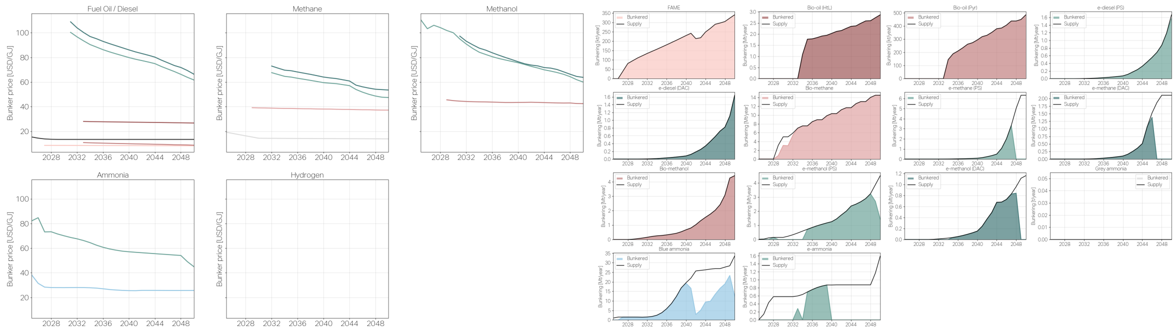


Figure I.5: Bunker fuel cost (left), and fuel supply and demand (right) in European ports.

Middle East

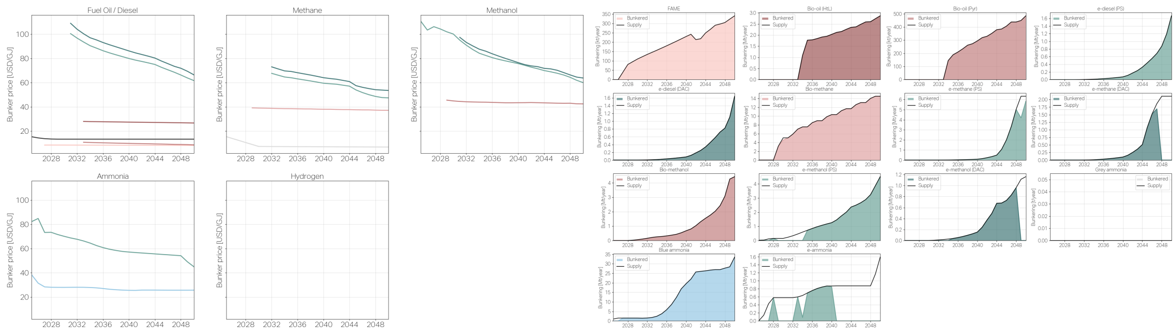


Figure I.6: Bunker fuel cost (left), and fuel supply and demand (right) in Middle Eastern ports.

Global Overview

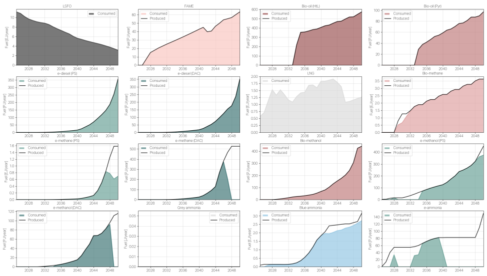


Figure I.7: Global fuel supply and demand overview for the Cost-Only scenario.

I.2.2 Fuel Supply and Bunker Prices – Emerging

Africa

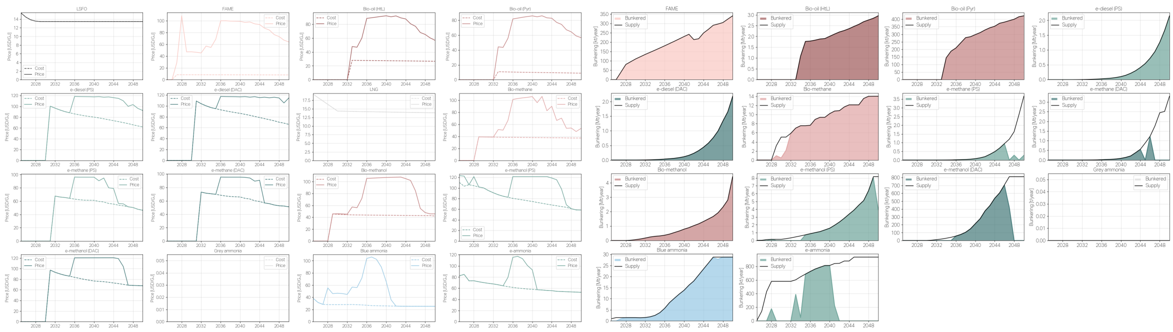


Figure I.8: Market price (left), and fuel supply and demand (right) in African ports under the Emerging configuration.

Americas

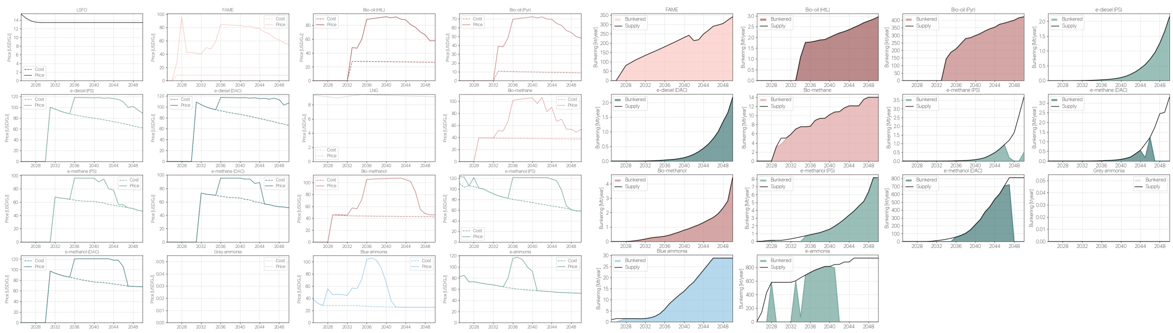


Figure I.9: Market price (left), and fuel supply and demand (right) in American ports under the Emerging configuration.

Asia

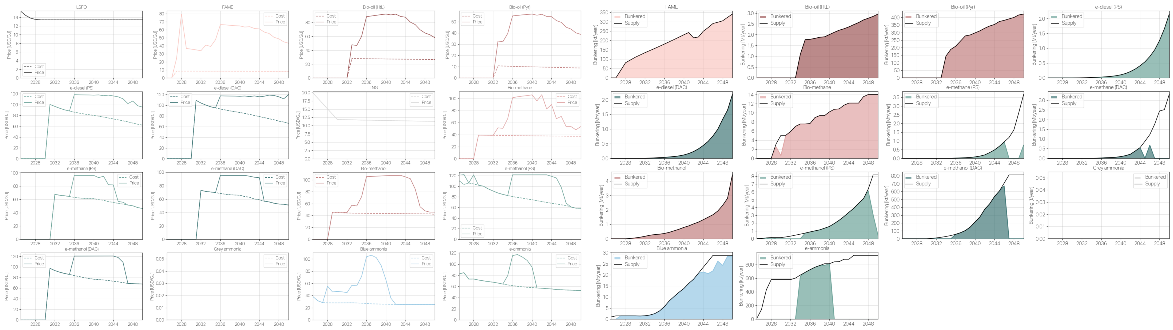


Figure I.10: Market price (left), and fuel supply and demand (right) in Asian ports under the Emerging configuration.

Europe

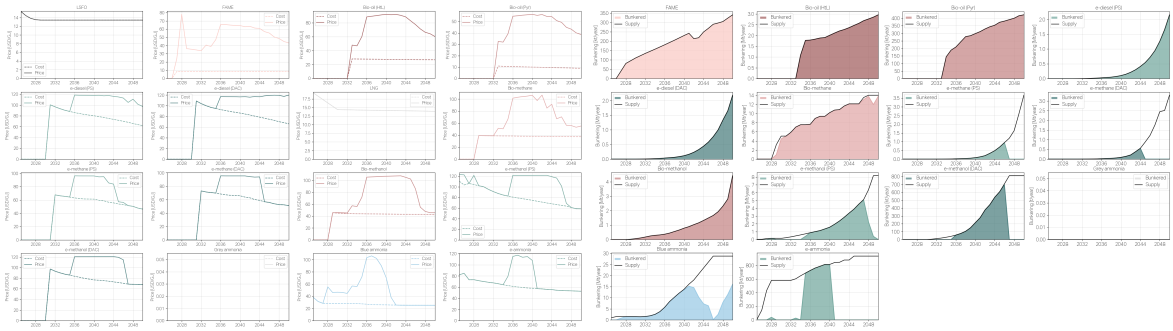


Figure I.11: Market price (left), and fuel supply and demand (right) in European ports under the Emerging configuration.

Middle East

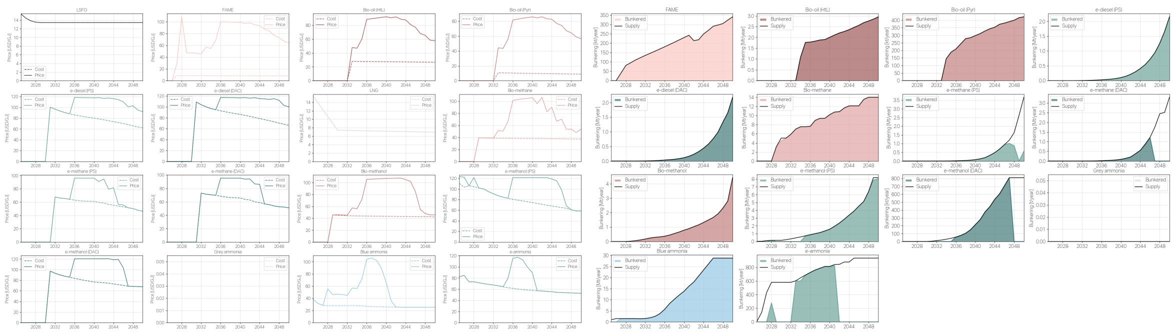


Figure I.12: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Emerging configuration.

Global Overview

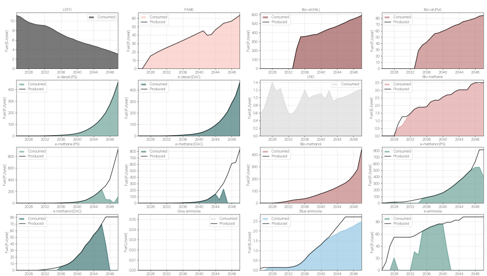


Figure I.13: Global fuel supply and demand overview for the Emerging configuration.

I.2.3 Fuel Supply and Bunker Prices – Global

Africa

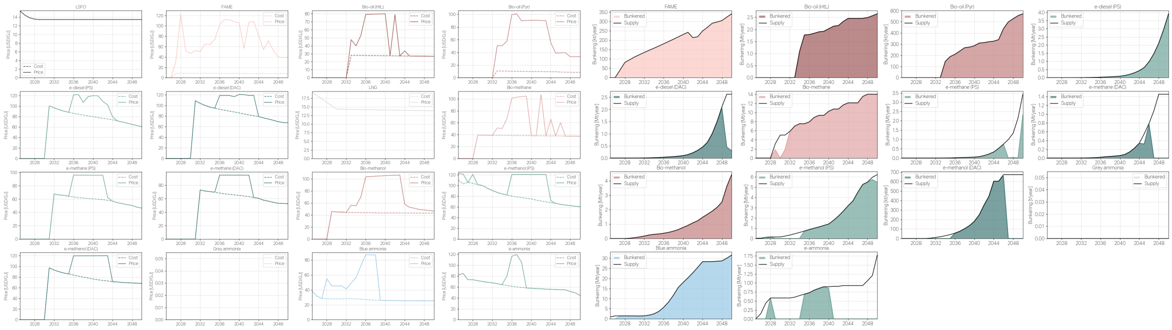


Figure I.14: Market price (left), and fuel supply and demand (right) in African ports under the Global configuration.

