Sustainable Bunkers

the changing bunker supply chain

J. F. de Vos

A hybrid model of the bunker supply chain to investigate the impact of sustainable fuels on the changing fuel supply chain on a bunkering hub-level.

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Preface

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This thesis was written to obtain my masters degree in Marine Technology focussed on the track Maritime Operations and Markets (MOM). With it, I will finish my period at the faculty of 3ME in Delft and start a new chapter in life.

Since I was a child, I have always been fascinated by everything related to water, particularly boats. However, I had no expectation that one day I would finish my thesis to become a naval architect. Therefore, I would like to thank my father for that fateful day he decided to join another campus tour in Delft, while I was attending a vastly different one. The one where they were talking about boats, was in his opinion far more interesting. After convincing me to join him on that tour, and are about to complete my master's degree, I can confidently say I couldn't agree with him more.

This project has challenged me in countless ways and taught me a great deal. In particular, I've learned that with enough optimism and creativity, the limited tools provided will suffice to tackle the challenges ahead.

I would like to express my gratitude to all the people who supported me throughout this period. First of all, I would like to thank Can Besev for providing me with his invaluable years of experience and his critical reflection on all aspects of life. I would like to thank Peninsula for the opportunity they provided me. Aside from the vast industry insights the company offered me, it also allowed me to meet phenomenal people throughout the entire project. I would like to thank my mentor Edwin van Hassel, who always provided me with the right input to keep me on track, was patient in getting me back on track and all the friendly conversations we had aside the topic of my project.

Lastly, I would like to thank my mother and friends, who have been kind and patient with me throughout this period. We celebrated all the milestones, but shared the difficult moments too. They provided me with invaluable feedback when I needed it.

Summary

The maritime industry faces the critical challenge to decarbonise, with alternative fuels offering a promising route towards being net-zero. While technical progress on these fuels continues to evolve rapidly, their introduction brings significant operational challenges. One of the most affected and overlooked areas is the bunker supply chain, which is essential to enabling global maritime logistics. This research focusses on quantifying the operational implications of implementing sustainable fuels in the ship-to-ship bunkering segment, with a specific focus via a case study on the bunkering hub of Gibraltar.

To provide this outlook, a hybrid-modelling approach was implemented, combining the dynamics of agent-based simulations with iterative optimisation. This model captures the dynamics involved in the ship-to-ship bunkering framework and the stakeholders involved under evolving supply and demand conditions. Actual operational data, provided through Peninsula a global physical bunker supplier, ensures that the model will produce outcomes that reflect the practical constraints and variability.

The results reveal that the implementation of sustainable fuels will introduce increased service times, higher operational complexity and a drastic increase in pressure on fleet utilisation. Supporting literature highlighted that segmentation of demand necessitates a transition from flexible, multi-fuel bunkering vessels to purpose built single-fuel assets, resulting in more individual and fragmented supply chains.

The scenario-based optimisation further underscores this as the requirement for maintaining reliable service levels will require significantly larger fleets, driven by diversification and not by demand. The extended service times revealed that for ship operators scheduling and port call planning may significantly be influenced and that bunker operations could transition from an additional port call activity to a critical path constraint.

To conclude, this research demonstrates that the effect of the transition to alternative fuels and in particular the segmentation of demand require a drastic reconfiguration of the bunker fleet and the bunker supply chain network. This thesis provides a quantitative framework for anticipating these stated challenges and support suppliers in planning for a service-oriented transition.

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Introduction

80% of global transport is performed by the maritime industry, a share expected to increase annually due to the ongoing increase in demand for transport capacity, resulting in substantial market expansion. However, the industry accounts for 3% of global emissions, and combined with the projected growth, an unsustainable outlook emerges.

This led to the development of a number of initiatives at the international and regional levels focused on mitigating the impact of the maritime sector on the environment. Yet, a lack of coordination between governing entities has led to overlapping and inconsistent regulations, creating a complex framework for shipowners, charterers and operators to operate in. Ultimately, creating uncertainty around the pathway for transitioning to a more sustainable industry.

Despite the uncertainty, the industry acknowledges the inevitability of transitioning to alternative fuels. While a multitude of alternatives have been marked as potential candidates, no single solution has emerged due to varied operational requirements, implementation constraints and scalability limitations. This segmentation introduces additional layers of complexities. Especially in the bunker supply chain, a key part of the maritime supply chain, responsible for the sourcing and distribution of the fuels that enable maritime transport. This introduces the need for diversification within the bunker supply chain due to the direct impact of the expected market segmentation in the marine fuel market, as it directly influences the two main aspects of ship-to-ship bunkering operations.

First, alternative fuels will transform the ship-to-ship delivery process and the corresponding bunker vessels. This due to the need to adapt to the new requirements for accommodating and handling these new fuels with different characteristics and safety requirements. Ultimately, resulting in a shift to purpose-built bunker vessels, designed to handle a single fuel type in contrast to the current compatibility and flexibility of a multi-fuel setup.

Second, the lower energy content of these fuels combined with the expected market expansion, which introduces additional and larger vessels to meet market demand, will require additional larger and longer ship-to-ship operations. This necessitates increased bunkering capacity through larger and additional bunker vessels, while handling extended operational times.

This outlook creates operational uncertainty for bunker suppliers, raising concerns about how day-to-day operations will evolve, whether the current fleet will be adequate in the future years, and what types and numbers of bunker vessels will be required. Questions also arise around the evolution of the supply chain and how demand will shift. These uncertainties have a direct impact on long-term policies aimed at keeping suppliers' service levels consistent. This study, conducted in partnership with Peninsula, attempts to quantify the challenges placed on the maritime fuel supply chain by identifying the significant changes in terms of demand, operations, and the scale of operation required.

2 1. Introduction

1.1. Problem Definition

The segmentation of the bunker market will introduce inevitable changes from a commercial and operational point of view, as demand will shift and diversify. Operational changes and complexities are attributed to the introduction of larger bunker quantities, more frequent supplies and the diverse requirements for fuel compatibility. Commercial changes are to be explained by the shift in fuel types, the demand to expect and a change in the size of operation. However, in order to anticipate these changes, invest timely and maintain the same level of service and maintain the maritime supply chain, a quantified outlook needs to be provided.

By analysing these changes systematically and translating them into a quantitative framework that provides insights into future operational scenarios, bunker suppliers would be enabled to anticipate the changes and possible challenges in future operations. This proactive approach would introduce a mutual benefit, as it would allow operators to transition smoothly to these new and more sustainable fuels and bunker suppliers to anticipate changes in a volatile market due to ever changing regulations.

1.2. Methodology

To address the implications of alternative fuel adoption in the bunker supply chain, this research follows a two step approach that begins with developing a comprehensive practical and theoretical foundation before developing the analytical tools.

First, a comprehensive overview of supporting literature was composed to fully comprehend the current working mechanisms of the bunker supply chain, operational processes and supply chain composition. Additionally, the review will also evaluate a number of research methods from similar research in supply chain analysis and transition studies to identify the most appropriate method of research in the bunker supply chain context.

Based on the foundation developed in the literature review, an analytical model will be developed, where the selected methodology will be implemented to analyse various transition scenarios and provide insights into operational changes, demand patterns and implications for the bunker suppliers in the Gibraltar hub.

1.3. Research Objective and Questions

The main objective of this research is to provide a quantified outlook into the operational implications of alternative fuel implementation in the bunker supply chain, this with a specific focus on the Gibraltar bunker hub due to it prominent presence as a global bunkering hub and Peninsula's centre of operations in this region. This cooperation with Peninsula enables access to real-world operational data and industry expertise, ensuring that the research addresses the practical challenges bunker suppliers face.

To encapsulate all previously stated and desired insights, the following main research question is proposed: What will the implications be of the implementation of sustainable fuels for the bunker industry on an operational level.

Guided by the following sub questions:

- What changes occur in the bunker supply chain in the transition to sustainable fuels?
- How can a model be developed to represent the future bunker supply chain under demand diversification?
- What are the projected operational impacts of different sustainable fuels on key stakeholder operations?
- How effective is a model to quantifying demand and supply chain diversification, and what insights does it provide for future operations?

In order to understand what challenges might be introduced with the transition to sustainable fuels in the bunker industry, a comprehensive overview of the bunker supply chain, possible alternative fuels and research methodologies needs to be established in order to determine potential, feasibility, compatibility and requirements. In the following chapter, an overview of supporting literature is provided in order to support all subsequent parts of the research.

2.1. Bunker Supply Chain

The global bunker supply chain can be broken down into two distinct phases, a global or regional sourcing phase, depending on the size of the operation, and a regional delivery phase [10]. The sourcing phase consists of collecting a specific fuel blend or different types of fuel grades to create the desired blend of fuel itself and delivering it to a regional storage facility. The secondary phase is the distribution of the fuels to the vessel by the bunker supplier. In figure 2.1 an overview of the most common combinations of the supply chain is depicted.

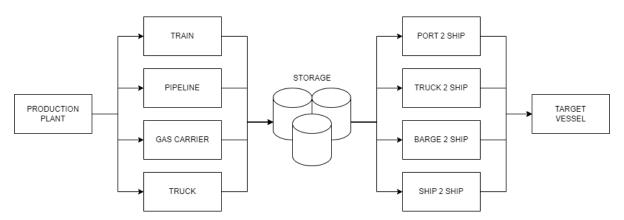


Figure 2.1: Global overview of the bunker supply chain

After evaluating the diagram of the most common combinations in the fuel supply chain, it should be noted that all types of distribution operations are performed, yet the most common type of operation performed is the ship-to-ship and barge-to-ship transaction in large bunker hubs globally. This is to be explained by the fact that these types of operations provide the ability to accommodate large quantities of fuel and offer operational flexibility in terms of location as they allow for a greater operational coverage [10].

2.2. Ship-to-Ship Bunkering Framework

After establishing the significance of the ship-to-ship bunkering operations in the maritime fuel supply chain, a comprehensive breakdown of the operation framework should be provided in order to fully comprehend all aspects that are involved and could be influenced in the transition to more sustainable marine fuels.

2.2.1. Bunkering Hubs

Most ship-to-ship bunkering operations are carried out in global bunkering hubs, which can be a single port, like Singapore, or multiple ports, such as the ARA (Antwerp-Rotterdam-Amsterdam) [53], [10], see illustration 2.2. In these locations, either a single bunker supplier or multiple bunker suppliers serve vessels requesting bunkers. The number of suppliers in a port or region is commonly determined by the amount of bunkering licenses issued for a specific fuel type by the local port authorities. The bunkering operation generally takes place at either an allocated anchorage or at a berth or terminal within the port. Based on location and the availability of infrastructure, these bunkering hubs can be classified into three categories: anchorage, port, and port-and-anchorage hubs. This classification determines how operations are organised among stakeholders, who the stakeholders are, the types of vessels requesting bunkers, and the capacity of these operations.

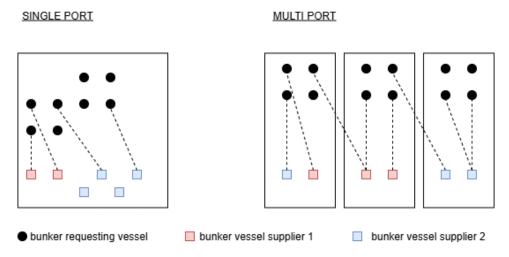


Figure 2.2: Simplified diagram of a bunkering hub

Evaluating global bunkering hubs, the observation can be made that these hubs mostly coincide with ports or regions that are exposed to highly dense marine traffic [34]. The concentrated nature of these bunkering hubs ultimately results in a highly concentrated demand for bunkers in specific locations. In turn, this concentrated demand results in a concentrated number of suppliers operating in these bunkering hubs, providing the requested bunkers to the vessel operators.

The multitude of bunker suppliers operating in these bunkering hubs may vary significantly in scale, covered region, fuel type offerings, bunker supplying vessels and operational organisation. Based on literature and industry insights the variation in fuel type offerings and scale of operation is to be explained by the supply chain configuration of the supplier in the specific bunkering hub [53], [26]. Variations in supply chain setup are to be traced back to access to local production capacity (refineries), storage configurations or the bunkering vessels deployed by the bunker suppliers, varying from a single fuel type offering to multi-fuel type configurations.

