Physics-Informed Digital Twins for Maritime Fleet Optimization under Regulatory Uncertainty: An EU ETS Case Study

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ABSTRACT

The global maritime industry is currently navigating a paradigm shift driven by decarbonization regulations, most notably the inclusion of shipping in the European Union Emissions Trading System (EU ETS) as of January 2024. This regulatory change transforms fuel consumption from a simple operational expense into a complex financial liability tied to stochastic carbon allowance prices. Existing fleet optimization models often fail to account for the dual challenges of market volatility and hydrodynamic heterogeneity across diverse vessel classes. This study proposes a novel "Digital Twin" framework that integrates first-principles naval architecture with data-driven machine learning to optimize voyage planning under uncertainty. We utilize a proprietary dataset of 1,440 voyages, enriched with physics-based synthetic features representing sea states, hull fouling, and engine load profiles. By contrasting a Linear Regression baseline with a physics-constrained Gradient Boosting (XGBoost) model, we demonstrate that the latter captures non-linear resistance regimes—such as the drag "hump" in planning hulls—with significantly higher accuracy (RMSE reduction of ~60%). Furthermore, we couple this predictive model with a Geometric Brownian Motion (GBM) simulation of carbon prices to derive optimal sailing speeds that minimize total voyage costs. The results highlight the necessity of adaptive slow steaming strategies in high-volatility carbon markets and offer a reproducible pathway for integrating regulatory risk into maritime operations.

1. INTRODUCTION

Maritime transport remains the backbone of the global economy, carrying approximately 80% of global trade by volume [1]. However, the sector's reliance on fossil fuels has drawn intense regulatory scrutiny. The extension of the EU Emissions Trading System (EU ETS) to the maritime sector marks a watershed moment for the industry [2]. As of January 2024, large vessels (≥5000 GT) entering EU ports must surrender allowances for their verified carbon emissions, effectively monetizing their environmental footprint.

This policy introduces a layer of "Regulatory Uncertainty" previously absent from voyage calculations. Unlike traditional bunker fuel markets, which are driven by supply and demand for crude oil, the price of EU Carbon Allowances (EUA) is influenced by legislative caps, cross-sectoral demand, and policy speculation. Historical data reveals extreme volatility, with prices exceeding €100/tCO_2 in early 2023 [8]. Consequently, ship operators can no longer optimize for fuel efficiency alone; they must optimize for a composite cost function where the "tax" rate is a stochastic variable.

Simultaneously, the operational reality of fleet management is complicated by vessel heterogeneity. A diversified fleet may contain displacement hulls (e.g., tankers), which follow cubic speed-power relationships, and planing crafts (e.g., crew transfer vessels), which exhibit complex, non-linear drag profiles. Traditional power-law models often fail to capture these distinctions, leading to suboptimal routing and speed selection.

This paper addresses these challenges by developing a **Physics-Informed Digital Twin**. By synthesizing domain knowledge (naval architecture) with advanced regression techniques (XGBoost), we answer two primary research questions:

1. How can machine learning models be constrained by physical laws to accurately predict fuel consumption across hydrodynamically distinct vessel classes?
2. How does stochastic volatility in carbon pricing alter the optimal operational profile of a diverse fleet?

2. LITERATURE REVIEW AND REGULATORY CONTEXT

2.1 The Evolving Regulatory Landscape

The inclusion of shipping in the EU ETS is phased, creating a dynamic compliance landscape. Regulations require shipping companies to surrender allowances for 40% of verified emissions in 2025 (covering 2024 data), rising to 70% in 2026, and reaching 100% by 2027 [3][4]. While currently applicable to cargo and passenger ships over 5000 GT [5], the scope is set to expand to offshore vessels of the same size by 2027 [6], with smaller general cargo and offshore vessels (400–5000 GT) entering the Monitoring, Reporting, and Verification (MRV) framework in 2025 [7]. This phased integration creates a temporal dimension to cost optimization, where the "cost of compliance" (ϕ) varies by year.

2.2 Fuel Consumption Modeling

Standard maritime fuel models rely heavily on the "Admiralty Coefficient" formula, assuming that power (and fuel) scales with the cube of speed (V^3). While accurate for large displacement vessels in calm water [9], this approximation degrades for high-speed crafts or vessels operating in adverse weather conditions. Planing hulls, for instance, experience a hydrodynamic "hump" where resistance increases sharply before flattening out at high speeds—a phenomenon poorly captured by simple polynomial regression.

Furthermore, "curve-fitting" approaches often ignore operational realities such as hull fouling (biological growth increasing drag) [10] and the "bathtub" curve of Specific Fuel Oil Consumption (SFOC), where engines become less efficient at very low loads. This study contributes to the literature by explicitly embedding these physical phenomena into the feature engineering process, creating a "Digital Twin" that respects first principles while leveraging the flexibility of non-parametric machine learning.

3. METHODOLOGY

Our methodology proceeds in three stages: constructing the Digital Twin dataset, training physics-constrained predictive models, and optimizing voyage speed under stochastic economic conditions.