Americas

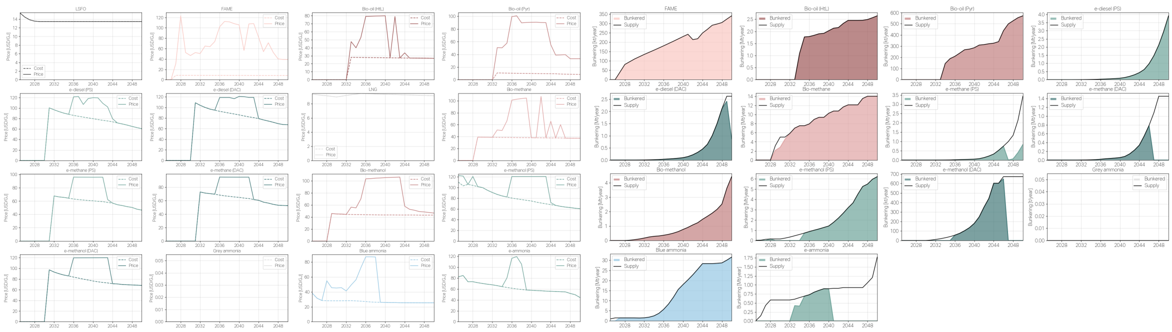


Figure I.15: Market price (left), and fuel supply and demand (right) in American ports under the Global configuration.

Asia

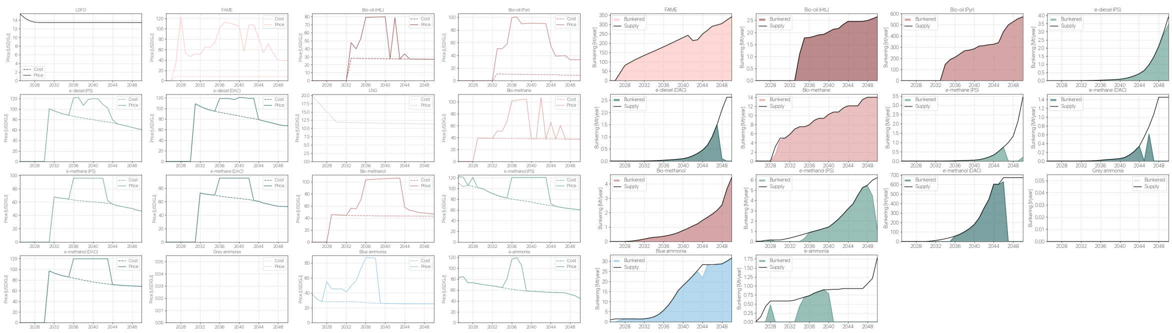


Figure I.16: Market price (left), and fuel supply and demand (right) in Asian ports under the Global configuration.

Europe

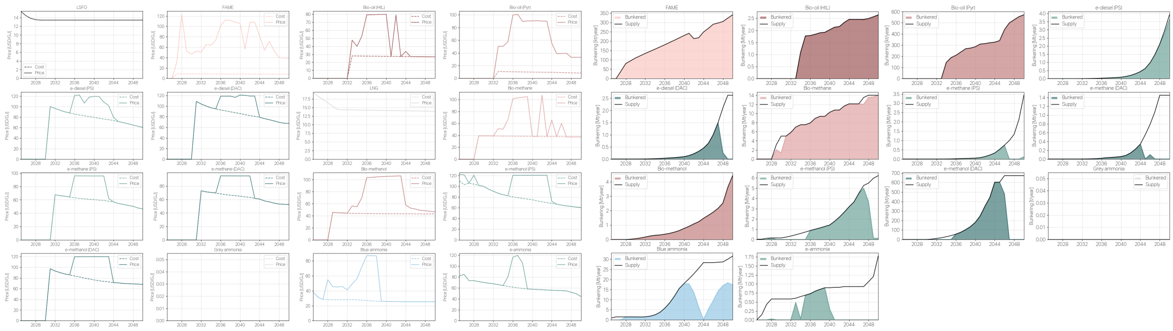


Figure I.17: Market price (left), and fuel supply and demand (right) in European ports under the Global configuration.

Middle East

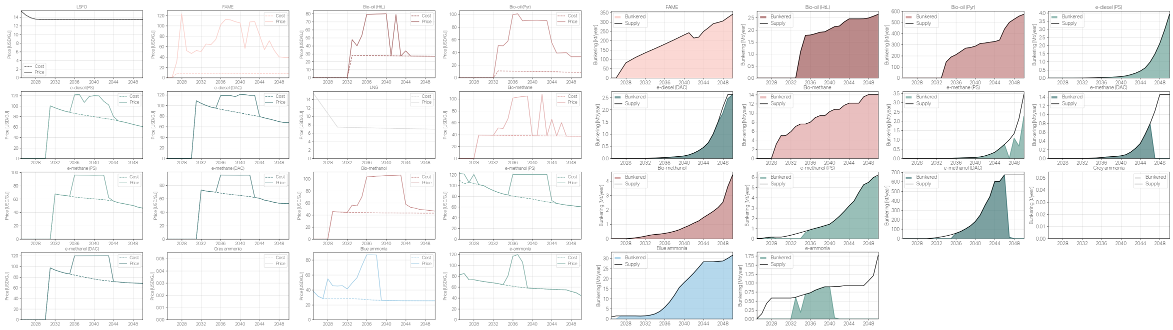


Figure I.18: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Global configuration.

Global Overview

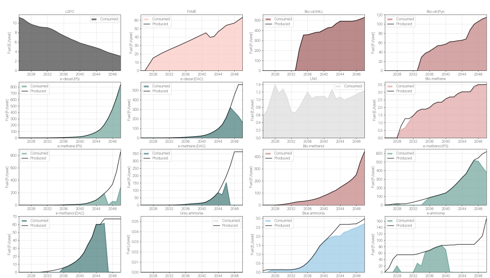


Figure I.19: Global fuel supply and demand overview for the Global configuration.

I.2.4 Fuel Supply and Bunker Prices – Local

Africa

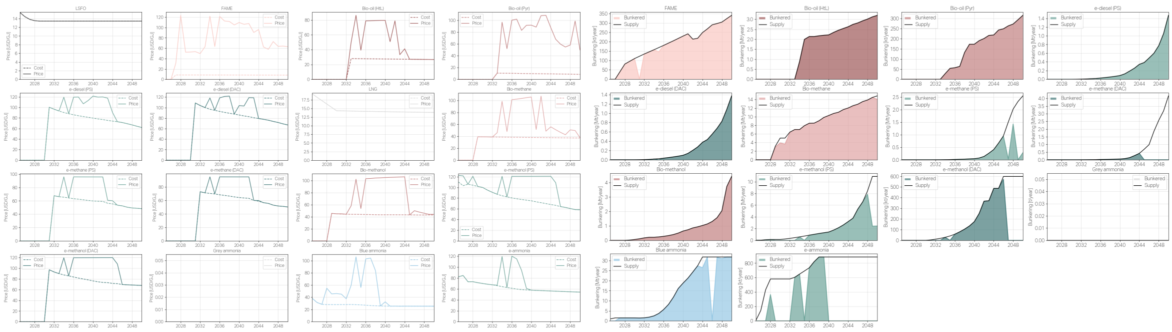


Figure I.20: Market price (left), and fuel supply and demand (right) in African ports under the Local configuration.

Americas

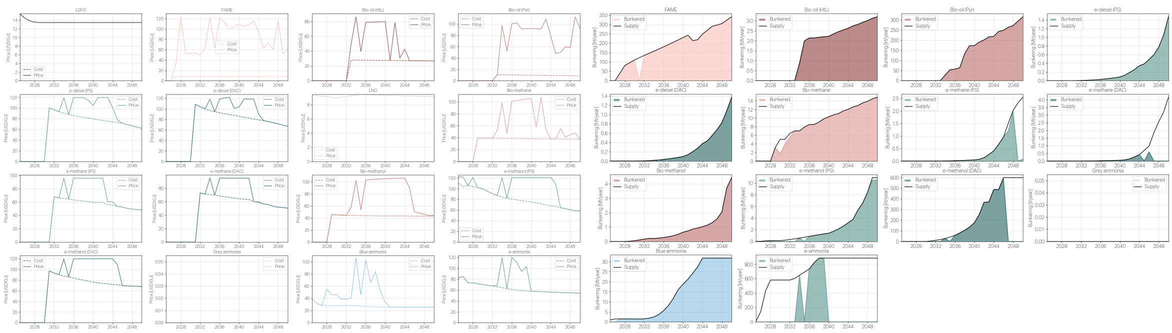


Figure I.21: Market price (left), and fuel supply and demand (right) in American ports under the Local configuration.

Asia

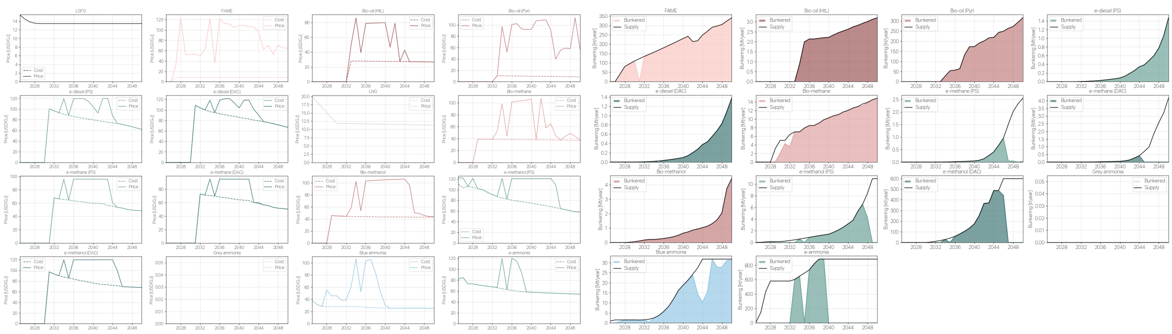


Figure I.22: Market price (left), and fuel supply and demand (right) in Asian ports under the Local configuration.

Europe

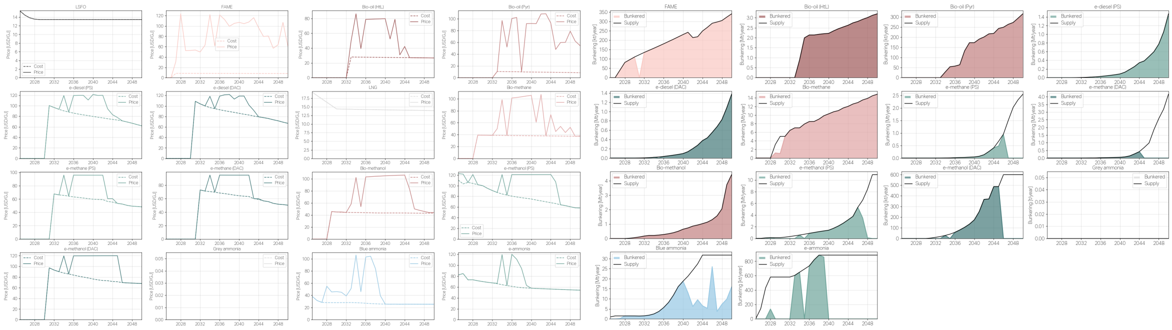


Figure I.23: Market price (left), and fuel supply and demand (right) in European ports under the Local configuration.

Middle East

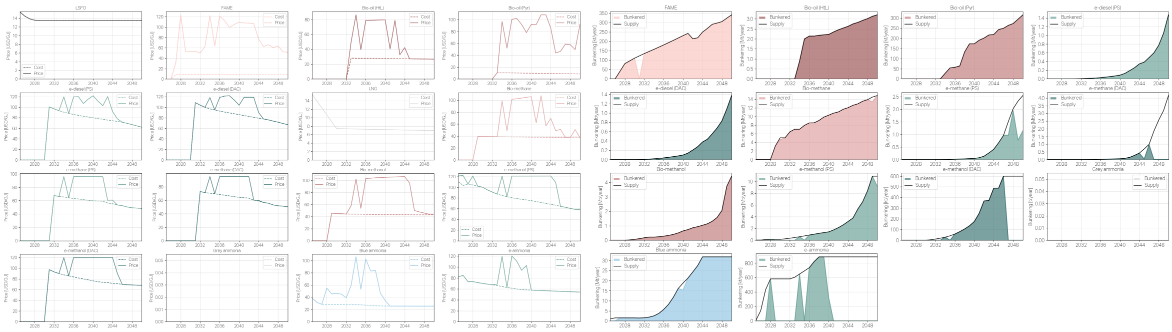


Figure I.24: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Local configuration.