2.2.2. Ship-to-Ship Bunkering Process

The ship-to-ship bunkering operation is most commonly performed between a bunker requesting vessel moored in port or at anchorage and a dedicated bunkering vessel. At anchorage or in port bunker supplies may occur simultaneously with other in port processes depending on the fuel type, the port of choice and the bunker requesting client. During the operation a bunker supplying vessel will moor alongside the receiving vessel in order to supply the requested bunkers. The entire bunkering process can consists of a single fuel type delivery or a more complex operation where multiple fuel types are requested by the receiving vessel. Based on the availability of fuel type, required quantity and available bunkering vessels, the operation will either be performed by a single bunkering vessel carrying a single or multiple fuel types or a number of bunkering vessels carrying various fuel types [10].

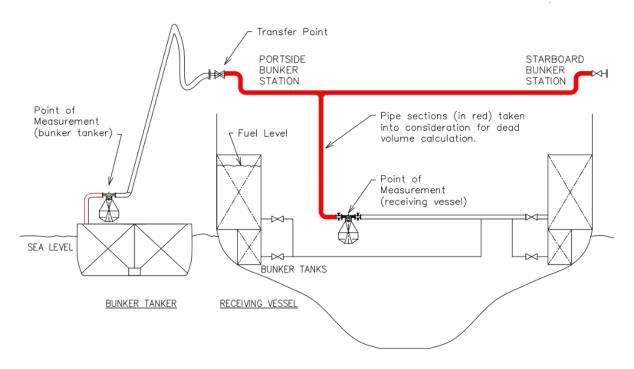


Figure 2.3: Diagram of bunker setup [2]

The transfer process is enabled by a connection with a flexible hydraulic hose between the supplying and the receiving vessel, as illustrated in figure 2.3. The supply process can either be performed by a single connection or multiple connections depending on the bunker station of the receiving vessel and the pump setup of the supplying vessel [10]. The rate of transfer is determined by the rated pressure of the receiving vessels piping system and the material properties of the delivered fuel type, this is to be explained by the various densities of the fuel types requested which influence the pressure introduced in the system when pumping and to mitigate the introduction of air into the fuel mixture, which is referred to as the 'cappuccino' effect within the industry. Highlighting the fact that the operation is dependent on the available infrastructure and the product being transferred. Measurement points can be utilised during the transfer process on either the supplying vessel, receiving vessel or both, yet are not mandatory. Common industry practice is verification of the delivered quantity by fuel level measurements from manholes, hence the reason air needs to be mitigated during the transfer process as additional air might influence fuel level readings and evoke disputes between supplier and client [26].

2.2.3. Ship-to-Ship Bunkering Stakeholders

As bunkering is an integrated subprocess of the global maritime supply chain which requires significant coordination between multiple stakeholders, a stakeholder framework needs to be evaluated that extends beyond the direct parties involved in the transfer process itself. Understanding the broader scope of this ecosystem of stakeholders becomes important for evaluating how alternative fuels will impact the entire bunkering operation and the maritime supply chain on an operational level.

The operational requirements of ship-to-ship bunkering operations create interdependent relationships between four primary stakeholders, each contributing on their own level by facilitating infrastructure or services while all aiming to maximise their own distinct operational priorities.

Bunker Suppliers facilitate the fuel transfer process described in the previous section. Their operations centre around coordinating the complex logistics between the vessel, bunker vessel and loading terminal under the time-sensitive constraints of global maritime operations. Therefore their focus lies on developing reliant and efficient supply chains. However, based on the fact that fuel costs represent 50-60% of the operational expenses of a vessel, cost management becomes equally critical, introducing the need to balance supply chain efficiency and cost-per-unit-delivered to maintain competitive positioning in the market [29], [34].

Lastly, based on the fact that client relationships are not solely based on price, yet on quality assurance and reliability. Bunker suppliers aim to maximise their assets and provide a reliable service in order to retain clients [26].

Ship Operators are the receiving party in the transfer process. Their main focus centres around maintaining reliable sailing schedules and a safe work environment. In general this results in minimising the turnaround times of vessels in port or at anchorage. Stakeholder research in bunkering operations further establishes this as service reliability was the primary differentiator aside from price in choosing a bunker provider, making reliable on time performance rates a key metric in bunkering operations [26], [34].

Terminal Operators provide infrastructure during port-call bunkering operations, where the vessel is moored at a terminal to load or unload cargo. Terminal operators centre their operations on providing infrastructure and services to port calling vessels, therefore their main priority is to maximise the berth allocation and their infrastructure availability [22]. Bunkering operations that may be performed simultaneously or sequentially directly impact their allocation strategies at berth [32].

Port Authorities provide the policies, infrastructure and possibly port services (e.g. towage) for anchorage bunkering calls in or outside of ports and provide infrastructure to enable bunkering in some ports. Based on limited availability of anchorages, berths and terminal availability, ports aim to maximise these assets in a similar way as terminal operators. Therefore their aim is to enable bunker processes with the shortest turnaround time possible while performed in a safe manner [26].

Based on the evaluated framework above the conclusion can be drawn that ship-to-ship bunkering operations create unique yet similar priorities in operations across all stakeholders. The interdependencies created by the simultaneous operations, safety requirements and other external factors result in a need for collaboration between all parties. Especially when these challenges are projected onto the implementation of alternative fuels, as the technical modifications required for the different fuel types could fundamentally alter operational parameters, safety requirements and the interactions between stakeholders outlined above. Furthermore, it could influence how each individual stakeholder will be influenced by the ship-to-ship bunkering operation in general.

2.3. Alternative Fuels 7

2.3. Alternative Fuels

As described in the previous section, the ship-to-ship bunkering operation is integrated in the entire global maritime supply chain and involves a number of stakeholders involved in the operation itself. Implementing new alternative fuels might significantly influence the operation and consequently all stakeholders. In the following section the most promising candidates for alternative fuel types are discussed based on multiple industry reports. This in order to establish all plausible new fuels that might be introduced in the supply chain, how they could integrate and their requirements to be integrated in the maritime fuel supply chain.

Biofuels

Biofuel, also known as B100, originates from biologically renewable resources such as plants, algae or second and third generation food waste, offering flexibility due to its ability to be blended with conventional fuels. The fuel can be classified as a 'drop-in fuel' as it requires minor modifications to be brought into practice, making it an attractive option due to it's low investment cost and barrier of entry [19]. The two most common types of biofuels produced to date are:

- FAME: Fatty Acid Methyl Ester (1st gen.)
- HVO: Hydrogenated Vegetable Oil (2nd & 3rd gen.)

By blending the fuel with conventional marine fuels in different percentages, different emission savings can be achieved, allowing for a gradual implementation [11]. However, high grades of biofuels are required for long-term compliance and deep decarbonisation. High grades of biofuels introduce the risk of bio-corrosion and fuel instability, especially in marine environments, introducing the need for tank lining and type I chemical tanks for transport [11], [12]. In addition, intra-competitiveness with the aerospace and automotive industry will limit availability [11].

LNG & Bio-LNG

Liquefied Natural Gas (LNG) is an already established and proven marine fuel in the industry. Produced from natural gas or derived from renewable sources by refining bio-methane. It is stored as a liquid at cryogenic temperatures (-162°C).

LNG enables a 20-25% reduction in CO_2 emissions on a TtW-basis [11]. It achieves a 90% reduction in SO_x , 85% reduction in particulate matter (PM), and up to 80% reduction in NO_x emissions. Implementing bio-LNG offers a carbon neutral solution on a WtW-basis [23]. However, methane slip during combustion and production emissions reduces its overall climate benefit on a WtW basis, being similar to HFO [63].

The energy density of LNG is approximately 50 MJ/kg being similar to HFO. However, its density as a liquid is 431kg/m³ meaning its storage requires 1.8 times more space than MDO or HFO. LNG's handling, storage, and safety requirements for pressurised storage create a vastly different set of requirements for bunkering operations, introducing additional safety requirements slowing down all procedures.

Methanol

Methanol is a fuel that can be produced from a variety of feedstocks, such as natural gas, biomass, or renewable energy sources, enabling flexible production. The fuel can be stored as a liquid at ambient temperatures, making it an easy to handle fuel. Operations can be performed either on stand alone methanol engines or on dual fuelled engines with a pilot fuel to promote combustion [47].

Methanol offers a 57% reduction in CO_2 emissions, a 99% reduction in SO_x and can cut up to 60% of NO_x emissions on a TtW-basis. Produced from renewables methanol has the ability to cut CO_2 by 95% on a WtW basis. Furthermore, methanol has the ability to be blended with all forms of methanol (grey, blue, green), allowing for a gradual transition in the usage of feedstocks [47], [23].

Due to the fuel handling characteristics methanol has a low barrier of entry for retrofit capabilities, enabling retrofit capabilities with most modern diesel engines [24]. However, the energy density of the

fuel is only 22MJ/kg, requiring additional fuel carrying capacity of around a factor of 2.2 to keep the vessel in the same operational window [48]. Furthermore, the toxicity and high flammability present challenges to the adaptation of the fuel. Ultimately this results in the type II chemical tanks for storage and handling.

Ammonia

Ammonia is a versatile option for the adaptation to cleaner combustion within shipping, as it can be sourced from a variety of production pathways such as natural gas, biomass, or renewables, offering flexible and scalable production. The fuel can be stored pressurised at 8 bar at ambient temperatures or as a liquid refrigerated at minus 30 degrees.

Ammonia offers a 100% reduction in CO_2 on a TtW-basis and has the potential of being net-zero on a WtW-basis (if produced from renewable energy), emits no SO_x and has a significant reduction in NO_x emissions depending on the efficiency of the engine cycle [11]. Incomplete combustion can lead to NO_x -slip, posing operational challenges. NO_x -slip can be avoided altogether with fuel cell usage.

However, ammonia's low energy density of 18.6 MJ/kg requires ships to carry 2.7 times more fuel compared to MDO or HFO [11]. Additionally, its toxicity, corrosiveness, and invisible flame during combustion present safety challenges. Yet, combustion can be promoted by introducing a catalyst such as methanol, circumnavigating some of the challenges presented by methanol and ammonia as a stand-alone fuel [64].

Hydrogen

Hydrogen is another alternative to mitigate emissions. The fuel can be sourced from a variety of production pathways such as natural gas (grey hydrogen), biomass (blue hydrogen), and renewable energy (green hydrogen). It is stored as a compressed gas or in liquid form at cryogenic temperatures (-253°C).

Hydrogen as a fuel offers 100% reduction in CO_2 and SO_x emissions during combustion or in fuel cell applications. NO_x emissions depend on the combustion method but can be mitigated with advanced technologies or avoided altogether in fuel cell [11].

Hydrogen has a high energy density of 120 MJ/kg (by mass), but a low volumetric energy density of 8.5 MJ/L (by volume). Resulting in significant challenges in fuel-storage (approximately 4.7 times more than HFO/MDO). This presents challenges for long-distance maritime operations, as onboard storage and infrastructure need substantial adaptation.

Nuclear

Powered by uranium or thorium as a fuel, Nuclear power eliminates CO_2 , SO_x , and NO_x emissions entirely during operation. Nuclear energy's high energy density allows vessels to operate for extended periods without refuelling, circumnavigating fuel supply chain dependency entirely [11].

However, due to the high capital expenses for the implementation of a reactor and the usually high energy output, it is unsuitable for most use-cases in the industry due to redundancy. Additionally, regulation and public concern pose challenges as well [4]. It can be viable option for VLBC, ULCC and offshore vessels as these usually have high hotel loads.

2.4. Fuel Viability 9

2.4. Fuel Viability

Due to the various options available to decarbonise the maritime industry, widespread analysis has been sparked to determine the most viable candidate. However, evaluating all options, the conclusion can be drawn that there is no 'one-size fits all' solution, as it depends on a mix of operational, technical, economical and environmental factors. Evaluating academic and industry reports, a number of frameworks have been proposed to asses fuel suitability:

- **Techno-economic models**: frameworks that compare fuels based on factors such as lifecycle emissions, fuel cost and availability [20], [33].
- **Feasibility matrices**: frameworks that evaluate (score) fuels in a matrix based on factors such as retrofit capabilities and/or costs, handling requirements and safety [57].
- **Scenario-based roadmaps**: frameworks that evaluate/project fuel adoption based on regulatory pressures and/or market conditions [50].