3.1 Digital Twin Dataset Construction

We utilize a dataset comprising 1,440 voyage records. To overcome the limitations of sparse raw data, we enrich this dataset with synthetic, physics-based features that mirror real-world complexity. The feature engineering process is detailed below.

3.1.1 Operational Profiles and Hydrodynamics

The fleet is heterogeneous, requiring distinct operational profiles for each ship type. We assign speed ranges and hydrodynamic regimes as follows:

Table 1: Operational Profiles for Synthetic Data Generation

Ship Type	**Hydrodynamic Regime**	**Typical Speed Range (knots)**	**Resistance Characteristics**
Tanker Ship	Displacement	10 – 14	Resistance $\propto V^3$
Fishing Trawler	Displacement/Trawling	8 – 12	High drag at low speeds
Oil Service Boat	Displacement	8 – 12	Moderate consistent drag
Surfer Boat	Planing	20 – 35	Non-linear "hump" transition

3.1.2 Environmental Proxies

Raw weather data is often categorical (e.g., "Calm", "Stormy"). To enable granular modeling, we map these categories to numeric spectral wave data proxies.

- **Significant Wave Height (H_s):** Drawn from a uniform distribution $U(a, b)$ based on sea state. For "Moderate" conditions, $H_s \sim U(0.5, 2.5)$ meters.
- **Wind Direction:** We introduce a directional feature (Head, Beam, Following). Head seas dramatically increase added resistance (and fuel consumption) according to ISO 15016 standards, while following seas may aid propulsion [9].

3.1.3 Engine and Hull Degradation

We model the efficiency loss of the main engine using an SFOC "bathtub" curve. Engines are designed for optimal efficiency at 75–85% Maximum Continuous Rating (MCR). We apply a penalty factor λ_{load} that increases fuel consumption when the engine load drops below 30% (slow steaming) or exceeds 90%.

Additionally, we simulate hull performance deterioration via a fouling index, $I_{fouling}$, representing days since the last drydock. Empirical evidence suggests biofouling can increase shaft power requirements by 10–20% [10].

3.2 Stochastic Carbon Pricing Model

To capture the financial risk of the EU ETS, we model the price of European Union Allowances (EUA), denoted S_t, as a Geometric Brownian Motion (GBM). This stochastic process accounts for the trend (drift) and uncertainty (volatility) of the market. The differential equation governing the price path is:

$$dS_t = \mu S_t\, dt + \sigma S_t\, dW_t$$

Where:

- S_t is the carbon price at time t.
- μ is the drift parameter (≅5%/year), reflecting regulatory tightening.
- σ is the volatility parameter (≅40%/year), reflecting market uncertainty [8].
- dW_t is a Wiener process.

The total carbon liability for a voyage is calculated as:

$$\text{Liability} = \text{Fuel} \times C_f \times S_t \times \phi_{\text{year}}$$

Where C_f is the carbon intensity of the fuel (3.114 tCO_2/t_{fuel}) and ϕ is the phase-in factor (0.4, 0.7, or 1.0) [3].

3.3 Predictive Modeling Framework

We define the prediction task as a regression problem: $Y = F(X)$ where Y is the adjusted fuel consumption and X is the feature vector including speed, weather proxies, and vessel characteristics.

3.3.1 Baseline: Linear Regression (OLS)

We establish a baseline using Ordinary Least Squares. While interpretable, OLS assumes a linear relationship between features and the target (or log-target). It is expected to struggle with the regime-switching behavior of planing hulls and the non-linear penalties of adverse weather.

3.3.2 Physics-Informed XGBoost

We employ XGBoost, a gradient-boosted decision tree algorithm capable of capturing complex non-linear interactions. Crucially, we enforce Monotonic Constraints on the speed feature.

Physics dictates that, all else being equal, increasing speed must increase fuel consumption. Standard ML models might violate this in sparse data regions. By enforcing a positive monotonicity constraint $(+1)$ on the speed feature, we ensure the model respects the first law of naval thermodynamics, preventing non-physical predictions.

3.4 Optimization Strategy

The trained model $\hat{F}(V)$ is embedded into a cost minimization function $J(V)$. For a voyage of distance D, the objective is to find the speed V that minimizes the sum of fuel costs, carbon taxes, and time-charter equivalent (opportunity) costs:

$$J(V) = \underbrace{P_{\text{fuel}} \cdot \hat{F}(V)}_{\text{Fuel Cost}} + \underbrace{P_{\text{carbon}} \cdot C_f \cdot \phi \cdot \hat{F}(V)}_{\text{Carbon Tax}} + \underbrace{\frac{D}{V} \cdot \text{TCE}}_{\text{Opportunity Cost}}$$

Where P_{fuel} is the bunker price and TCE is the daily Time Charter Equivalent rate.

4. RESULTS

4.1 Predictive Performance

The models were trained on an 80/20 train-test split. Table 2 summarizes the performance metrics on the test set.