Global Overview

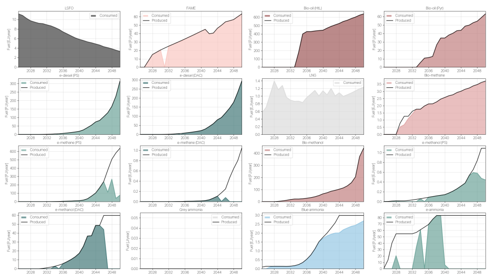
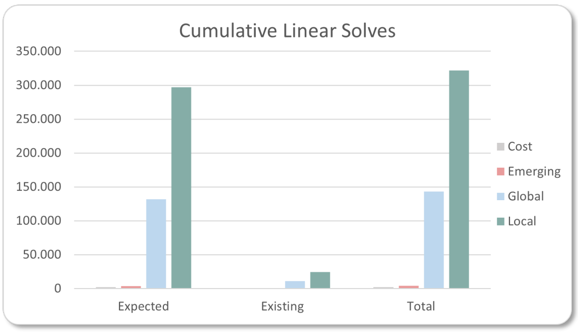


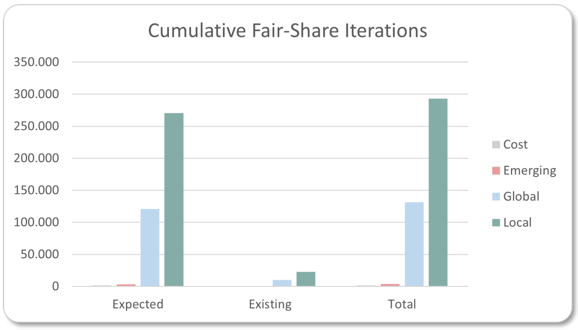
Figure I.25: Global fuel supply and demand overview for the Local configuration.

J Regulation w/o Flexibility - Results

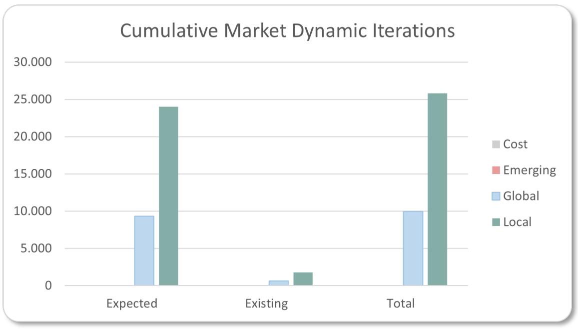
J.1 Performance Diagnostics



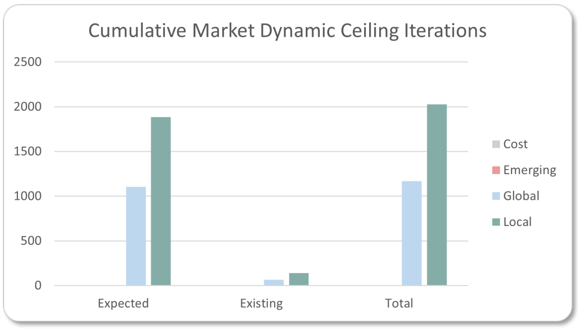
(a) Linear Solves



(b) Fair-Share Iterations



(c) Market Dynamic Iterations



(d) Ceiling Iterations

Figure J.1: Cumulative expected, existing and total solver calls and iteration counts under the `Regulation without Flexibility` scenario across all model runs.

J.2 Market Dynamics

J.2.1 Fuel Supply and Bunker Prices – Cost-Only, Regulation without Flexibility 1200

Africa

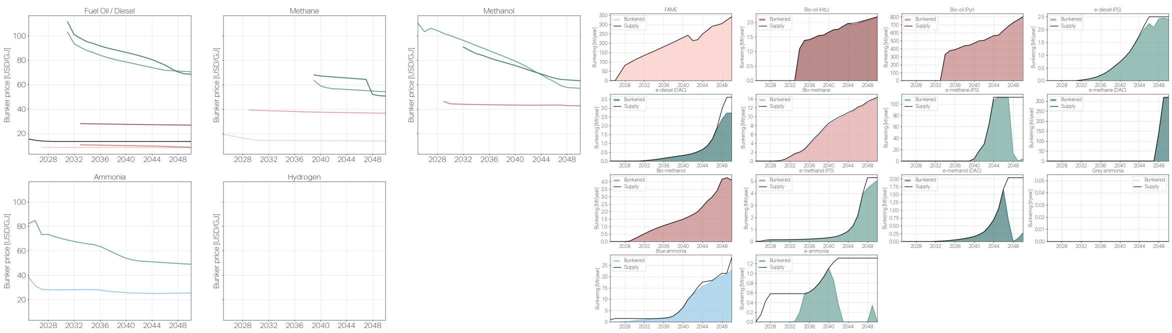


Figure J.2: Market price (left), and fuel supply and demand (right) in African ports under the Cost- Only configuration.

Americas

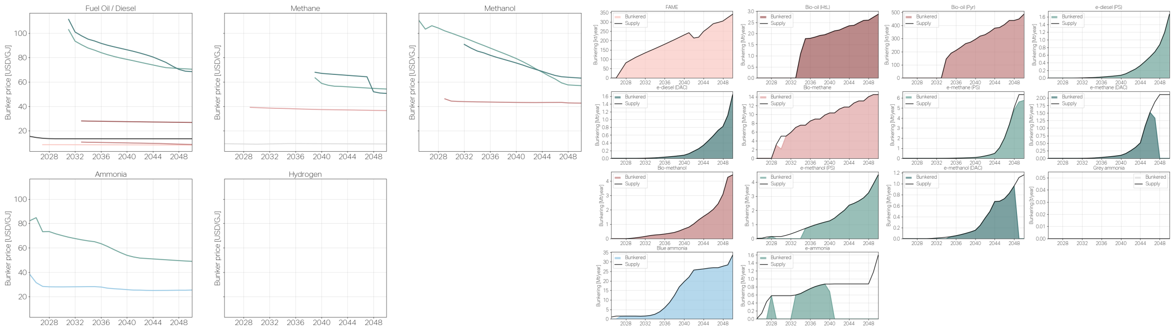


Figure J.3: Market price (left), and fuel supply and demand (right) in American ports under the Cost- Only configuration.

Asia

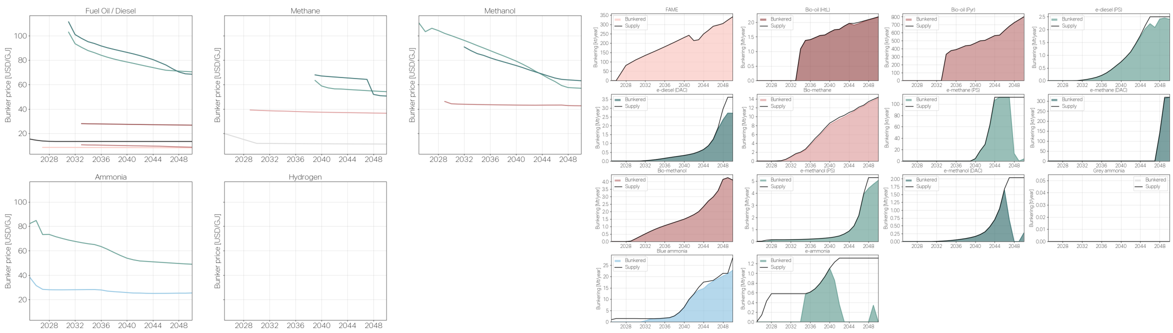


Figure J.4: Market price (left), and fuel supply and demand (right) in Asian ports under the Cost- Only configuration.

Europe

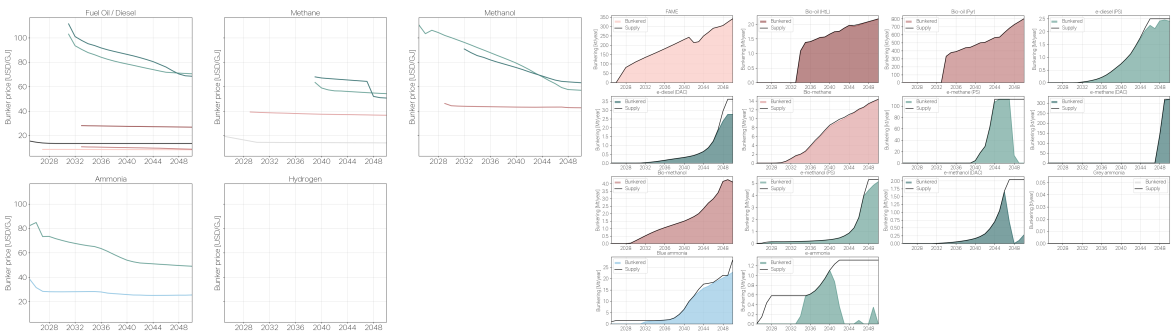


Figure J.5: Market price (left), and fuel supply and demand (right) in European ports under the Cost- Only configuration.

Middle East

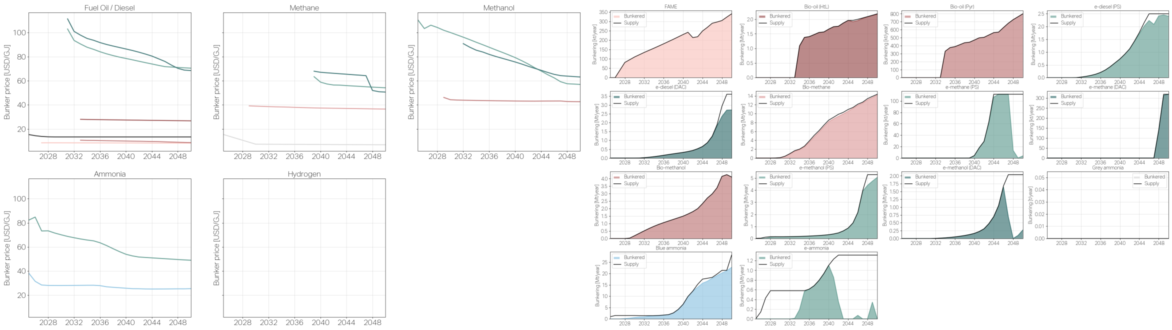


Figure J.6: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Cost-Only configuration.

Global Overview

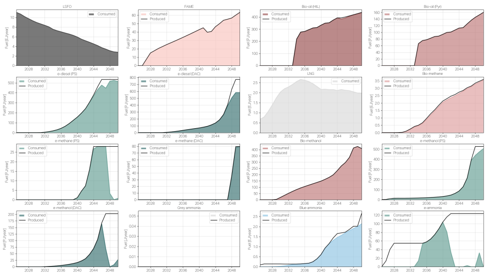


Figure J.7: Global fuel supply and demand overview for the Cost-Only scenario.