While these various approaches provide a vast number of insights on all fuel types, a more operationally constrained framework would benefit this research, specifically focussing on:

- **Energy demand**: Evaluate the required energy based on vessel parameters such as size, type and sailing route deployed on.
- **Scalability**: Evaluate the scalability of a fuel, defined as the combined feasibility of sourcing transporting and distribution at scale in the maritime fuel supply chain context.

The proposed method introduces an application-specific, bottom-up framework for fuel selection, based on individual energy demand and fuel scalability. Compared to top-down strategies, the proposed method aligns fuel choice with operational and infrastructure constraints, making it well-suited for supply chain analysis and bunker demand modelling. By segmenting the fleet into short-sea and deep-sea categories based on technical and logistical feasibility rather than abstract preference, the framework enables a more direct planning of future fleet composition and the required bunker infrastructure.

The proposed framework builds on prior work such as Smith et al. [56] and the IEA's route specific assessments [iea2022], by projecting a similar segmentation framework onto the evaluation of the bunker supply chain of the hub of Gibraltar. Here vessel diversity, demand uncertainty and infrastructure variation are influential factors [53], making a bottom-up and operationally constrained approach necessary for accurate scenario development.

Short Sea Shipping

Characterised by small to medium vessels, capable of navigating maritime choke holds such as the Suez and Panama Canal and mostly responsible for the transportation of goods on a regional level [31]. For these vessels the following alternatives are to be considered as the most suitable alternatives: biofuels and methanol. This is based on the following assumptions:

- **Energy demand**: deployed on shorter routes, the total energy requirement is lower for operations performed [31], [18].
- Routing: deployed on shorter coastal routes, these vessels have more flexible options for refuelling allowing the accommodation of less energy dense fuels [53].
- Technological Scalability: based on the size, the barrier of entry for scaling and successfully implementing the technology becomes smaller [47].
- **Compliance**: often constrained to regional trade, regional regulations apply. Necessitating short and long term compliance [16],[1].

Deep Sea Shipping

Consisting of large vessels such as ULCC and ULBC that transport goods on a global scale, deep-sea liners have a different set of requirements for feasible integration of alternative fuels. For decarbonising this segment of the maritime market, the following fuels are to be considered as the most viable alternatives for deep-sea applications: ammonia, methanol and LNG. This selection is based on the following assumptions:

- Energy Demand: deployed on longer routes and with higher daily energy consumption, the total energy necessitated for transport is significant, requiring either energy dense fuels or fuels with the ability to be blended [31].
- Routing: depending on the vessel type long sailing trajectories apply, limiting access to bunkering facilities [31]. Additionally it introduces the need for stable fuel types, due to the longer voyages on which these vessels are deployed.
- Global Availability: with the greater introduced energy demand, greater volumes of fuel are needed not only per vessel but sufficient availability of a specified fuel is necessitated on a global scale [40].

Based on the most prominent discussed operational requirements for the short-sea and deep-sea shipping segments, the following fuel evaluation matrix was composed to determine the most plausible/viable fuel applications in figure 2.4. The fuel evaluation matrix is limited to the most viable alternatives and highlights the supporting characteristics needed for the specified segment.

FUEL	ENERGY [HFOeq]	IMPLEMENTATION AVAILABILITY	USECASE SCALABILITY	STABILITY	AVAILABILITY/ SCALABILTY	DECARBONISATION EFFECT
BIOFUEL	~ 1.1 - 1.2	DROP-IN DIRECT	LIMITED	BIO-CORROSION	LIMITED	100% WtW
METHANOL	~ 2.2	DIESEL RETROFIT	SMALL TO LARGE SCALE	STABLE	GLOBALLY SCALABLE	60% - 90% WtW
AMMONIA	~ 2.7	NEW BUILD	HIGHLY SCALABLE (THEORETICALLY)	STABLE	GLOBALLY SCALABLE	100% WtW
LNG	~ 1.8	NEW BUILD	HIGHLY SCALABLE (PROVEN)	STABLE	GLOBALLY AVAILABLE	20-40% TtW
SHORT SEA SHIPPING DEEP SEA SHIPPING						

Figure 2.4: Fuel Selection Matrix

Evaluating the viability matrix, the observation can be made that multiple fuel types share the same operational requirements for both segments highlighting the viability for multiple fuel types per segment. Based on the results from the operational requirements the following fuel segmentation is proposed for applicability in an operational context for ship operators:

- Short-Sea: are most likely to adopt biofuels and methanol in the fuel mix in the energy transition
- Deep-Sea: are most likely to adopt methanol, ammonia and LNG in the energy transition

Based on this segmentation the conclusion can be drawn that ship owners will have a variety of options available to decarbonise their operations. However, as previously mentioned and illustrated in the fuel selection matrix 2.4, this will mostly depend on operational factors, indicating a possible diversification in fuel adoption strategies.

2.4. Fuel Viability 11

To operationalise these projections, the segmentation between short-sea and deep-sea shipping was projected onto commonly used vessels classes. This mapping, based on DWT and data from Peninusla, offers a more tangible perspective on fuel compatibility (table 2.1) [53], [15].

Vessel Type	DWT Range	Bio	Methanol	Ammonia	LNG
Feeder /	10,000–25,000	Yes	Yes	No	No
Feedermax	DWT				
Baby Bulker / NN	10,000–25,000	Yes	Yes	No	No
	DWT				
Handysize (Small	10,000–35,000	Yes	Yes	No	No
Handy)	DWT				
Handymax /	35,000–60,000	No	Yes	Yes	Yes
Supramax	DWT				
MR / MR1 / MR2	45,000–55,000	No	Yes	Yes	Yes
	DWT				
Panamax /	60,000–85,000	No	Yes	Yes	Yes
Kamsarmax	DWT				
Aframax / LR Type	75,000–120,000	No	Yes	Yes	Yes
	DWT				
Post-Panamax /	85,000–120,000	No	Yes	Yes	Yes
Mini Capesize	DWT				
Mini Capesize	100,000–130,000	No	Yes	Yes	Yes
	DWT				
Suezmax	120,000–200,000	No	Yes	Yes	Yes
	DWT				
Capesize / VLOC	130,000–200,000+	No	Yes	Yes	Yes
	DWT				
Newcastlemax	180,000–200,000	No	Yes	Yes	Yes
	DWT				
VLCC	150,000–320,000	No	Yes	Yes	Yes
	DWT				
ULCC	>320,000 DWT	No	Yes	Yes	Yes

Table 2.1: Vessel Types and Fuel Compatibility based on DWT classification from [15].

Industry Alignment

While the vessel-based segmentation provides a technical outlook on fuel compatibility, it is useful to compare/validate these assumptions with current industry reports. Table 2.2 provides an overview of how maritime forecasts anticipate fuel adoption across the various segments and validates the previously discussed segmentation.

Fuel	Short-Sea / Small Vessels	Deep-Sea / Large Vessels	Industry Insight (key takeaway)
Bio	Yes – Preferred (drop-in) [11]	No – Costly at scale [11]	Biofuels seen as drop-in for near term, especially in short-sea shipping [21].
Methanol	Yes – Easy retrofit [21]	Yes – Growing adoption (Maersk, COSCO) [15]	Methanol emerging as a cross-segment contender [49].
Ammonia	No – Toxicity/safety concerns [21]	Yes – High energy density and long-haul suitability [61]	Suitable for deep-sea, bulk, and tankers [61].
LNG	No – Storage inefficiency [33]	Yes – Transitional fuel for larger vessels [30]	Still dominant transitional fuel for deep-sea newbuilds [30].

Table 2.2: Industry-aligned fuel adoption outlook by vessel segment.

2.5. Implications On The Ship-to-Ship Bunkering Framework

As illustrated in the previous section 2.4, a single and universal transition path will remain elusive. Instead, market segmentation is to be expected, with fuel selection based on vessel size, vessel type, operational profile, regional fuel supply, and costs. Ultimately, this will result in specific market segments embracing different fuel options based on their unique constraints. However, based on the discussed characteristics of all viable candidates, a number of general implications can be deduced that will impact the ship-to-ship bunkering framework.

A shared challenge across all viable alternatives is their lower energy density compared to conventional fuels, which in turn will result in a significant increase in individual demanded fuel quantity in order to maintain identical or similar operational windows. This translates into shipowners facing trade-off between fuel storage, cargo capacity and deployed voyages. In many cases this will result in larger or additional fuel tanks, reducing the cargo space or lead to increased vessel sizes, especially for deep-sea shipping where long voyages are performed on a single fuelling operation. Short-sea operations could see more frequent refuelling patterns as shipowners aim to retain as much cargo space as possible to minimise cost per transported capacity.

Additionally, when assessing the handling and storage needs of these new fuels, it becomes apparent that they vary considerably from each other: LNG and Hydrogen introduce the need for cryogenic storage, ammonia and methanol require corrosion-resistant and/or pressurised storage and high grades of biofuels introduce the need for tank liners due to the challenge of bio-corrosion and fuel instability. In turn this will result in significantly different infrastructure per operated fuel type aboard vessels (bunkering station, operational procedures and storage infrastructure), resulting in a greater variety of operational procedures. When projected onto the ship-to-ship bunkering framework, fuel specific compatibility is introduced with this diversification of demand.

This fuel specific compatibility has a significant and immediate impact on the bunker supply chain infrastructure, as the current fleet of conventional bunkering vessels, storage facilities and safety procedures will not be compatible with all the alternatives expected to enter the market. Instead, a fleet of fuel-specific bunker vessels, each designed to meet their unique containment, pressurisation, insulation and safety standards specific to the intended fuel it carries is to be expected. Evaluating the most viable fuel types outlined in section 2.4, the following compatibility requirements are introduced in order to offer all fuel types [11], [21]:

FUEL	TANK MATERIAL	STORAGE	EQUIPMENT	VESSEL CLASS
BIOFUEL	TANK LINERS	LIQUID	STIRRING & HEATING	CHEMICAL CLASS I
METHANOL	ANTI-CORROSIVE	LIQUID	ANTI-LEAK FLAME-MITGATION	CHEMICAL CLASS II
AMMONIA	HIGH-INTEGRITY	LIQUID/ PRESSURISED	RELIQUEFICATION ANTI-LEAK TOXIC-EXOPURE	~ GAS CARRIER
LNG	HIGH-INTEGRITY	CRYOGENIC	RELIQUEFICATION VENTING	LNG CARRIER

Figure 2.5: Overview of bunker requirements per selected fuel type

Evaluating the bunker vessel requirement matrix 2.5, the observation can be made that across all fuel types little overlap is to be found in terms of requirements and specified vessel classes provided by classification societies. Ultimately, this will result in the inevitable requirement of fuel-specific bunkering vessels or highly complex multi-fuel combinations.

As a result, diversification of the bunker fleet will be inevitable with the introduction of these fuel-specific vessels, leading to an increased complexity in fuel logistics, the requirement for redeveloping the supporting infrastructure, and an increased complexity in operational protocols in terms of fuel handling and safety, impacting the entire bunker supply chain and consequently the global maritime supply chain.

The complexity of this diversification becomes particularly apparent when examining the compatibility requirements between bunker supply vessels and receiving vessels for alternative fuels. The compatibility matrix presented in the figure 2.6 demonstrates how market segmentation could alter the existing ship-to-ship operation framework, in particular when balancing supply capabilities with demand requirements. The industry could be forced to transition from a unified single-asset model to a diversified five-vessel-type system, each serving distinct market segments within the maritime fuel market.