Table 2: Model Performance Comparison

Model	**RMSE (tonnes)**	**R2 Score**
Linear Regression (OLS)	1054.11	0.964
Physics-Informed XGBoost	417.71	0.994

The XGBoost model achieves a significantly lower Root Mean Square Error (RMSE), reducing prediction error by approximately 60% compared to the linear baseline. This confirms the hypothesis that ship hydrodynamics—particularly across diverse classes like tankers and surfer boats—are inherently non-linear and require high-capacity models to capture effectively.

4.2 Physics-Based Validation

To ensure the model is not merely overfitting but learning valid physics, we analyzed the **Admiralty Coefficient Proxy** (A_c') for the predictions:

$$A_c' = \frac{V^3}{\hat{F}}$$

For displacement hulls, A_c' should remain relatively stable. For planing hulls, it should increase significantly at high speeds as the vessel lifts out of the water, reducing drag.

- **Observation:** The XGBoost predictions yielded a physically plausible spread. Displacement vessels (Tankers) clustered around moderate A_c' values. Surfer Boats at high speeds (>30 kts) showed significantly higher A_c values, correctly reflecting the hydrodynamic efficiency gain of the planing regime.
- **Weather Sensitivity:** The model successfully differentiated between "Head" and "Following" seas. Voyages with "Head" wind direction were predicted to consume higher fuel than identical voyages with "Following" wind, validating the efficacy of the numeric weather proxies.

4.3 Optimization under Uncertainty

Using the trained model and the cost function $J(V)$, we calculated the optimal cruising speeds for each vessel type under current market conditions ($P_{fuel} = , TCE = , \phi$).

Table 3: Optimal Speed Results by Vessel Type

Ship Type	Realistic Range (kts)	Optimal Speed (kts)	Minimized Voyage Cost ($)
Oil Service Boat	8.0 – 12.0	**12.00**	2,293,040
Fishing Trawler	8.0 – 12.0	**11.59**	1,477,980
Surfer Boat	20.0 – 35.0	**34.69**	1,097,959
Tanker Ship	10.0 – 15.0	**14.80**	10,435,936

The optimization results reveal distinct strategies. High-value assets like Tankers and Surfer Boats tend to operate near their maximum speeds to minimize opportunity costs (TCE), as the cost of delay outweighs the incremental fuel and carbon tax. Conversely, Fishing Trawlers show an optimal speed (11.59 kts) slightly below their maximum, indicating a sensitivity where "slow steaming" begins to yield marginal returns against the carbon tax.

5. DISCUSSION

5.1 The Role of Non-Linearity in Compliance

The superior performance of XGBoost over Linear Regression highlights the danger of using simplistic fuel models for regulatory compliance. A linear model systematically underestimates fuel consumption in the high-resistance "hump" region of planning crafts and overestimates efficiency in adverse weather. Under the EU ETS, such errors translate directly into financial risk—underestimating fuel burn leads to an under-purchase of carbon allowances, exposing the operator to penalties or higher spot prices later.

5.2 Operational Implications of Carbon Pricing

The Digital Twin demonstrates that carbon pricing acts as a friction on speed. As the phase-in factor ϕ increases from 0.4 (2025) to 1.0 (2027), the "Carbon Tax" term in our cost function $J(V)$ will more than double. This will shift the optimal speeds found in Table 3 downwards. Operators of older, less efficient tonnage (like the Trawlers in our dataset) will be forced to slow steam more aggressively than modern, efficient vessels to remain profitable.

5.3 Limitations and Future Work

While the Geometric Brownian Motion (GBM) used for carbon pricing provides a robust baseline for volatility, it assumes a random walk. Real carbon markets often exhibit **mean-reverting** behavior, where prices fluctuate around a long-term equilibrium driven by policy supply caps. Future research should explore Ornstein-Uhlenbeck processes to model this behavior more accurately. Additionally, while our weather proxies captured head/following sea effects, integrating real-time satellite oceanographic data could further refine the environmental resistance components of the model.

6. CONCLUSION

This study presents a rigorous, physics-informed framework for maritime fleet optimization in the era of the EU ETS. By replacing static assumptions with a Digital Twin that incorporates vessel-specific hydrodynamics, weather impacts, and stochastic regulatory costs, we provide a granular view of voyage economics.

Our results confirm that machine learning models, when constrained by monotonic physical laws, significantly outperform traditional regression in predicting fuel consumption for heterogeneous fleets. The integration of these models into a cost-optimization loop reveals that optimal sailing speeds are highly sensitive to the interplay between hydrodynamic efficiency and regulatory taxation. As the EU ETS phase-in progresses toward 100% coverage in 2027, such adaptive, data-driven tools will be essential for the maritime industry to balance profitability with decarbonization mandates.

DATA CODE AND AVAILABILITY

The complete Python implementation, including the Digital Twin generation logic, XGBoost model configuration, and the synthetic dataset used in this study, is available in the following public repository to facilitate reproducibility: https://github.com/akash-dj/Maritime-Fleet-Optimization-under-Regulatory-Uncertainty.git

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