J.2.2 Fuel Supply and Bunker Prices – Emerging

Africa

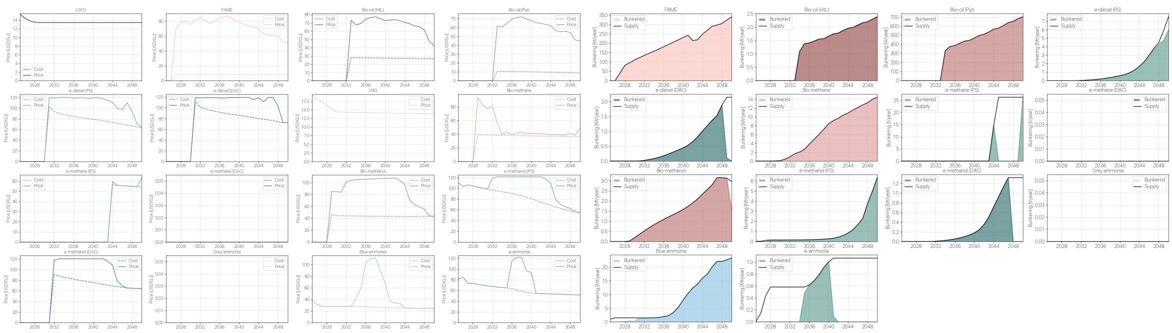


Figure J.8: Market price (left), and fuel supply and demand (right) in African ports under the Emerging configuration.

Americas

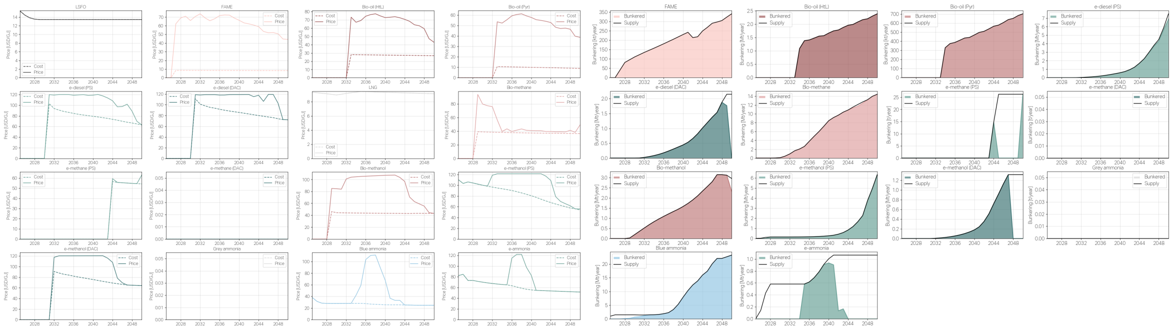


Figure J.9: Market price (left), and fuel supply and demand (right) in American ports under the Emerging configuration.

Asia

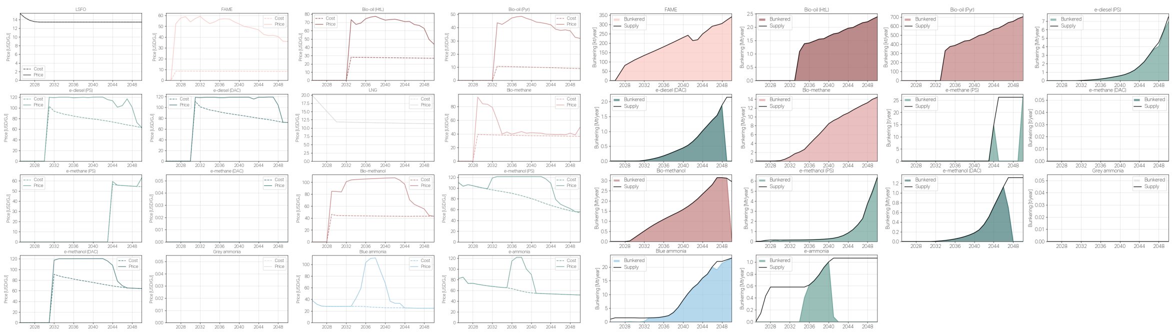


Figure J.10: Market price (left), and fuel supply and demand (right) in Asian ports under the Emerging configuration.

Europe

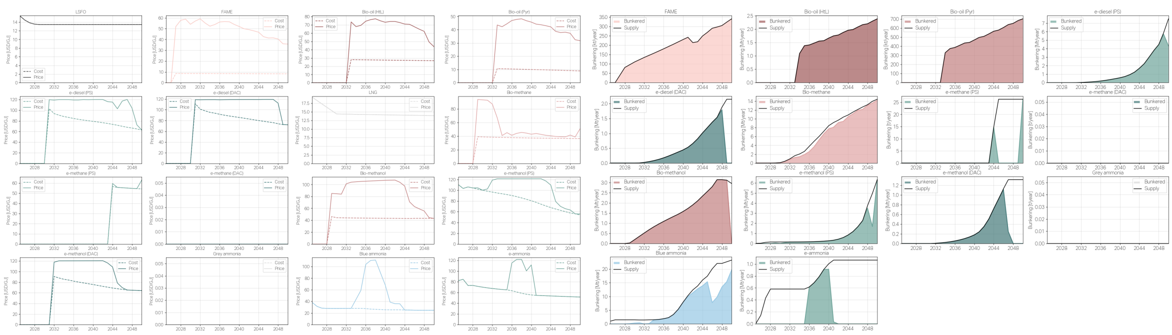


Figure J.11: Market price (left), and fuel supply and demand (right) in European ports under the Emerging configuration.

Middle East

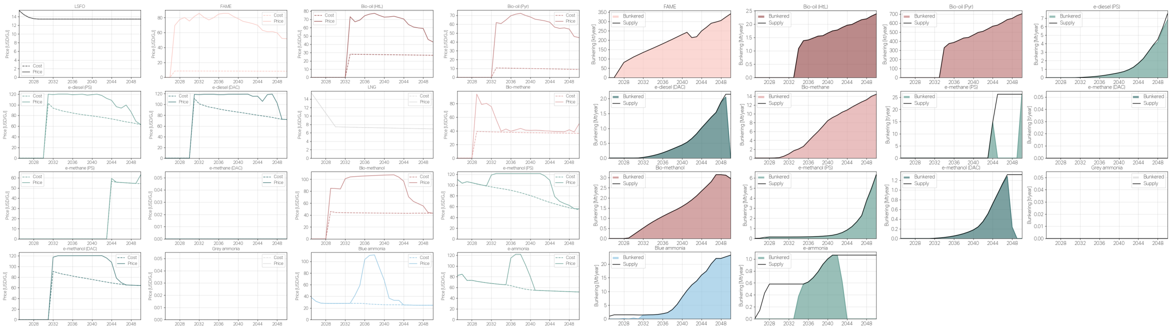


Figure J.12: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Emerging configuration.

Global Overview

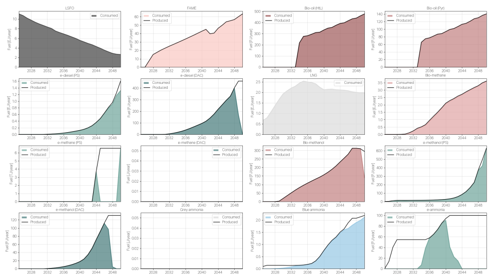


Figure J.13: Global fuel supply and demand overview for the Emerging scenario.

J.2.3 Fuel Supply and Bunker Prices – Global

Africa

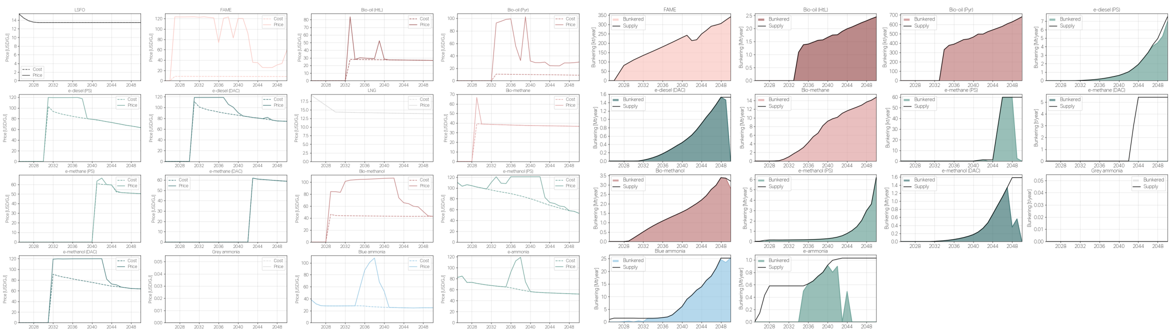


Figure J.14: Market price (left), and fuel supply and demand (right) in African ports under the Global configuration.

Americas

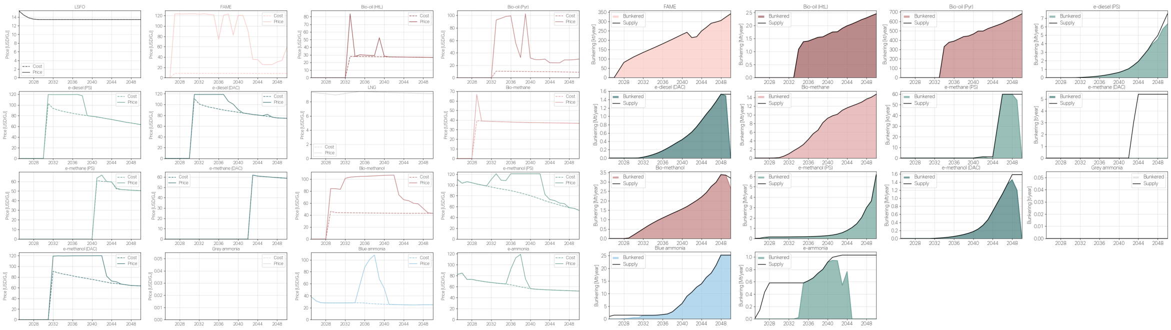


Figure J.15: Market price (left), and fuel supply and demand (right) in American ports under the Global configuration.

Asia

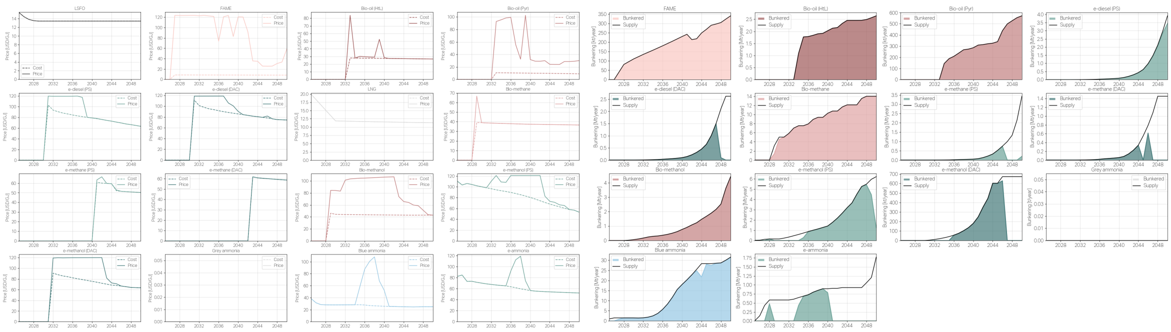


Figure J.16: Market price (left), and fuel supply and demand (right) in Asian ports under the Global configuration.

Europe

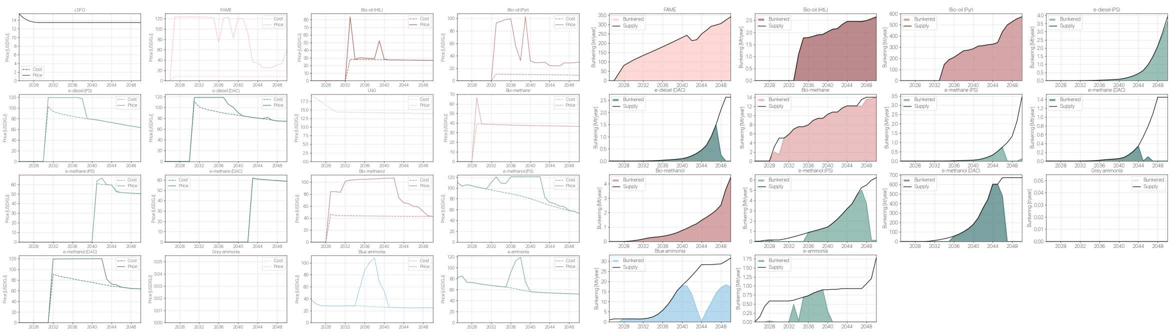


Figure J.17: Market price (left), and fuel supply and demand (right) in European ports under the Global configuration.