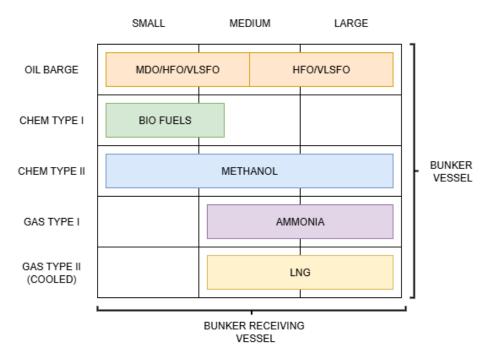


Figure 2.6: Compatibility Diagram of Bunker supplier and receiver

This diversification extends beyond immediate operational challenges during ship-to-ship bunkering operations. When examining the broader infrastructure implications, a comprehensive analysis of the complete bunker supply chain reveals a potential fragmentation from one integrated system into five separate, independent supply chains. Each chain will require specialised infrastructure, dedicated storage facilities, unique handling procedures, and distinct safety protocols, representing a fundamental shift in organisation of operations for large bunker suppliers worldwide.

This highlights the primary challenge of integrating sustainable fuels into the maritime supply chain: the shift from a uniform and integrated, multi-fuel-based system to a network of parallel, fuel-specific supply chains. Each of these individual supply chains will require dedicated infrastructure, fuel-specific bunkering vessels and operational procedures, redefining the current bunker supply chain and the ship-to-ship bunkering framework. This challenge is further amplified by the need to synchronise these parallel systems within existing port operations, where space, infrastructure and operational schedules are already highly constrained. Aside from infrastructure, performance, vulnerabilities and resilience of these projected supply chains should be evaluated, particularly under the conditions of fluctuating demand and marine traffic typical to a bunkering hub. Understanding how these systems perform within the broader maritime network and among diverse stakeholders is therefore essential and this research aims to quantify these changes.

2.6. Research Gap

The maritime industry's shift towards alternative fuels presents significant challenges in infrastructure, supply chain management, and operations, particularly at the port level. While existing literature offers valuable insights through techno-economic comparison and high-level scenario modelling, they often fall short in representing the dynamics of bunkering, infrastructure compatibility and multi-fuel supply chain coordination.

Most existing literature simplifies the bunkering transition by assuming homogenous fuel adoption, uniform demand across vessel types and static infrastructure readiness. These assumptions limit their ability to guide decisions on bunker-hub specific infrastructure planning, bunker fleet composition or the quantification of parallel supply chains. In addition, current frameworks generally apply generic assessments of fuel adaption. This often leads to exclusion of taking into consideration of how vessel-level energy demand and refuelling opportunities influence the technical and logistical feasibility of adopting specific fuels. particularly when they vary across the two main segments of shipping.

Several methods have been applied to explore maritime supply chains, which include:

- Scenario-based techno-economic models: aimed at offering macro-level insights of systems but often lack environmental and stakeholder behaviour detail.
- Linear and network optimisation models: aimed at addressing routing, transport capacity or infrastructure requirements but do not capture vessel interactions or system feedback.
- Simulation-based models: aimed at providing higher operational detail, yet are often disconnected from fuel adoption frameworks or demand segmentation (focus on a single fuel or process).

What is missing is a modelling framework that dynamically links the segmented fuel demand with the constraints and behaviours of future bunkering hubs and fuel supply chains. What the framework should be incorporating/taking into account:

- · the diversity and variability of vessel operations in bunkering hubs
- · the infrastructure requirements of multiple fuel types
- the dynamics of ship-to-ship bunkering operations in bunkering hubs.

This thesis aims to develop such a framework, building on the fuel market segmentation and bunker supply chain considerations in the ship-to-ship bunkering context, outlined in the previous sections. The following sections will define the modelling method, objectives and structure used to evaluate the impact of a multi-fuel maritime context on the bunker supply chain.

2.7. Method

The modelling framework selected to evaluate the future of bunker supply chains under a multi-fuel transition scenario should support the main goal of this research: to assess how the maritime fuel supply chain can be maintained reliably with alternative fuels, while accounting for fuel diversity, infrastructure and operational limitations. The model should replicate the key dynamics of a bunkering hub, described in section 2.1. In particular, the dynamics of the ship-to-ship bunkering operation in the context of segmented fuel demand, fuel compatibility constraints and specialised supply infrastructure. To capture these important details, the modelling approach should reflect the following principles:

- **Fleet diversity**: account for a diverse fleet, segmented by operational constraints (short-sea vs. deep-sea) and their respective energy demand.
- Fuel diversity: account for multiple fuel types, each with unique bunkering and compatibility requirements.
- Bunker fleet performance: account for achieving vessel servicing within realistic time and capacity constraints. In addition, it should quantify the effect of fleet composition on system wide performance and individual bunker vessel performance.

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Based on the stated requirements, the model should not only simulate bunker hub-level refuelling operations, but evaluate the relative performance of different fleet configurations and bunker vessels as well. This enables the development of a comprehensive understanding of individual supply chain performance and fleet requirements. In order to develop the desired framework, the following section evaluates recent and relevant modelling approaches for supply chain analysis. This in order to apply the most relevant modelling technique to account for all the stated requirements.

2.7.1. Supply Chain Modelling Techniques

In order to develop an effective quantitative framework that meets the requirements for modelling fleet composition and performance evaluation, a comprehensive review of existing literature on supply chain modelling techniques is required. The main goal is to determine how the bunker supply chain can be reliably maintained with the integration of alternative fuels, taking into account fuel diversity, infrastructure, compatibility and operational constraints. The complexity of the transition to sustainable fuels, which requires a reorganisation of the bunker fleet and supply chain network, results in an asset allocation problem: determining the required types and respective number of bunker vessels needed for future operations.

As a result, recent literature on supply chain modelling techniques for asset allocation problems have been evaluated and can be broadly classified into three categories for strategy: analytical models, system-level simulation approaches, and agent-level simulation frameworks. When applied to the context of maritime logistics systems, each method offers its own set of pros and disadvantages.

Mathematical Formulation Approaches

Analytical methods represent the most commonly applied approach to fleet composition and deployment problems in maritime logistics. Linear programming, mixed-integer programming, and their variants have been extensively applied to fleet sizing and capacity allocation decisions [13], [39]. These mathematically formulated models excel at determining globally optimal solutions under well-defined problem constraints, providing convergence guarantees and sensitivity analysis options to support the validity of the obtained solution [44].

However, pure optimisation approaches face significant limitations in the bunker supply chain context. First, the assumption of perfect information inherent in a deterministic approach stands in contrast to the stochastic and dynamic nature of bunker hubs described in section 2.1, especially in combination with the shifting demand of the energy transition [3]. Second, optimisation models assume centralised decision-making where a single entity controls all system variables, fundamentally misrepresenting the bunker supply chain where multiple independent stakeholders make autonomous decision based on individual objectives [34], [58]. Third, these models fail to capture the dynamics of ship-to-ship bunkering operations and time-varying demand patterns.

System-Level Simulation Approaches

System dynamics modelling accommodates for the integration of complex dynamics such as feedback loops and delays within supply chain systems. This approach enables to capture aggregate system behaviour and non-linear relationships that are typically associated with supply chains over extended timelines [59], [25]. However, system dynamics operates at aggregated level system where individual stakeholder behaviour and individual operational behaviour are obscured, treating system components as homogeneous entities [42]. This abstraction eliminates the vessel-specific operational details and stakeholders interactions that are critical in bunker fleet composition decisions.

Discrete-event simulations provides more granular modelling of individual operational processes while accommodating stochastic elements characteristic of maritime logistics. This approach effectively represents fluctuations in market conditions and operational variability including vessel arrival patterns, service variability, and resource allocation conflicts [36], [7]. Discrete-event simulation can capture the operational complexity of ship-to-ship bunkering, including queue dynamics, service time variations, and capacity constraints. However, conventional discrete-event simulations employ static decision processes and fixed sequential operational parameters that fail to capture the stochastic decision processes characterised in the system described in section 2.1 [51].

Agent-Level Simulation Approach

The stakeholder framework described in section 2.1 indicates an asymmetry in operational structure among supply chain participants. The bunker supplier operates as a collection of individual vessels that continuously adapt their behaviour on fuel demand and service requirements, due to their role as a service provider. In contrast, other stakeholders (vessel operators, terminal operators and port authorities) maintain consistent operational frameworks enforced regulatory requirements, established infrastructure constraints and optimised operational cycles per adopted fuel technology [7], [46].

Agent-based modelling provides the necessary provides the necessary framework for representing this mixed system of adaptive and non-adaptive entities. In this context, individual bunker vessels function as agents with predetermined fuel type capabilities, capacity constraints and operational parameters making decisions regarding operational execution based on assigned objectives [37], [8]. Complex system behaviour is created by the interactions between the various bunkering vessels and the static operational patterns of other stakeholders, creating realistic representations of resource allocation and operational conflicts.

This approach captures the three required aspects absent in the other evaluated modelling techniques. First, it represents the diversity in capabilities, operational characteristics and performance constraints of various bunker vessels for various fuel types that characterise real bunker fleets. Second, it models the effects of individual vessel operations on system-wide performance, including queue formation, service reliability and capacity utilisation patters. Third, it provides the simulation framework within which fleet composition decisions can be evaluated and/or optimised based on operational performance feedback. Therefore the conclusion can be drawn that agent-based can directly address the fuel transition challenge and should be the appropriate modelling technique for the outlined problem.

2.7.2. Optimising Agent-Based Discrete Event Simulation

While the agent-based discrete-event simulation effectively captures the operational dynamics and interactions, the core research challenge requires to determine optimal fleet compositions under various fuel demand scenarios. This introduced the need for the integration of optimisation capabilities that allow for adaptations in fleet composition in response to performance feedback.

Multi-Objective Framework

The stakeholder framework demonstrates that bunker suppliers face a multi-objective optimisation problem characterised by three primary components: maximising asset utilisation, maximising capacity utilisation and maintaining service reliability across various supply chains. Industry surveys indicate that service reliability takes priority over cost in supplier-client relationships [34],[26]. When projected onto scenarios where alternative fuels enter the market with distinct operational characteristics and infrastructure requirements, suppliers must adapt fleet composition to ensure reliable service levels while avoiding redundant assets.

Therefore, the optimisation problem becomes determining the minimal fleet composition that maintains acceptable service levels across all fuel types while maximising individual asset utilisation. Ultimately, this becomes a constraint satisfaction problem with performance thresholds rather than unconstrained optimisation.

Performance-Bounded Optimisation Framework

The ship-to-ship bunkering framework exhibits fundamental efficiency thresholds imposed by physical constraints (vessel capacity, transfer rates, infrastructure), operational limitations (fuel handling protocols) and market dynamics (demand variability) [26]. These system level-constraints create performance boundaries beyond which fleet composition adjustments cannot improve service reliability.

These efficiency thresholds enable performance-bounded optimisation that utilises system performance metrics rather than attempting to mathematically formulate the underlying dynamics [43], [66]. This approach recognises that bunker supply chains operate within the bounded feasibility regions where service reliability and asset utilisation reach natural limits imposed by infrastructure and operations. Therefore the optimisation objective transforms into identifying fleet compositions that operate near these efficiency thresholds while maintaining service reliability above acceptable levels.

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Gradient-Based Fleet Optimisation

The performance-bounded characteristics of the bunker supply chain align with gradient-based optimisation properties, as the outlined system cannot indefinitely reduce fleet requirements beyond the limits imposed by the infrastructure and satisfy service reliability constraints [6]. This characteristic enables iterative adjustments in fleet compositions based on performance indicators derived from simulation outputs until locally optimal configurations are achieved within the feasible decision space [9].

This output-based approach transforms the fleet composition challenge into a dynamic programming problem where optimal configurations for specific demand scenarios are determined through iterative optimisation cycles [5]. The system constraints and reliability thresholds provide natural stopping criteria when further fleet reductions would deteriorate service reliability levels. A review of recent literature, applying a similar hybrid-optimisation approach, validates the effectiveness for asset allocation problems in supply chain systems [66], [45].

Proposed Strategy Framework

The hybrid simulation-optimisation approach would operate on an evaluation-cycle basis, as illustrated in figure 2.7. In each iteration a simulation is performed using a certain fleet composition. The system provides returns performance indicators such as service time and asset utilisation after each simulation. Based on the obtained results, the optimisation module modifies the fleet composition and feeds it back into the simulation. This process is repeated until a near optimal configuration is achieved for each fuel type.