Middle East

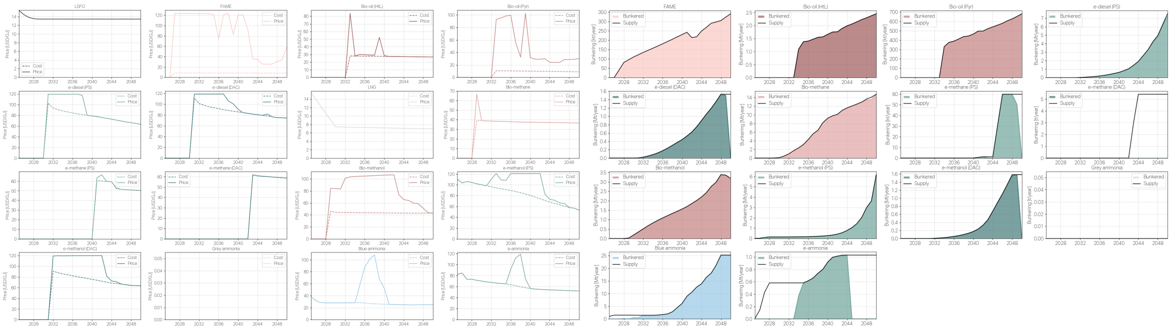


Figure J.18: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Global configuration.

Global Overview

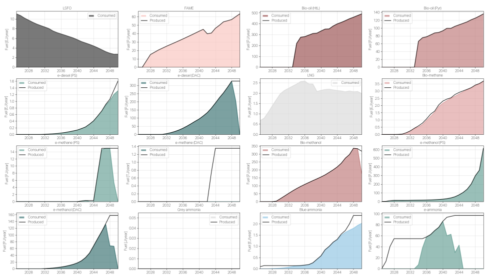


Figure J.19: Global fuel supply and demand overview for the Global scenario.

J.2.4 Fuel Supply and Bunker Prices – Local

Africa

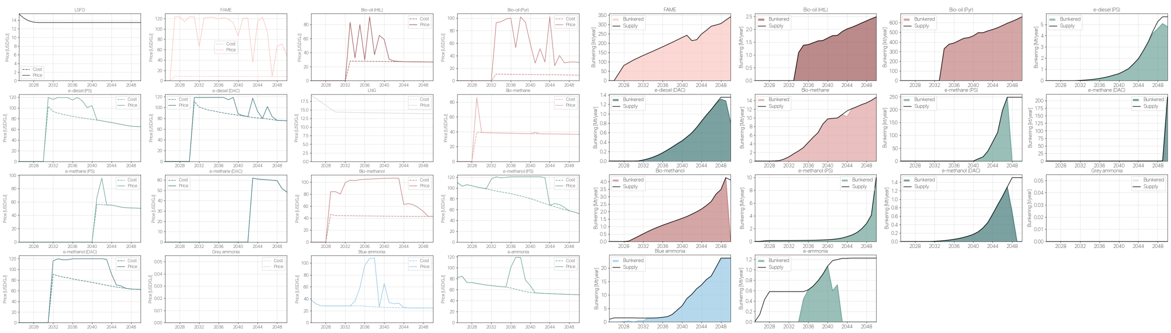


Figure J.20: Market price (left), and fuel supply and demand (right) in African ports under the Local configuration.

Americas

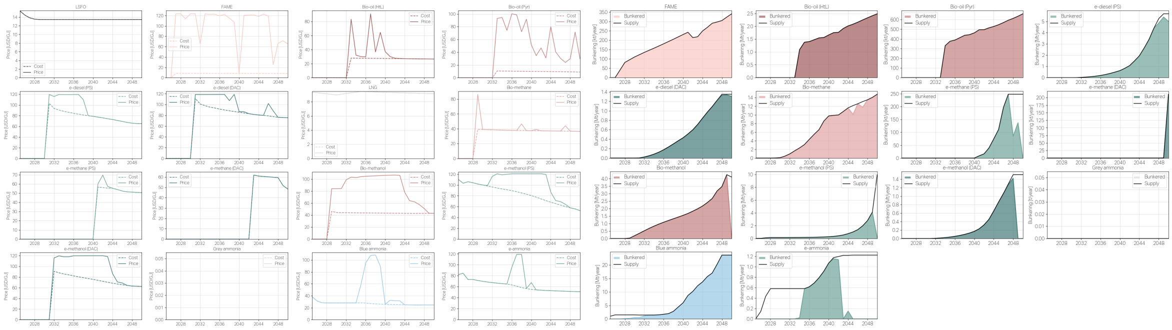


Figure J.21: Market price (left), and fuel supply and demand (right) in Asian ports under the Local configuration.

Asia

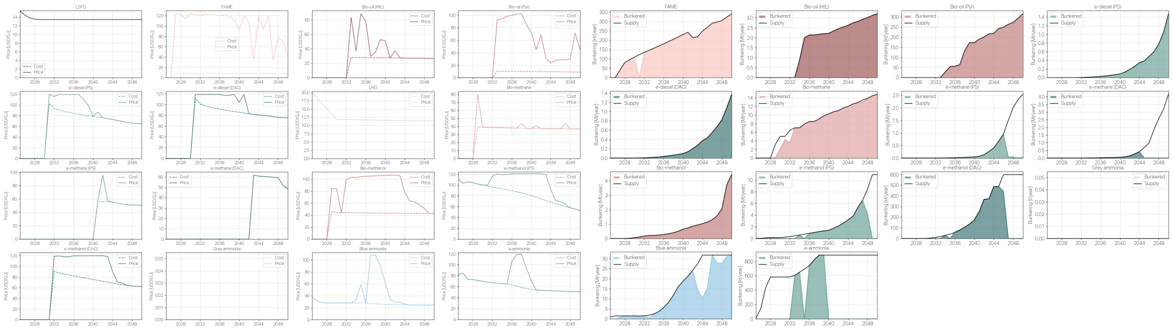


Figure J.22: Market price and fuel supply in Asian ports under the Local configuration.

Europe

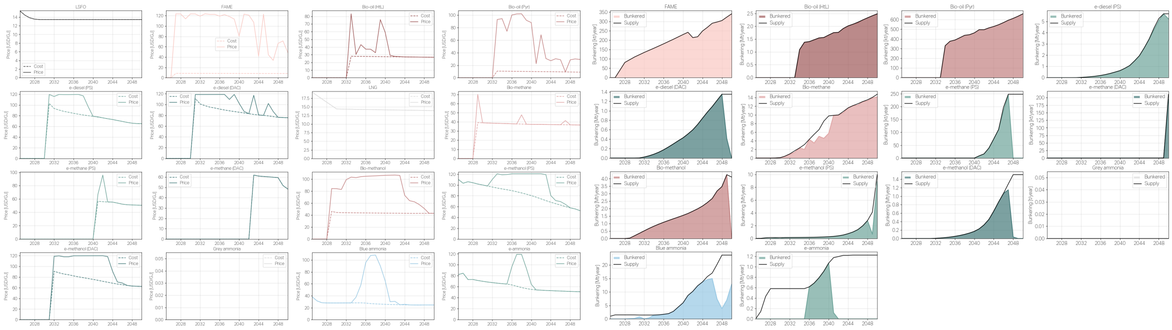


Figure J.23: Market price (left), and fuel supply and demand (right) in European ports under the Local configuration.

Middle East

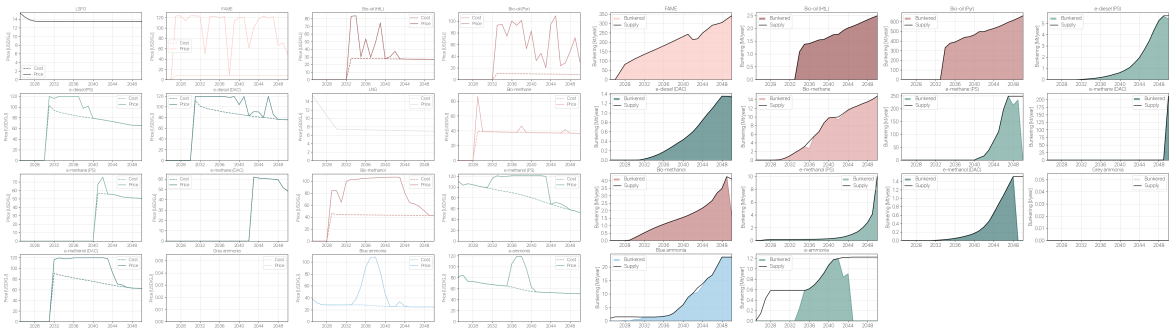


Figure J.24: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Local configuration.

Global Overview

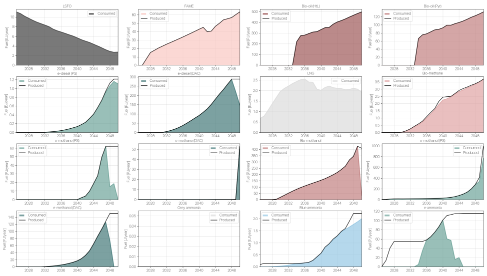
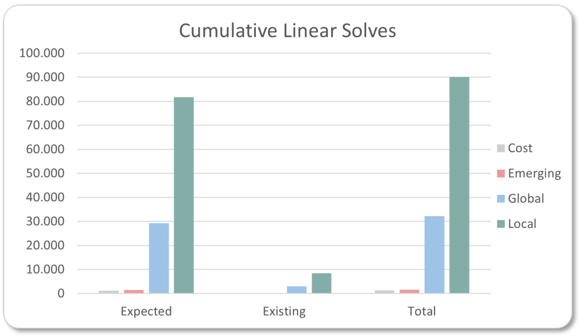


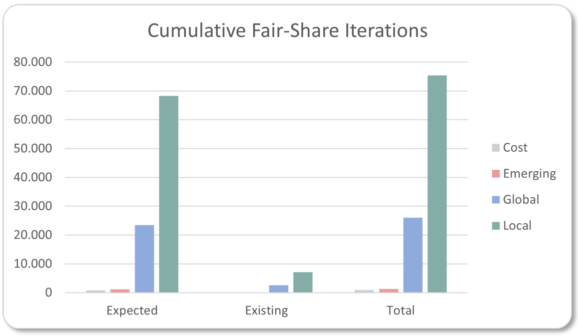
Figure J.25: Global fuel supply and demand overview for the Local scenario.

K Levy-Based Regulation - Results

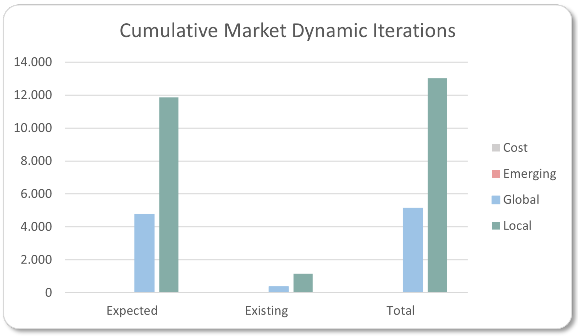
K.1 Performance Diagnostics



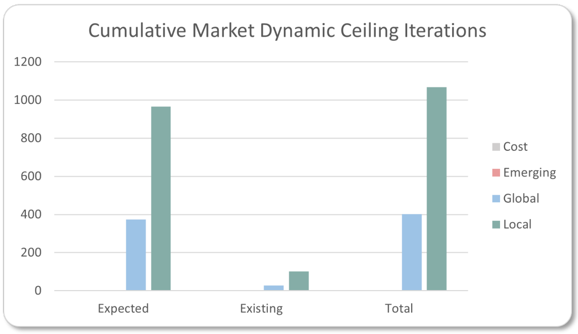
(a) Linear Solves



(b) Fair-Share Iterations



(c) Market Dynamic Iterations



(d) Ceiling Iterations

Figure K.1: Cumulative expected, existing and total solver calls and iteration counts under the `Levy-Based` scenario across all model runs.