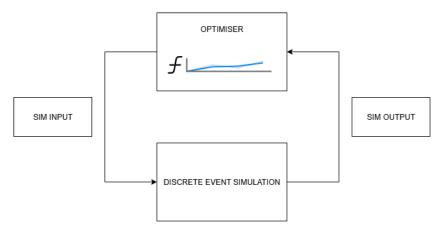


Figure 2.7: outline of proposed strategy

This framework would incorporate three capabilities that are often absent in reviewed approaches:

- 1. **Operational realism**: the simulation module enables the framework to closely replicate actual stakeholder behaviour, compatibility constraints and ship-to-ship bunkering dynamics.
- 2. **Adaptive optimisation**: the optimisation module enables the framework to respond to changing fuel demand by iterative adjustments in fleet composition.
- Performance evaluation/validation: key output metrics enable the framework to quantify the system's ability to maintain service reliability across multiple fuel types and evaluate individual performance.

By linking segmented fuel demand to infrastructure requirements and constraints on an operational level, this framework directly addresses the outlined research gap. It offers a structured, scenario- and bottom-up approach to determining how the bunker supply chain may need to evolve in response to fuel demand diversification.

Model

3.1. System and Model Architecture

This section outlines the structure of the framework and the implementation. It includes the system architecture, essential assumptions and discusses the input and output parameters.

3.1.1. System Description

The system represented in the simulation is the bunker supply chain in the Strait of Gibraltar, which consists of several actors and dynamics. However, evaluating the entire system, two distinct phases can be determined in the supply chain: a loading-phase where the bunker vessel gathers product from the terminal and a supply-phase where the same bunker vessel distributes the product among bunker receiving vessels. A general overview of the system can be seen in figure 3.1 below.

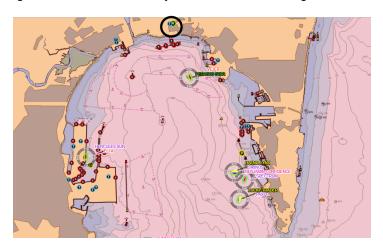


Figure 3.1: Overview of the Gibraltar Bunkering Hub [52]

The **loading-phase** consists out of the interaction between the bunker vessel and the loading terminal, the Cepsa refinery circled in black in figure 3.1, where bunkering vessels gather various grades of product from the refinery. This interaction is mostly dependent on two factors: terminal availability and product availability. The loading-phase will be defined as the refuelling process in the structuring of the simulation and from this point onwards will refer to the corresponding phase of the supply chain.

The **supply-phase** consists out of the interaction between the bunker vessel and the bunker receiving vessel at anchorage, circled in gray in figure 2.1. The operation is dependent on a number factors such as the fuel-type, the quantity and the receiving rate of the vessel requesting bunkers, as outlined in section 2.1. The supply-phase will be defined as the supply process in the structuring in the simulation and from this point onwards will refer to the corresponding phase of the system operation.

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3.1.2. Agent Behaviour and Interactions

According to the stakeholder framework in section 2.1 and the system description from the previous section, the simulation must include five main agents. Each of these agents should have certain attributes, behaviours, interaction patterns, and processes to accurately represent the environment discussed earlier. The following subsection will discuss all these required components and their core processes.

Terminal

The terminal will act as the access, storage and production point of the corresponding fuel types for the bunker vessels to distribute during operation. The terminal will have two processes running simultaneously, the production process, which will create product to be distributed in the system (figure 3.2) and an allocation process, responsible for managing gueues and terminal loading slots (figure 3.3).

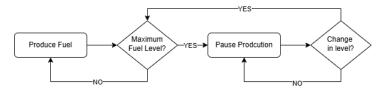


Figure 3.2: Closed production loop

Based on available information, the operational profile of the Cepsa refinery, highlighted in the system description, was determined to be continuous [65], therefore a production loop was chosen as process. The production loop as depicted in figure 3.2 is mathematically formulated as the following function in terms of level of availability in the simulation environment per refinery entity:

$$l_f(t) = \begin{cases} l_f(t-1) - d_f(t) + r_f, & l_i(t) < c_f \\ c_f - d_f(t), & l_f(t-1) > c_f \end{cases}$$

Where:

f: Fuel type

 r_f : Production rate for fuel type f formulated as $r_f = t_f * \Delta_{sim}$ where t_f is the average daily production and Δ_{sim} is the time step of the simulation

 c_f : Storage capacity for fuel type f

 $d_f(t)$: Demand for fuel type f at time t

 $l_f(t)$: Level of fuel type f in storage at time t

The terminal class will initiate with the previously mentioned properties in terms of production rate, storage capacities and fuel types. In addition, terminal capacity needs to be defined as well, this in order to define the number of vessels that can be accommodated for refuelling simultaneously. When the terminal is at full capacity a queue will be handled as described in 3.3. Queue management will be performed using a First in, First Out technique, preserving the sequence of arrival at the terminal.



Figure 3.3: Terminal allocation process diagram

Within the environment, a classification can be made between 4 types of terminals: fossil fuels (MDO, HFO, VLSFO), LNG, ammonia and methanol terminals. These are all attributed to their individual classes due to the segmentation of infrastructure outlined in chapter 2.

Vessel

The vessel will initiate all other processes in the simulation, as this process interacts with the bunker vessels who will interact with the vessel and terminal. The vessel is initiated with a single process, requesting resources from the environment until a bunker vessel is allocated and the delivery is processed. A simple overview of this process can be seen in figure 3.4 below.

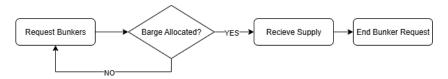


Figure 3.4: vessel process diagram

When initiated the vessel class is attributed with a number of key specifications needed in all subprocesses to replicate the bunkering process and market conditions.

- **size:** when initiated the vessel class will be attributed with a random size class i drawn from the vessel sizes distribution vector \vec{p} , which was derived from the historical data from PTA and S&P Mint, see appendix A.
- type: based on the allocated size of the vessel the vessel type will be defined based on the vessel
 type distribution of each size class drawn from row i of the matrix C, this distribution was obtained
 from the fleet register and S&P Mint, see appendix A.
- fuel: based on size and type a specific fuel type will be allocated to the vessel class, defining its compatibility. See appendix A.
- quantity: based on the previously allocated vessel size, the quantity demanded by the vessel will be drawn from a deal size matrix $Q_{f,i}$ for the corresponding vessel size and fuel-type, see appendix A.
- **receiving rate:** based on the type of vessel *j* the corresponding receiving rate will be allocated based on the fuel type *f* and vessel type *j* from the matrix *R*, where *f* represents the column for fuel type and *j* the type of vessel, please see appendix A.

Vessel Generator

In order to replicate the current market structure a subprocess is initiated in the environment responsible for generating the correct number of bunker enquiries. This is achieved by modelling the inter-arrival times of vessels as a stochastic process. T_i denotes the inter-arrival time between the i-th and (i+1)-th vessel. The model assumes:

$$T_i = LogNormal(\mu_a, \sigma_a^2)$$

where μ_a and σ_a are the log-scale mean and standard deviation estimated from the historical market data (see appendix A). The arrival rate can then be approximated as:

$$\lambda_s = \frac{1}{\mathbb{E}[T_i]} = \frac{1}{\exp(\mu_a + \frac{\sigma_a^2}{2})}$$

This formulation allows vessel arrivals to be spaced over time, while capturing the variability of demanded bunker enquiries. The subprocess follows the logic illustrated in figure 3.5.

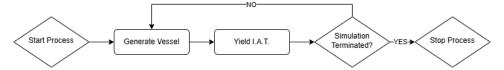


Figure 3.5: vessel generation flow

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Bunker Vessels

The bunker vessels will act as the connection between the terminal and the vessels requesting bunkers, by delivering the required fuel type in the desired quantities to the vessels. Evaluating bunker vessels, the conclusion could be drawn that they all vary in size, setup and specification. However, a classification can be applied to liquid & gaseous bunkering operations, due to the inherent differences of the fuel handling requirements. The same classification is applied in the system, resulting in a distinct liquids and gas bunkering vessel.

Liquid bunkering vessels will consists of a multi-tank and multi-compatibility specification. This results in bunker vessels with the ability to carry various types of products simultaneously. In the simulation the number of tanks, tank size and product per tank are allocated. See figure 3.6 for an simple overview of a possible the tank setup.

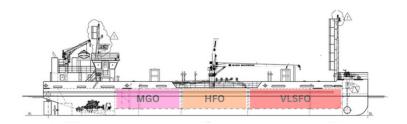


Figure 3.6: simplified structure of a liquid/conventional bunker vessel [54]

Gas bunkering vessels will consist of a single or multi-tank specification with a single fuel compatibility. This results in a bunkering vessel able to carry a single fuel type. This is mostly due to the different storage handling requirements. In addition this vessel class will be equipped with an additional process, simulating the boil off gases that occur during storage. See figure 3.7 for an simple overview of a possible the tank setup.

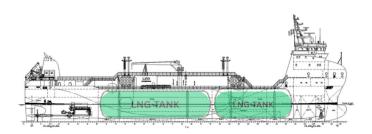


Figure 3.7: simplified structure of a gas bunker vessel [28]

Supply process both class types will follow the same supply logic when allocated to a vessel requiring bunkers. However, during the process the classes will draw process durations from distributions allocated to liquid or gas operations, which were derived from the operational logs, see figure 3.8 for a process overview.

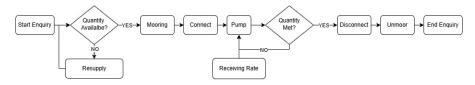


Figure 3.8: overview of the supply process by the bunker barge

When translating this process to a discrete timeline in the simulation, the following mathematical description is formulated in order to yield the correct service time by the bunker vessel for delivering quantity q:

$$T_{\text{service},f} = \begin{cases} s(q,r) + 2t_m + 2t_c + t_s + r(q_r, r_b), & l_f < q \\ s(q,r) + 2t_m + 2t_c + t_s, & l_f > q \end{cases}$$

The individual components are given by:

$$s(q, r_{f,j}) = \frac{q}{r_{f,j}}, \quad r(q_r, r_b) = \frac{q}{r_b} + 2t_m + 2t_c + 2t_s$$

where:

- $T_{\text{service},f}$ is the total service time for the bunkering operation for fuel type f.
- l_f the fuel level of requested fuel type f.
- $s(q, r_{f,j})$ is the pumping time, with q the quantity and $r_{f,j}$ the receiving rate for fuel type f and vessel type j.
- t_m is the mooring or unmooring time for STS-operations, drawn from the distribution for mooring and unmooring of the corresponding bunkering type.
- t_c is the connecting or disconnecting time for STS-operations, drawn from distribution for connecting and disconnecting of the corresponding bunkering type.
- t_s is the sailing time between bunkering operations, drawn from the distribution of the corresponding bunkering type.
- $r(q_r, r_b)$ is the resupply time, with r_b the barge resupply rate for quantity q_r for a complete resupply.

In addition to the supply process, the bunkering vessel also partakes in a pro-active bunkering strategy. This ultimately results in the vessel automatically engaging in the resupply process below a specified fuel-level threshold. This threshold has been specified as $t_{fl,f}$ for fuel type f which is derived from the lower quartile of the combined probability of the quantity matrix $Q_{f,j}$ and the vessel size probability vector \vec{p} . This process is aimed to trigger a resupply for a non-operational bunkering vessel when 75% of possible bunker enquiries can not be fulfilled by current fuel levels on board the vessel, this is in line with Peninsula's operational strategy. This is determined by calculating the following distribution:

$$\tilde{Q}_f = \sum_{j=1}^J p_j \cdot Q_{f,j}$$

The calculated distribution allows to determine the fuel-level threshold, which is defined as the lower quartile of \tilde{Q}_f for specified fuel type f:

$$t_{fl,f} = \mathsf{Q}_1(\tilde{Q}_f)$$

The process logic for this subprocess is outlined in figure 3.9, which first verifies that the vessel is non-operational before performing the threshold check for the bunkering vessel.