K.2 Market Dynamics

K.2.1 Fuel Supply and Bunker Prices – Cost-Only, Levies Africa

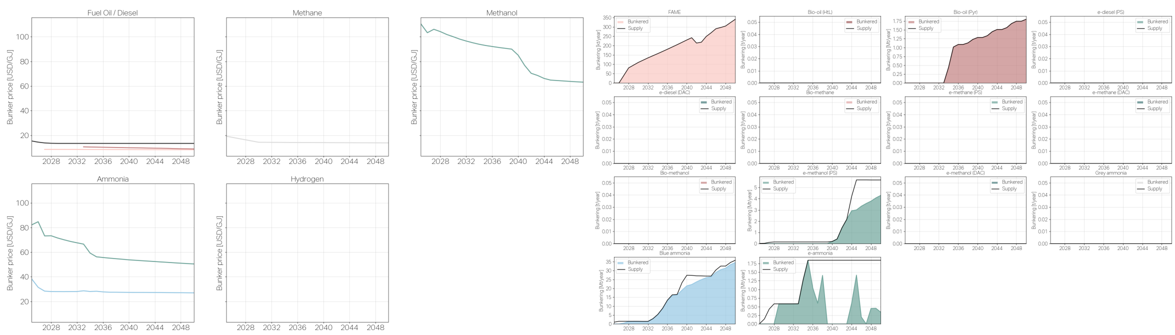


Figure K.2: Market price (left), and fuel supply and demand (right) in African ports under the Cost-Only configuration.

Americas

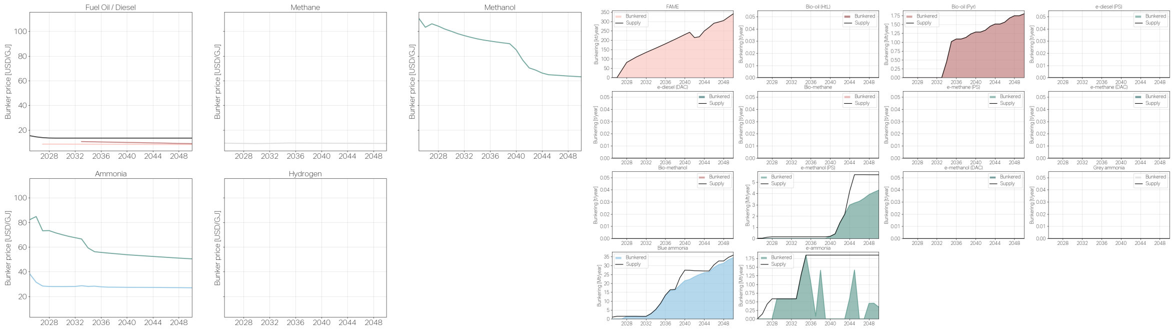


Figure K.3: Market price (left), and fuel supply and demand (right) in American ports under the Cost-Only configuration.

Asia

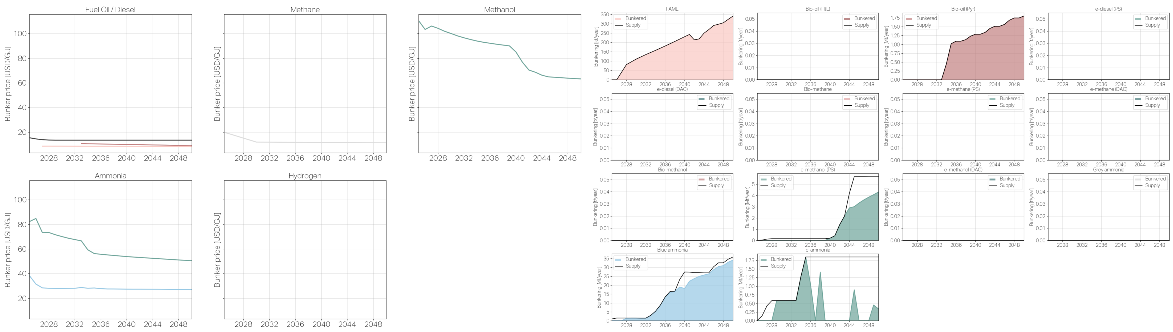


Figure K.4: Market price (left), and fuel supply and demand (right) in Asian ports under the Cost-Only configuration.

Europe

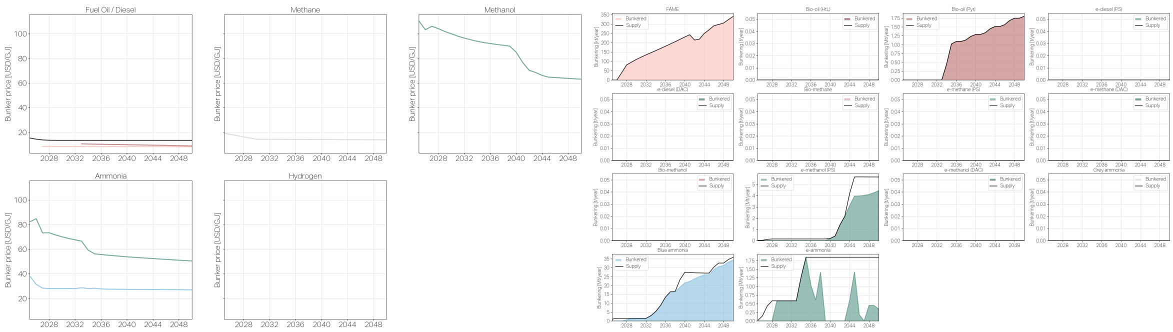


Figure K.5: Market price (left), and fuel supply and demand (right) in European ports under the Cost-Only configuration.

Middle East

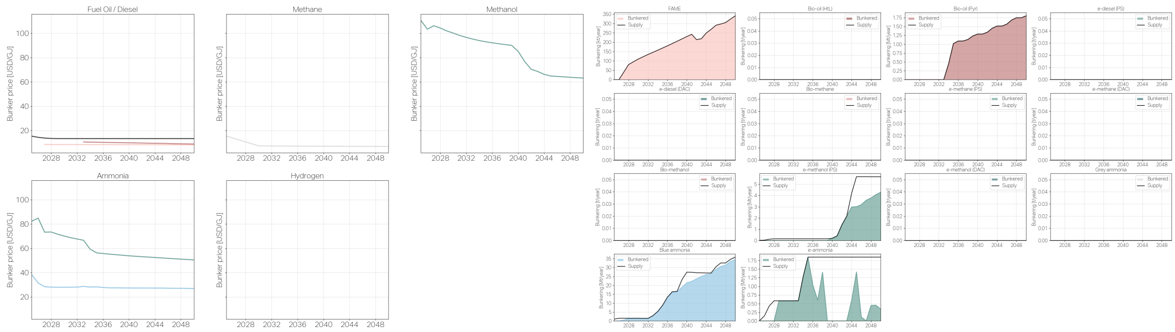


Figure K.6: Bunker price and fuel supply in Middle Eastern ports.

Global Overview

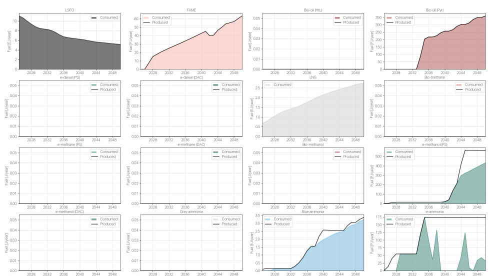


Figure K.7: Global fuel supply and demand overview for the Cost-Only scenario.

K.2.2 Fuel Supply and Bunker Prices – Emerging

Africa

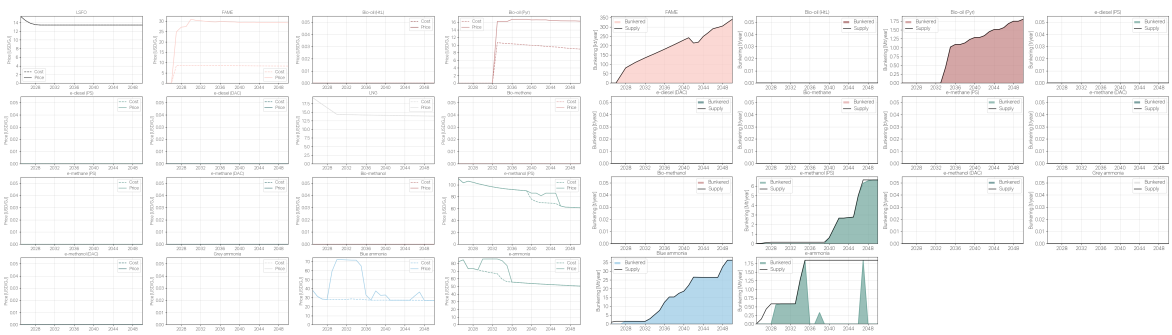


Figure K.8: Market price (left), and fuel supply and demand (right) in African ports under the Emerging configuration.

Americas

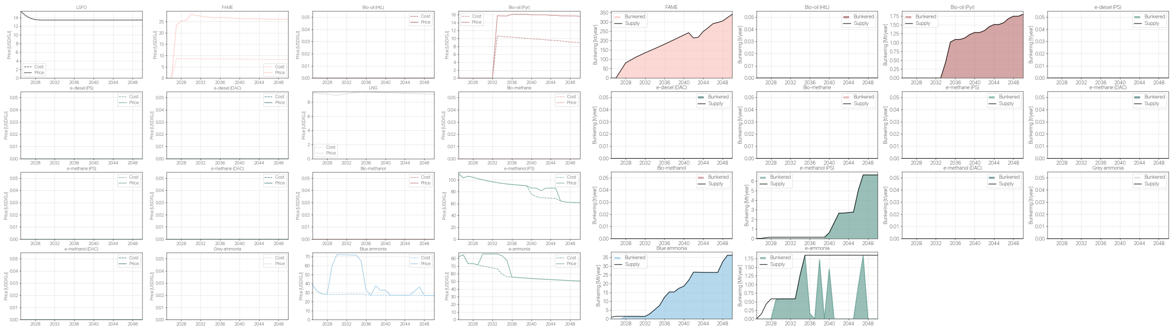


Figure K.9: Market price (left), and fuel supply and demand (right) in American ports under the Emerging configuration.

Asia

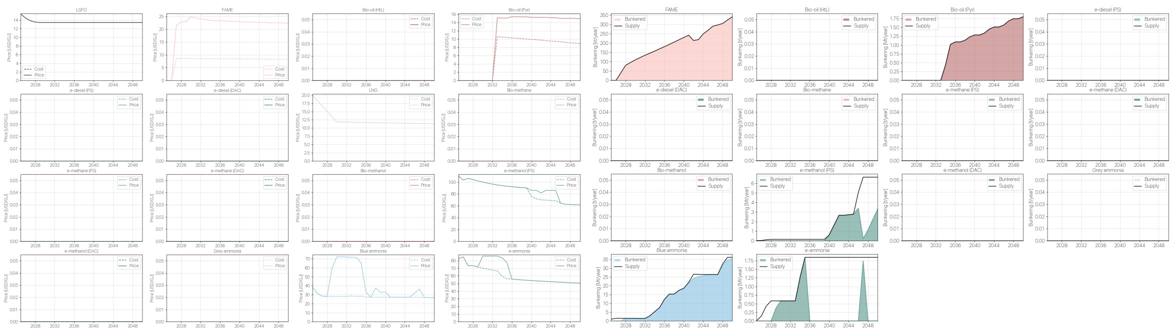


Figure K.10: Market price (left), and fuel supply and demand (right) in Asian ports under the Emerging configuration.

Europe

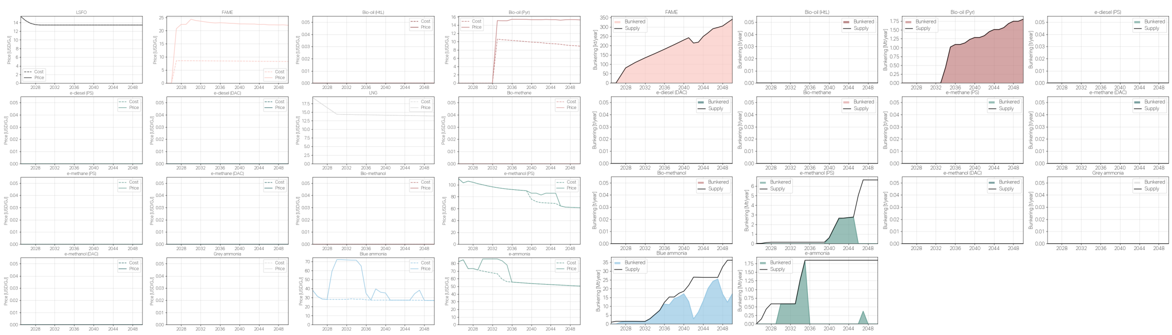


Figure K.11: Market price (left), and fuel supply and demand (right) in European ports under the Emerging configuration.

Middle East

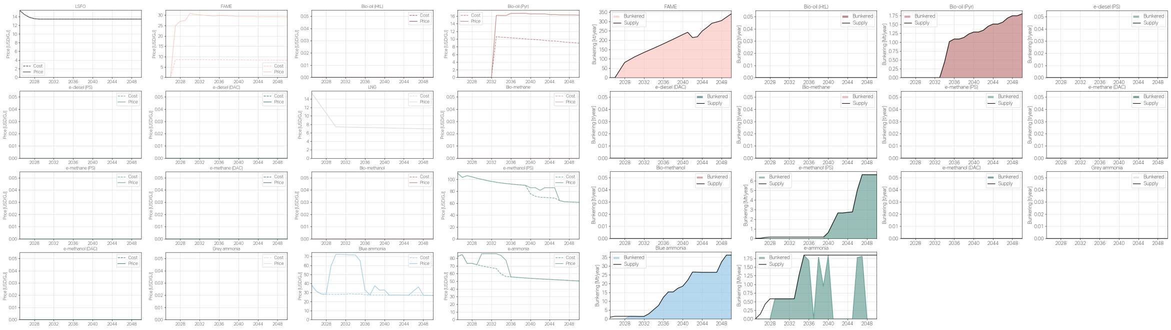


Figure K.12: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Emerging configuration.

Global Overview

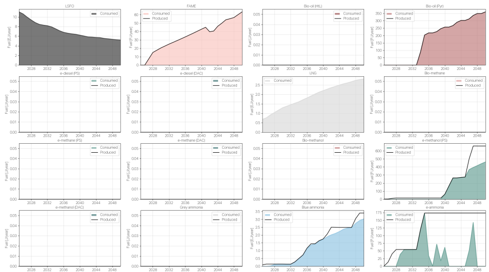


Figure K.13: Global fuel supply and demand overview for the Emerging scenario.

K.2.3 Fuel Supply and Bunker Prices – Global

Africa

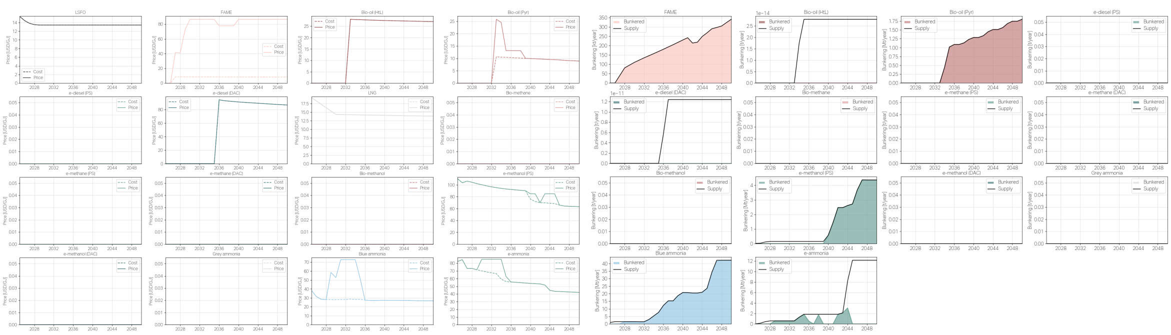


Figure K.14: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Global configuration.

Americas

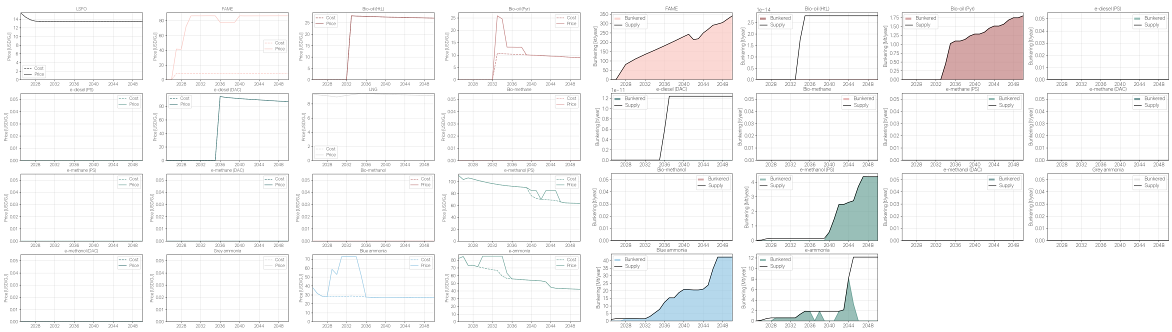


Figure K.15: Market price (left), and fuel supply and demand (right) in American ports under the Global configuration.

Asia

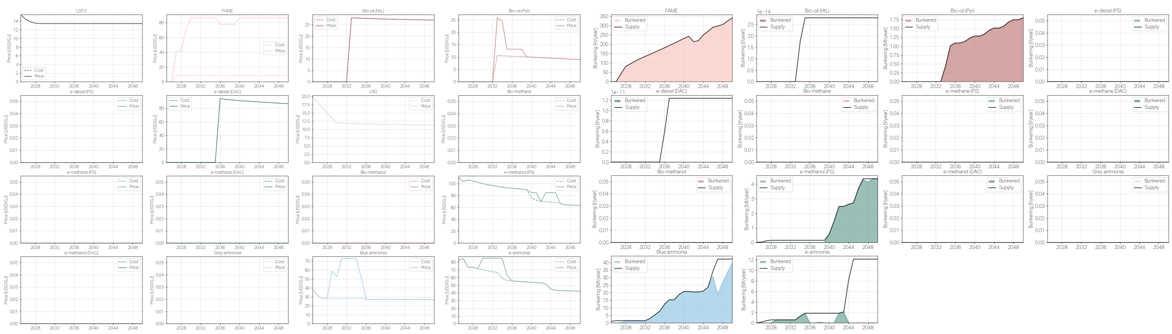


Figure K.16: Market price (left), and fuel supply and demand (right) in Asian ports under the Global configuration.

Europe

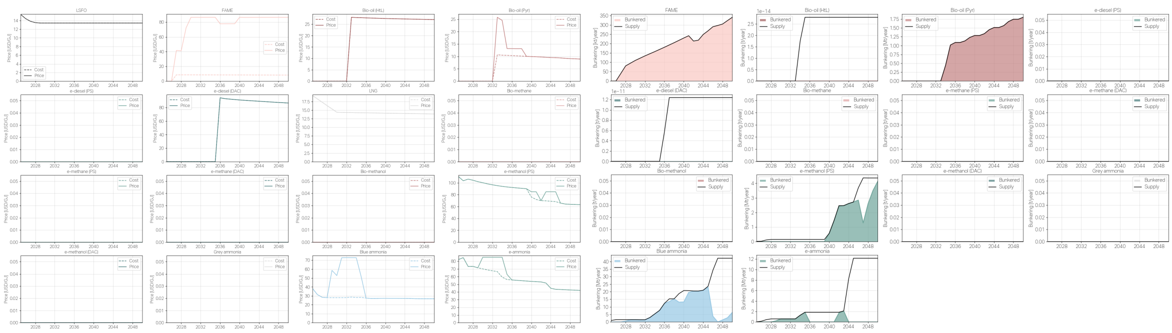


Figure K.17: Market price (left), and fuel supply and demand (right) in European ports under the Global configuration.

Middle East

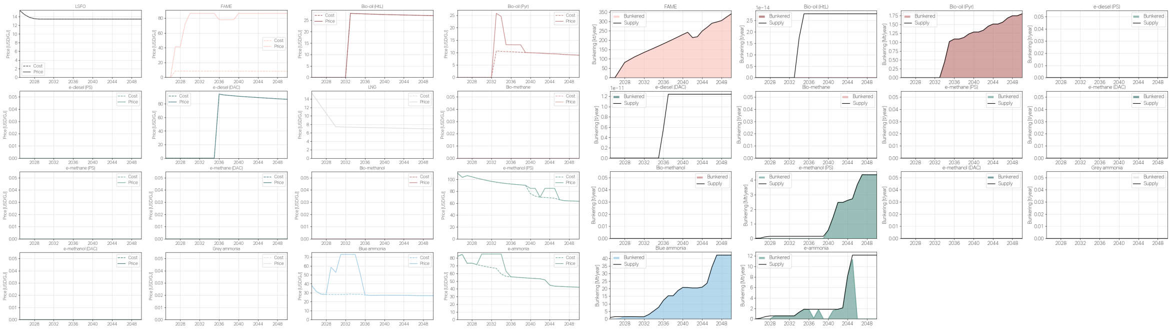


Figure K.18: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Global configuration.

Global Overview

Figure K.19: Global fuel supply and demand overview for the Global configuration.

K.2.4 Fuel Supply and Bunker Prices – Local

Africa

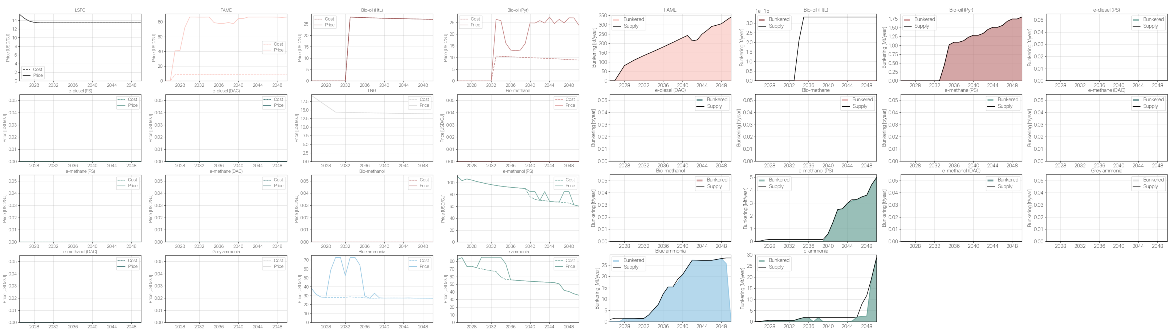


Figure K.20: Market price (left), and fuel supply and demand (right) in African ports under the Local configuration.

Americas

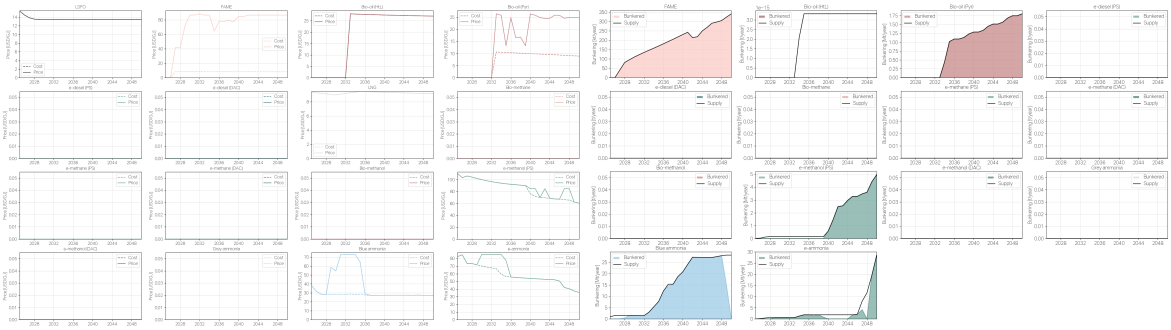


Figure K.21: Market price (left), and fuel supply and demand (right) in American ports under the Local configuration.