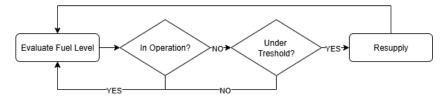


Figure 3.9: Fuel Evaluation Loop

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Barge Pool

The final class implemented in the scheme is the barge pool. Representing several bunker operators who assign their boats to nominated bunker enquiries. The barge pool class will receive the vessel's inquiry and assign a compatible and available vessel with adequate capacity and the appropriate fuel type to that asset. The following diagram 3.10 depicts the process logic for allocation.

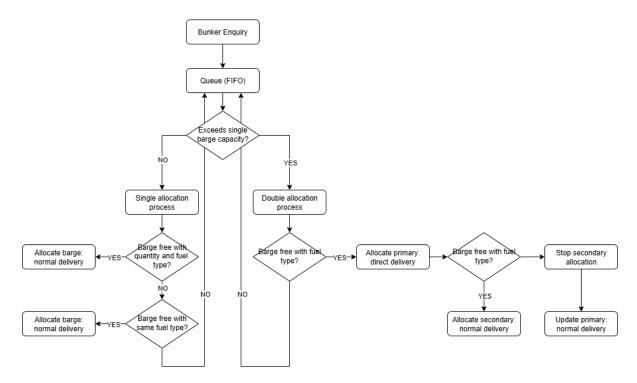


Figure 3.10: allocation process diagram

Evaluating the allocation diagram, the enquiry for bunkers enters the queue process. This queue operates on a first in first out principle. From this queue process two distinct flows are to be observed. A process flow for single allocation of resources and a flow for double allocation of resources, this is in place in order to replicate the current challenge of accommodating larger bunker enquiries, where the bunker enquiry is fulfilled by two vessels. After allocation the vessel will leave the queue and the process is handed over to the allocated bunkering vessel.

Diving deeper into the double allocation branch, two types of delivery modes are to be observed. A direct supply mode and the normal supply mode, the normal supply mode follows the logic as shown in diagram 3.8. The direct supply mode of the system follows the same logic for supplying the bunker vessel, yet does not have access to the resupply loop resulting in directly delivering the maximum level of fuel the vessel has in its tanks. Based on this division of tasks the delivered quantities will be allocated to the bunker supplying vessels in order to fulfil the bunker enquiry.

Lastly, another flow can be observed where double allocation is not possible due to insufficient capacity of bunker vessels operating in the system. In this case, the primary assigned barge will revert back to the normal supply mode delivering as much as possible to the bunker requesting vessel. Ultimately, this results in an incomplete delivery by the bunker operator due to an under-capacitated system due to a possible combination of unavailability of the required assets and under-capacitated assets.

3.1.3. System Logic

Integrating all individual processes, a comprehensive operational framework is established that integrates all aspects involved in ship-to-ship operations in a bunkering hub. This framework captures the sequential logic and interactions among system components. The complete system logic is illustrated in the swim-lane diagram 3.11, which visualises the sequential flow and interactions between system components.

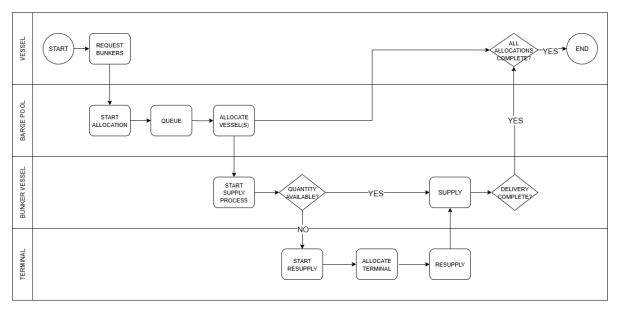


Figure 3.11: system overview swim lane model

The diagram (Figure 3.11) depicts the lifecycle of a bunker inquiry within the simulated system, managed from beginning to end. The inquiry operates according to these procedural steps:

- 1. **Vessel initialisation**: a vessel class is instantiated in the simulated environment, characterised by the following attributes:
 - Required fuel type
 - · Requested fuel quantity
 - · Vessel's receiving rate
- 2. **Inquiry queuing and allocation**: the generated inquiry is transferred to the barge pool, where the vessel enters a service queue. It waits for either a single or double allocation, depending on:
 - · Fuel type compatibility
 - · Requested quantity
- 3. **Supply Process**: after allocation, the vessel exits the queue and interacts with the assigned bunker vessel(s), which triggers the supply process. Two scenarios are possible:
 - (a) Sufficient fuel levels: the bunker vessel delivers the requested amount directly.
 - (b) **Insufficient fuel levels**: initiates a resupply request with a terminal. The terminal handles the allocation of fuel and the resupply operation. After resupply, the bunker vessel resumes the delivery process.
- 4. **Completion**: after all assigned bunker vessels confirm the completion of their respective supply operation, the enquiry is marked as complete.

Once all processes are completed, the system will terminate the vessel class and handle the next enquiry in the system. This cycle continues until the simulation reaches the predefined duration.

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3.2. Model Metrics

After establishing a complete description of all operations and the system's architecture, the model is nearly ready for implementation. This is because the system's input parameters, as well as the system's output and key performance indicators (KPIs), must be established in order to report performance and provide the needed input for the optimisation module.

3.2.1. System Input

Based on the previous chapter's requirements, a number of inputs must be defined in order to execute a simulation that closely resembles reality. The following input parameters were defined to run the simulation for current and future scenarios.

Base Parameters

in order to set up the environment a number of base parameters should be specified based on operational and commercial data:

 σ_a : the inter arrival time distribution between vessels, drawing the inter arrival time λ_0

 \vec{p}_s : the probability mass function of vessel sizes in vector: $\vec{p}_s = (p_1, p_2, ..., p_K)$, with $\sum_{k=1}^K p_k = 1$

C: the composition of the fleet represented as a matrix $C \in \mathbb{R}^{I \times J}$, translating the normalised probability of vessel type j in vessel size category i.

Fleet Growth

as market expansion will increase transport capacity demand, the number of vessels in operation will increase. This was mathematically formulated as:

$$\mu_a' = \mu_a/f \rightarrow \lambda_s = \lambda_0/f$$

Where the new inter-arrival time λ_s , λ_0 is the base inter-arrival time and f is the frequency factor.

Vessel Size

Aside from expansion of the fleet in absolute numbers, an increase in general vessel size is expected due to economies of scale and regulations such as EEDI. This is implemented through the following vector transformation:

$$\vec{p_s'} = \vec{v} \circ \vec{p_s}$$

Where \vec{p}_s' is the new size probability vector, \vec{v} is the growth vector and \vec{p}_s is the original size probability vector. Shifting the probability of vessel sizes to larger vessels, while taking into account port limitations, as \vec{p} to derived from port data.

Fleet composition:

as the energy transition may introduce a shift in types of vessels, the model should be able to handle and process a shift in vessel types. This is represented in the following matrix transformation:

$$C' = TC$$

Where C' is the transformed composition matrix, T the transformation matrix and C the original composition matrix.

Demand

The entire demand distribution is represented as a matrix D where each element $d_{i,j}$ represents the possibility of demand for fuel type j by vessel size i. The global demand fractions are given by vector \vec{T} , which transforms matrix D into D', while applying the fuel adoption segmentation outlined in section 2.4:

$$T = [t_{\text{fossil}}, t_{\text{bio}}, t_{\text{MeOH}}, t_{\text{NH}_3}, t_{\text{LNG}}] \qquad D'_{i,f} = \Phi_{i,f}, \quad T_f = \frac{\displaystyle\sum_{i=1}^n \Phi_{i,f} \; p_i \, \bar{q}_i \, \text{LCV}_f}{\displaystyle\sum_{i=1}^n \sum_{k=1}^m \Phi_{i,k} \, p_i \, \bar{q}_i \, \text{LCV}_k}$$

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3.2.2. Performance Indicators

After the simulation is ran, a number of performance indicators in the system need to be reported. These will be grouped into two categories. The performance indicators for the vessel operators and the performance indicators for the bunker operators as these are the main stakeholders involved in the ship-to-ship bunkering operation, as outlined in section 2.1.

Bunker Operators

For bunker operators the following performance indicators are introduced in order to define performance of the system that is being simulated which are relevant to their stakeholder priorities:

 average operation time: the operation time is the main measure for the efficiency of the bunker operations, as it provides insights into the average duration per enquiry. This also doubles as a measure for service reliability. In the system this measure is calculated as follows:

$$\bar{T}_{\text{oper},f} = \frac{1}{n_f} \sum_{k=1}^{n_f} T_{\text{service},f}^{(k)}$$

where $T_{\mathsf{service},f}$ is the service time for the k^th operation involving fuel type f, and n_f is the number of such operations for type f.

• bunker vessel downtime: downtime of a bunker vessel is defined as the time the vessel is not performing operations, as the it will be waiting until the next operation. This measure represents the asset utilisation. In the system this measure is calculated as follows:

$$f_{\text{downtime},f} = 1 - \frac{\sum_{f \in \mathcal{F}} \sum_{k=1}^{n_f} T_{\text{service},f}^{(k)}}{\sum_{f \in \mathcal{F}} \textit{x}_f \cdot T_{\text{sim}}}$$

Where $T_{simulation}$ represents the total simulation duration, $T_{service,f}$ the time of the bunker vessel performing refuelling operations and where x_f is the number of bunker vessels assigned to fuel type f.

• tank utilisation: tank utilisation is an important measure nowadays, as it allows for a tangible way to measure the utilisation of tank capacity before engaging in a refuelling operation. This measure represents the capacity utilisation. In the system this is mathematically described by the following fraction:

$$f_{u,f} = 1 - \frac{l_f}{c_f}$$

Where l_f represents the fuel level and c_f the tank capacity for fuel type f of the bunker supplying vessel.

• double allocations: important to know if the current vessel sizes are insufficient to deliver the necessitated capacity needed for the supply. This measure will be numerically tracked by the barge pool as follows:

$$n_{d,f} = \sum_{k=1}^{n_f} \mathbb{1}\left\{a_f^{(k)} \ge 2\right\}$$

where $a_f^{(k)}$ is the number of vessels allocated for the k-th delivery of fuel type f, and $\mathbb{1}\{\cdot\}$ is the indicator function.

• **insufficient capacity**: A discrete count of failed deliveries where available bunker vessel capacity was insufficient to meet demand for fuel type *f*. Similar to the service this measure provides feedback for service reliability.

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Operators

For vessel operators a set of different requirements for reporting performance is defined. These are mostly focussed on how fast and reliable a vessel can be serviced in order to continue its operation, as outlined in section 2.1..

average waiting time: the waiting time of the vessel has a significant impact for operators as
they would be out of operation awaiting a refuel. This could lead to vessel operators opting to
taking fuels at another port. This is a measure for reliability.

$$\bar{T}_{\text{wait},f} = \frac{1}{n_f} \sum_{k=1}^{n_f} T_{\text{wait},f}^{(k)} \mid T_{\text{wait},f}^{(k)} = t_{\text{a},f}^{(k)} - t_{\text{s},f}^{(k)}$$

where $t_{a,f}^{(k)}$ is the system time at which a bunker vessel is allocated, and $t_{s,f}^{(k)}$ is the system time for the start of the enquiry of the k^{th} request involving fuel f.

average service time: the expected service time for operators is an important measure as it
gives an indication into how long the bunker operation will take. This is a measure for efficiency.

$$\bar{T}_{\text{service},f} = \frac{1}{n_f} \sum_{k=1}^{n_f} t_{t,f}^{(k)} - t_{\mathsf{a},f}^{(k)} \mid T_{\text{service},f}^{(k)} = t_{t,f}^{(k)} - t_{\mathsf{a},f}^{(k)}$$

where $t_{t,f}^{(k)}$ represents the system time the bunker enquiry is terminated and $t_{a,f}^{(k)}$ represents the system time the bunker vessel(s) where allocated for the k^{th} operation involving fuel f.

 average turnaround time: the turnaround time, consolidates the waiting time and service time, including the possibility of a barge refuel before operation. This is a performance measure for efficiency and reliability.

$$\bar{T}_{\text{turnaround},f} = \frac{1}{n_f} \sum_{i=1}^{n_f} T_{\text{turnaround},f}^{(k)} \quad | \quad T_{\text{turnaround},f}^{(k)} = T_{\text{wait},f}^{(k)} + T_{\text{service},f}^{(k)}$$

3.2.3. Desired output and objective

Lastly, the system should report a number of global outputs in order to report trends and verify results. The following outputs were defined:

• **local demand** the local demand will be defined as the total demanded quantities in the system for each fuel type for a given scenario. In the system this is defined as follows:

$$Q_f = \sum_{k=1}^{n_i} q_f^{(k)}$$

where q_f represents the quantity demanded for the k-th bunker enquiry for fuel type f.

global turnaround time is defined as the average turnaround time of all operations performed
in the system, aimed a tracking the global system performance. In the system this is defined as
follows:

$$\bar{T}_{\text{turnaround}} = \frac{1}{N} \sum_{f \in \mathcal{F}} \sum_{k=1}^{n_f} T_{\text{turnaround},f}^{(k)}$$

where $T_{\text{turnaround},f}^{(k)}$ is the turnaround time for the k-th operation involving fuel type f, and $N = \sum_{f \in \mathcal{F}} n_f$ is the total number of operations across all fuel types.

• **optimal bunker fleet composition** The optimal number of bunker vessels x_f required to maintain service levels for fuel type f, as determined by the optimisation model.

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3.3. Data

Once all the components, as well as the input and output parameters for the simulation framework, are defined, the essential operational input can be derived to develop the entire system. Before building the discrete-event simulation, datasets were gathered to establish the basis for all model components. This section outlines the different data sources, processing techniques, and data quality considerations.

3.3.1. Operational Data

For developing a representative approach to model the ship-to-ship bunkering operation, a combination of input based calculations and distributions will be used, as outlined in the agent processes in section 3.1.2. In order to derive all the corresponding distributions for the stochastic processes and the required inputs for the processes in function of time, two operational datasets were used:

Conventional-bunkering: The operational data for conventional marine fuels or liquid fuels (VLSFO, HFO and MGO) was obtained from Peninsula's internal CRM system (PTA). The original dataset included records of 10000 operations from the Gibraltar bunker hub. Each entry detailed the quantity provided, pumping duration, mooring/unmooring times, connection/disconnection times and times between start of operation to arrival at vessel. Data filtering excluded incomplete or inconsistent entries, decreasing the usable dataset to 5000 entries. Fuel and vessel-type pumping rates were calculated based on these records using the relationship between quantity and pumping duration. Standard statistical approaches were used to fit distributions to fit the observed distributions of all subprocesses.

LNG-bunkering: Gas-based operations were analysed using the operational logs from Peninusla's LNG vessel Levante. This dataset included 140 entries, which represents the whole operational lifecycle of the vessel to date. The LNG dataset provided timing breakdowns for all subprocesses and receiving vessel characteristics such as connecting time, disconnecting time, pumping time, receiving vessel size, vessel type and receiving rates for gas-based systems. Receiving rates for gas-based systems were extracted per vessel type, and similar to the conventional bunkering operations standard statistical approaches were used to fit distributions to fit based on the data of all subprocesses.

For a complete overview of the exact fitted distributions for all subprocesses for the gas- and liquid bunkering operations, please see appendix A.

3.3.2. Commercial Data

For developing realistic demand patterns corresponding to the various vessels, the dataset of size and type specific fuel-type and quantity demanded was developed. Individual demand patterns were analysed based on the same operational data-sets from PTA and the Levante to develop fuel-specific demand distributions and vessel compatibility matrices.

Fuel Compatibility Matrix: To establish a baseline for fuel types demanded by different vessels, a fuel preference matrix was constructed using the PTA dataset. This resulted in a demand probability matrix D, where $d_{i,f}$ represents the likelihood of vessel size i preferring fuel type f. This matrix captures current market preferences and serves as a reference for alternative fuel adoption scenarios.

Individual Demand: To establish a baseline for energy demanded by various sizes of vessels, dealsize distributions were derived from both conventional and LNG datasets by comparing the delivered quantities to vessel size classifications. These entries resulted in distributions with the primary variable being the vessel size, with separate distributions per fuel type. Distribution selection was based on fit testing across multiple distributions. 30 3. Model

3.3.3. Shipping Data

To create representative market conditions, a dataset on market characteristics was constructed. Vessel arrival patterns and fleet composition were analysed using S&P Global's MINT platform [52], which includes market intelligence reports on bunkering activities in the Gibraltar Strait. The dataset included recorded bunkering activities from the period between 01/01/2024 - 31/12/2024.

Vessel Arrival Patterns: In order to create representative market conditions, realistic vessel arrival patterns for bunkering needed to be developed. The shipping dataset initially included 8,500 reported ship-to-ship bunkering operations. However, quality and validity assessment removed operations lasting less than 4 hours and those performed by vessels other than bunkering vessels (e.g. STS operations by slop barges or wrong reports), resulting in a dataset of around 4,850 verified operations. Based on the data the following three distributions were extracted to develop realistic arrival patterns:

- Inter-arrival time distribution (σ_a): To accurately model the frequency of ship-to-ship operations at the bunker-hub, the inter-arrival time between reported operations was analysed. By fitting a distribution to the time intervals between logged bunkering operations, the simulation can generate realistic inter-arrival times λ_s for vessels.
- Vessel Size Distribution (\vec{p}):To effectively model vessel sizes requesting bunkers, the probability vector \vec{p} was designed to represent the likelihood of any vessel size i arriving at the bunker hub. The vector \vec{p} was based on the frequency of arriving vessel sizes.
- **Vessel Type Matrix** (*C*): To capture the variety of vessel types arriving in the bunker hub, the vessel type matrix *C* was constructed. This matrix maps the probability of vessel types *j* in each size category *i*, where element $c_{i,j}$ represents the probability of vessel type *j* for vessel size *i*. The matrix is based on the frequency of vessel type *j* in vessel size *i*.

The combination of these three elements allows for realistic simulation of market conditions in a given bunker hub for a given duration. It also provides the necessary input for the operational and commercial parameters from the previous subsection, which in turn provide the correct input for the processes outlined in section 3.1.2. Appendix A provides a comprehensive summary of all derived distributions and data fit.

3.3.4. Data Quality

After accumulating all of the data required for the simulation's foundation, a thorough evaluation should be conducted to assess the data's reliability, as data quality has a substantial impact on model correctness. When evaluating all datasets used, a number of remarks should be in place regarding data quality:

Data Collection Issues: Due to partial entries, missing timestamps and inconsistent entries, the conventional dataset had to be filtered down from 10000 entries to 5000 acceptable records. This 50% rejection rate illustrates the current challenge of digitalisation in the bunker industry. The LNG dataset, while complete and accurate, only has 140 entries due to the short lifespan of gas bunkering operations within Peninsula. These observations in both datasets should introduce a careful bias when interpreting the obtained results.

Alternative Fuel Extrapolation: Extrapolation of normal operations, vessel design requirements based on engineering principles and limited pilot project data, yielded operational requirements for methanol, ammonia and biofuel. This strategy involves uncertainty yet is the best available practice given the early stages of alternative fuel operations.

Despite the limitations, the datasets capture the operational complexity and market dynamics that are typical of large bunker hubs. The model's emphasis on relative changes and system transformation patterns, rather than absolute forecast, makes it able to stand to data limitations. The breadth of the data collected gives a solid foundation for understanding the amount and nature of bunker hubs and to project the adjustments required for sustainable fuel implementation in bunkering operations.

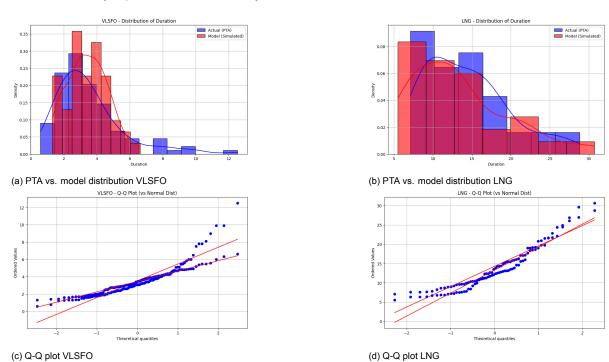
3.4. Validation:

3.4. Validation:

Prior to developing the optimisation module, the simulation framework must be validated against historical operational data to confirm its accurate representation of the modelled processes and consistency to produce reliable results.

3.4.1. Process verification

To validate the simulated processes, a subset of the initial datasets was reserved and used as input for the model to replicate similar operating conditions. Given the stochastic nature of the simulation, the model's validity needs to be assessed through distributional analysis rather than point-by-point comparison, which would naturally showcase individual deviations. Figure 3.16c–3.16d show the distribution comparisons for both VLSFO and LNG fuel types fitted with KDE-curves and Q-Q plots for both fuel types. These fuels were selected as they provide the foundation for all types of liquid and gaseous bunkering operations. The VLSFO- and LNG-simulation were verified against 250 and 75 data points respectively. Visually, the simulated distributions align closely with the actual data, suggesting that the model effectively reproduces the variability of the real world.



In order to quantitatively assess the similarity between the actual and simulated distributions, the Kolmogorov-Smirnov (K-S) test was performed. This metric highlights the maximum distance between the cumulative distribution functions (CDFs) of two samples, while the corresponding p-value tests the null hypothesis of both samples being drawn from the same distribution.

Fuel Type	K-S Statistic	P-value (K-S)
LNG	0.2167	0.1198
VLSFO	0.1731	0.0887

Table 3.1: Distribution Comparison for Stochastic Fuel Simulations (K-S Test Results)

Table 3.1 shows that both LNG and VLSFO have p-values that exceed the 0.05 threshold, indicating no statistically significant difference between the simulated and actual distributions. This shows that the model accurately simulates the statistical properties of real-world processes. The LNG instance produces a p-value of 0.1198, which exceeds the more cautious 0.1 threshold indicative of significant distributional resemblance [38]. While the VLSFO result (p = 0.0887) is slightly lower than this level, it is still within an acceptable range, indicating the model's overall validity.

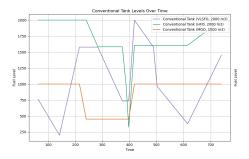
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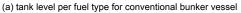
3.4.2. Agent Behaviour

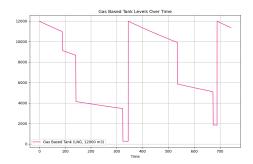
After verifying the accuracy of the individual processes implemented in the simulation, the individual agent behaviour needs to be evaluated. This in order to evaluate if the agents behave according to their predefined processes.

Bunker Vessels

The bunker vessel agents demonstrated consistent and realistic behaviour throughout testing. Tank levels shown in figures 3.13a and 3.13b illustrate expected operational cycles, with clear supply operations visible at various timestamps and resupply events occurring at appropriate moments (conventional vessels at timestamp 400, gas-type vessels at timestamps 350 and 690). The gradual depletion of tank levels and the resupply events align with the predefined processes in section 3.1.2, confirming that the agent behaves as intended and reflects the operational profiles and responds to system demands.



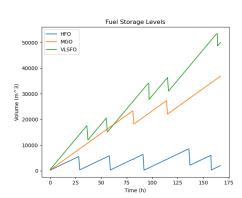




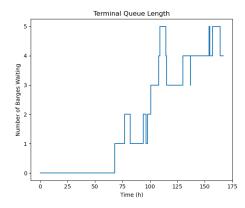
(b) tank level over time for gas-type bunker vessel

Product Terminals

For the modelled terminal the results vary significantly. The terminal agent displayed sensitive and unrealistic behaviour at baseline conditions that raising significant concerns about the underlying data used for modelling the terminal processes and infrastructure. Figure 3.14a depicts how terminal fuel levels increase for two of the three fuel kinds. Furthermore, when analysing 3.14b the observation can be made that the queue length grows over time, with vessels queuing up to 60 hours. Based on both observations made in the simulation, the conclusion can be drawn that the model produced for the refinery is built on inadequate data as it is not able to replicate real world operations in the baseline scenario.