Asia

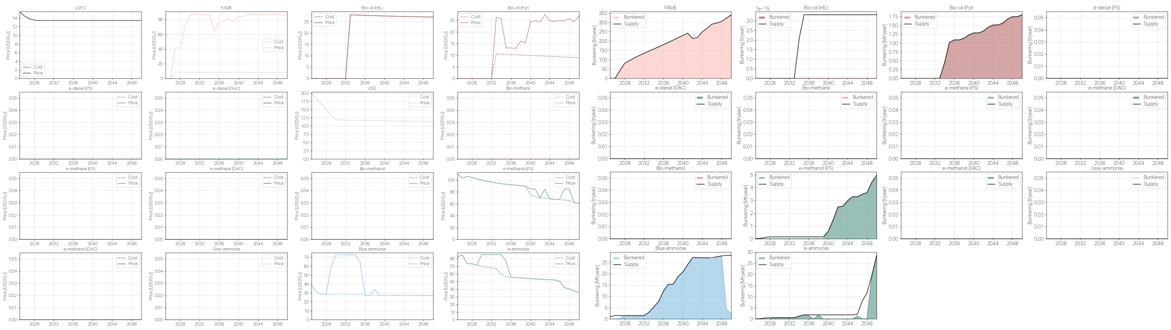


Figure K.22: Market price (left), and fuel supply and demand (right) in Asian ports under the Local configuration.

Europe

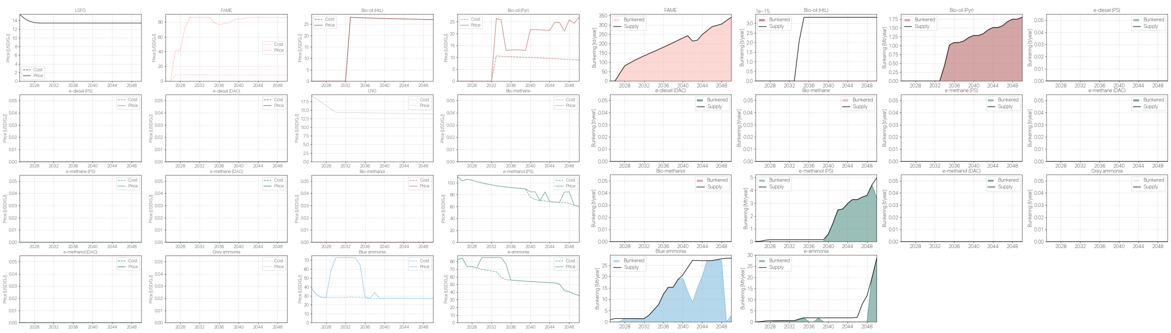


Figure K.23: Market price (left), and fuel supply and demand (right) in European ports under the Local configuration.

Middle East

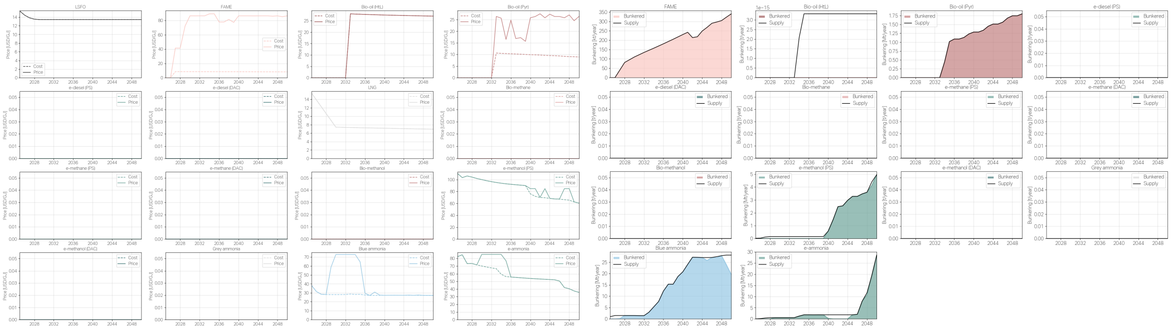


Figure K.24: Market price (left), and fuel supply and demand (right) in Middle Eastern ports under the Local configuration.

Global Overview

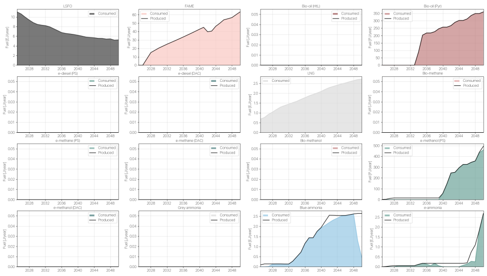


Figure K.25: Global fuel supply and demand overview for the Local configuration.

L Numeric Performance Analytics Results

Indicator	No Regulation	Reg. Flex 380	Reg. Flex 1200	Reg. No Flex	Levy-Based
			Total Runtime (s)		
Cost-Only	3,176.19	5,054.86	4,411.90	5,054.86	4,677.31
Global	12,966.62	12,966.62	46,174.57	41,457.37	8,787.99
Local	17,970.77	17,970.77	85,578.09	85,729.03	29,888.34
Emerging	5,397.78	5,397.78	4,508.61	4,590.55	2,299.54
			Build Time (s)		
Cost-Only	2,669.96	2,978.50	2,961.06	2,978.50	3,126.16
Global	12,218.36	3,325.38	3,313.44	3,325.38	2,364.08
Local	17,296.78	2,899.23	3,583.71	2,899.23	4,121.30
Emerging	4,541.82	2,913.45	3,004.93	2,913.45	1,649.01
			Solve Time (s)		
Cost-Only	506.23	1,421.04	770.44	1,421.04	672.03
Global	748.26	37,410.71	42,102	37,410.71	5,224.74
Local	674.00	80,471.98	81,199.50	80,471.98	22,541.63
Emerging	855.96	1,019.93	801.71	1,019.93	246.28

Table L.1: Cross-scenario comparison: Runtime and Model Size.

Indicator	No Regulation	Reg. Flex 380	Reg. Flex 1200	Reg. No Flex	Levy-Based
			LP Variables		
Cost-Only	2,487,034	2,225,561	2,224,796	2,493,095	2,491,329
Global	2,221,710	2,224,796	2,224,796	2,226,536	2,226,300
Local	2,221,710	2,224,796	2,224,796	2,226,536	2,226,300
Emerging	2,220,945	2,224,796	2,224,796	2,226,536	2,224,770
			LP Constraints		
Cost-Only	1,253,299	927,385	927,056	1,358,070	1,255,539
Global	925,714	32,999	927,056	928,796	927,688
Local	925,714	57,886	927,056	928,796	927,688
Emerging	925,385	927,056	927,056	928,796	927,030
			Linear Solves		
Cost-Only	919	1,744	3,113	2,165	1,272
Global	9,107	35,791	116,396	143,018	32,275
Local	11,044	63,823	206,335	321,690	90,190
Emerging	936	1,800	3,284	4,274	1,617

Table L.2: Cross-scenario comparison: LP Size and Linear Solves.

Indicator	No Regulation	Reg. Flex 380	Reg. Flex 1200	Reg. No Flex	Levy-Based
Fair-Share Iterations					
Cost-Only	568	1,393	2,762	1,814	921
Global	5,743	28,190	104,150	131,198	26,030
Local	7,025	51,514	181,506	293,150	75,395
Emerging	585	1,449	2,933	3,923	1,266
Market Dynamic Iterations					
Cost-Only	0	0	0	0	0
Global	2,308	6,526	10,491	9,949	5,141
Local	2,935	11,031	22,445	25,813	13,026
Emerging	0	0	0	0	0
Ceiling Iterations					
Cost-Only	0	0	0	0	0
Global	354	373	1,053	1,169	402
Local	382	576	1,682	2,025	1,067
Emerging	0	0	0	0	0

Table L.3: Cross-scenario comparison: Iterations Statistics.

M Numeric Market Dynamic Results

Scenario	Metric	Cost-Only	Global Market	Local Market	Emerging Market
4*No Regulation	Cost (M USD)	690,719.43	690,719.33	778,085.34	690,719.34
	Price (USD/t)	0.00	713,501.44	805,344.65	725,865.82
	Supply (t)	369,281,258	369,286,186	369,071,577	369,285,872
	Demand (t)	8,487,192,726	8,484,704,279	8,478,843,319	8,476,645,787
4*Reg. w/ Flex (380 USD)	Cost	966,477.22	964,334.17	964,696.03	964,335.60
	Price	0.00	1,213,406.49	1,232,522.76	1,215,866.54
	Supply	2,714,684,620	2,704,209,913	2,759,435,249	2,671,962,598
	Demand	8,045,589,671	8,024,744,465	8,023,802,091	7,977,805,540
4*Reg. w/ Flex (1200 USD)	Cost	2,490,767.94	2,487,124.34	2,487,890.55	2,486,688.02
	Price	0.00	3,570,903.77	3,773,112.60	3,905,451.29
	Supply	3,773,956,265	3,773,829,322	3,941,909,638	3,628,544,662
	Demand	8,478,770,347	8,274,803,009	8,279,792,441	8,075,026,520
4*Reg. No Flex (1200 USD)	Cost	2,255,091.24	2,160,127.27	2,151,375.34	1,998,938.66
	Price	0.00	2,991,541.88	3,174,417.87	3,120,385.72
	Supply	2,802,349,106	2,784,245,401	2,775,875,916	2,785,968,196
	Demand	7,801,511,169	7,698,372,354	7,664,615,429	7,706,438,704
4*Levies (800)	Cost	656,800.46	1,037,688.64	750,356.90	655,218.78
	Price	0.00	1,407,899.18	1,160,963.22	806,261.76
	Supply	2,667,937,884	2,928,833,184	2,695,560,265	2,505,444,697
	Demand	7,801,568,467	7,736,061,708	7,774,773,067	7,683,880,042

Table M.1: Comparison of aggregated system indicators across all policy scenarios and market typologies.

N Numeric Expenses Results

Indicator	No Regulation	Reg. Flex 380	Reg. Flex 1200	Reg. No Flex	Levy-Based
			Total Fuel Related Expenses (EUR)		
Cost-Only	4.30268×10^{12}	5.43144×10^{12}	6.57223×10^{12}	5.80×10^{12}	1.41207×10^{13}
Global	4.31067×10^{12}	5.46669×10^{12}	8.03188×10^{12}	6.22×10^{12}	1.43008×10^{13}
Local	4.31318×10^{12}	5.47554×10^{12}	8.45076×10^{12}	6.37×10^{12}	1.43254×10^{13}
Emerging	4.31892×10^{12}	5.54100×10^{12}	9.23706×10^{12}	6.81×10^{12}	1.43898×10^{13}
			Vessel Related Expenses (EUR)		
Cost-Only	1.36084×10^{13}	1.47585×10^{13}	1.48015×10^{13}	1.49272×10^{13}	1.56244×10^{13}
Global	1.36097×10^{13}	1.47693×10^{13}	1.49448×10^{13}	1.49803×10^{13}	1.56354×10^{13}
Local	1.36143×10^{13}	1.47721×10^{13}	1.49823×10^{13}	1.50008×10^{13}	1.56346×10^{13}
Emerging	1.36154×10^{13}	1.47959×10^{13}	1.50536×10^{13}	1.50184×10^{13}	1.56561×10^{13}
			Regulation Expenses (EUR)		
Cost-Only	0	1.19951×10^{12}	9.14584×10^{11}	2.60573×10^{12}	0
Global	0	1.19308×10^{12}	6.05848×10^{11}	2.27767×10^{12}	0
Local	0	1.19458×10^{12}	7.18097×10^{11}	2.23543×10^{12}	0
Emerging	0	1.22515×10^{12}	7.33278×10^{11}	2.30779×10^{12}	0

Table N.1: Cross-scenario comparison of all expenses across five policy settings and four market typologies.

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