(a) tank level per fuel type at terminal over time



(b) queue length at terminal over time

Model Scope Refinement: Based on the observed behaviour, the decision was made to exclude the terminal operations from the final simulation model. This change ensures model integrity by focussing on components with validated behaviour while avoiding potentially misleading results from problematic agents. The accuracy of the discrete event simulation is largely dependent on the quality of input data and the validity of the model's assumptions. As a result, fuel availability was regarded as an external parameter, allowing the simulation to focus on proven supply-phase operations.

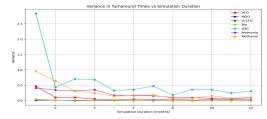
3.4. Validation:

3.4.3. Stability

Before assessing other aspects of the simulation, stability assessment is crucial to determine the reliability across single or multiple simulation runs. This reflection is necessary due to the stochastic nature of the simulation, which introduces a certain level of variance based on the input. Evaluating variance and consistency is therefore mandatory.

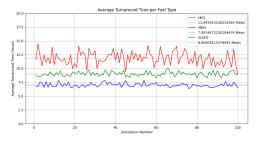
The parameter having the most significant impact on system noise is identified to be the duration of the simulation. This parameter can be tuned to minimise, yet never completely eliminate system noise. This is to be explained by the statistical variations that occur in every run, making noise inherently part of every simulation result.





- (a) Variance in simulation based on duration for conventional
- (b) Variance in simulation based on duration for alternatives

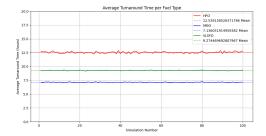
As shown in figures 3.15a and 3.15b, the variance in the system reduces over longer simulation durations. This could be explained by the fact that the system is reaching a 'steady-state' during extended periods. Based on the variance results, the decision was made to implement all further simulations for a duration of 6 months and to exclude the first month. This due to presented steady variance. In table 3.2 the reduction of variance between 100 iterations of 1 month vs. 6 months can be observed.

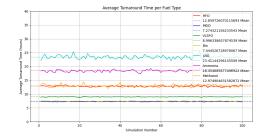




(a) 100 iterations of a simulation duration of 1 month for conventional







- (c) 100 iterations of a simulation duration of 1 year for conventional
- (d) 100 iterations of a simulation duration of 1 year for alternative

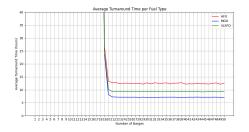
Table 3.2: Variance of Fuel Types for Different Simulation Durations

Group	Sim. Duration	HFO	MGO	VLSFO	Bio	LNG	Ammonia	Methanol
Conventional	1		0.0289	0.0330	-	-	-	-
	6	0.0316	0.0020	0.0028	_	_	_	
Alternative	1	0.2563	0.0224	0.0382	0.0314	2.7921	1.0304	0.8217
	6	0.0587	0.0046	0.0088	0.0089	0.4221	0.2083	0.1921

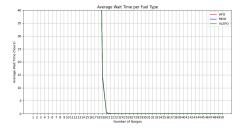
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3.4.4. Commercial verification

To validate the system's representation of the current market and the systems expected behaviour to fleet changes, a saturation test was performed and verified against the commercial data made available from the business origination division from Peninsula and commercial data available from the platform S&P CI MINT on the operating region the system is representing. During this test, the number of bunker vessels in operation was increased incrementally with a step size of one bunker vessel while logging the system's turnaround and waiting time. This approach allowed to determine when the system should be operating at an 'optimum' (the point where an increase in additional vessels had no significant impact on turnaround times). The obtained values will be used to verify how accurate the simulation represents current market dynamics and present a baseline reference for the optimisation later implemented in the simulation.



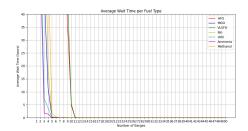
(a) number of conventional bunker vessels vs. turnaround time



(c) number of conventional bunker vessels vs. waiting time



(b) number of alternative bunker vessels vs. turnaround time



(d) number of alternative bunker vessels vs. waiting time

Evaluating figure 3.17a-3.17d two conclusions can be drawn. The first key takeaway is the direct correlation between the waiting time of the system and the turnaround time of the system, highlighting the relation of a near optimal turnaround time when the system showcases no waiting time. The second takeaway from these saturation tests is the fact that the turnaround time can be optimised beyond the point of an optimal waiting time. Which emphasises the fact that the turnaround time should be the decisive KPI for determining an optimum in the system.

When evaluating both figures 3.17a and 3.17c an optimum can be determined by identifying the saturation point or knee in the turnaround time graph. Based on this analysis, the optimal number of bunker vessels operating in the Gibraltar straight should be 20 vessels. However, the combined commercial data provided by the business origination team and the data from S&P Market Intelligence indicates that 25 vessels currently operate as bunker suppliers in the region [52]. This discrepancy between simulation results and actual market results is to be explained by several factors, the first being that the saturation test optimises with one type of bunker vessel, while the market consists of a variety of vessels with different specifications. Secondly external factors such as market dynamics, weather conditions and operational challenges necessitate system redundancy.

Lastly, the total demanded quantity for conventional fuels was obtained from the system performance indicators and compared to the reported estimated quantity of the modelled year of 2024. The model reported a total demanded tonnage of 4.7 mT, while estimates state a demand varying between 4.5 mT and 5mT [53], [26]. This overlap highlights the potential validity of the modelled bottom-up approach for demand, yet is unfortunately unverifiable due to no verified total bunker demand figure.

3.5. Optimisation 35

3.5. Optimisation

After constructing and verifying the simulation model of the framework, the optimisation module needs to be integrated. As outlined in the literature review and verified by the performed saturation test in the previous section, gradient-based optimisation based on simulation outputs should be employed to determine the optimal fleet configuration.

Evaluating all defined output parameters, the conclusion could be drawn that the turnaround time and waiting time should be optimised by varying the number of bunker vessels in operation, as these are the most important KPIs for vessel and bunker operators aside from bunker price, as outlined in the stakeholder framework in section 2.1. According to graphs 3.17a and 3.17c, a strong correlation between these parameters is observed. When evaluating both parameters individually, the conclusion can be drawn that the turnaround time can be optimised beyond the point of the optimal waiting time. This highlights that turnaround time should be optimised with a hard constraint for waiting time.

Method

In order to determine the optimal fleet composition based on the turnaround time of the system a gradient-based optimisation method was employed [17], this due to underlying characteristics outlined in section 2.1 and the behaviour the system showcased in the saturation test. Figure 3.17a and 3.17b illustrate a distinct gradient change in which the system deteriorates in performance near the optimal number of vessels in operation. Additionally, the method accommodates heterogeneity across optimisation vectors, as was highlighted in the variance in responses for different fuel types shown in the same figures.

Mathematical Formulation

Implementing the gradient-based optimisation strategy in the simulation requires a vector-based approach in order to determine all the various saturation points for all fuel types. This led to the following objective function $\mathbf{f}(x)$, which represents the multi-objective optimisation problem focused on minimising turnaround times across all fuel types:

$$\mathbf{f}(x) = \begin{bmatrix} T_1(x) \\ T_2(x) \\ \vdots \\ T_N(x) \end{bmatrix}$$
(3.1)

Subject to the following constraints for optimisation, where constraint 3.2 represents the optimisation constraint for the gradient of the turnaround time and equation 3.3 represents the hard constraint for the waiting time:

$$\nabla_n(x) \le \nabla_{\text{ref},n} \quad \forall n \in \{1, \dots, N\}$$
 (3.2)

$$W_n(x) \le \tau \qquad \forall n \in \{1, \dots, N\}$$
 (3.3)

$$x \in \mathbb{Z}^+ \tag{3.4}$$

Where:

- x Number of bunker vessels in operation (decision variable)
- n Fuel type index, $n \in \{1, ..., N\}$
- $T_n(x)$ Turnaround time function for fuel type n
- $W_n(x)$ Waiting time function for fuel type n
- $\nabla_n(x)$ Gradient of turnaround time for fuel n
- ∇_{ref,n} Gradient threshold for fuel n
- τ Maximum allowable waiting time
- $\mathbf{f}(x)$ Vector-valued objective function: all $T_n(x)$

36 3. Model

Noise

Evaluating the stability test, the observation can be made that the system showcased some level of variability due to the stochastic nature of the simulation. In order to determine an optimal solution, the influence of this noise should be minimised. To mitigate this system noise the following solutions were implemented:

- A coarse-to-fine search strategy to identify plausible solutions across the entire optimisation domain, aimed at mitigating local optima and improving computational time. Follows the logic of optimisation theory [60].
- Exponential smoothing to reduce the noise showcased in the turnaround time curve measurements, aimed at improving curve detection. Follows the logic of noise in time measurements in systems [27].
- 3. Weighted moving average in the gradient evaluation, prioritising the most recent trend in the turnaround time curve. Follows the logic of noise reduction in signal processing [55].
- 4. Multiple simulation runs at potential optima to increase confidence in results, this in order to minimise the effect of variance. Follows the logic of stochastic simulation theory [35].
- 5. Fuel-specific sensitivity factors to account for different responses to fleet size changes and the difference in variance showcased per fuel type in table 3.2. Follows the potential of adaptive optimisation [66].

Adaptive Knee Detection

Different fuel types exhibited varying degrees of variance in the stability test, which leads to different responses to changes in the number of bunker vessels in operation. In order to mitigate this, fuel specific gradients were introduced.

$$\nabla_{\mathsf{ref},n} = \nabla_{\mathsf{base}} \cdot f_n$$

Where the base threshold (∇_{base}) is defined by the optimisation constraint of the simulation, the fuel factor (f_n) by the variance in the stability results from table 3.2.

Exponential Smoothing

To reduce the impact of noise in the turnaround measurements obtained from the simulation, exponential smoothing was applied to the return values from turnaround time:

$$S_n(x) = \alpha \times T_n(x) + (1 - \alpha) \times S_n(x - 1)$$
, for $x > 0$

Transforming the value $T_n(x)$ observed at point x in the number of barges and returning the smoothed value $S_n(x)$ by applying the smoothing factor $\alpha=0.3$. This factor alpha preserves the underlying trends of the simulation model while reducing noise observed in the system, this value was determined by iterative testing of different values for α .

Weighted Moving Average

As observed in figure 3.17a and 3.17b, the change of gradient of the turnaround slope is aggressive. In order to accommodate for this, a weighted moving average was implemented to give a higher priority to recent changes in trends.

$$\nabla_n(x) = 0.6 \times \frac{\delta S_n(x)}{\delta x} + 0.3 \times \frac{\delta S_n(x-1)}{\delta x} + 0.1 \times \frac{\delta S_n(x-2)}{\delta x}$$

This method allows for a more responsive detection of the knee point, while still maintaining the advantage of filtering out system noise. Identifying the optimal number of vessels in operation before deterioration in the system occurs.

3.5. Optimisation 37

Coarse-to-Fine Search

In order to efficiently identify the optimal fleet composition over the entire solution space, a two-phase search strategy was implemented:

- 1. **Phase 1 (Coarse Search)**: Evaluate the solution space by larger step sizes (3 vessels) in order to identify plausible regions where the system gradient increases significantly, while minimising the number of computations.
- 2. **Phase 2 (Fine-grained Search)**: Evaluate the identified regions with the smallest step size in combination with multiple simulation runs evaluating the same point. The increased number of runs is aimed at increasing the confidence of the results, allowing for a more detailed and accurate analysis.

This strategy allows for a significant reduction in computational time by reducing the number of computations while maintaining high accuracy in determining the optimal fleet composition.

Implementation

Combining all previous steps, the following optimisation procedure is implemented:

- 1. Initiate the optimisation at the starting point, which is the maximum number of bunker vessels in the solution space, defined by the input of the user.
- 2. Reduce the number of barges in a coarse step size, identifying the regions of a potential optimum.
- 3. For each region identified to have a plausible optimum, execute a fine grained search according to the following principles:
 - · Multiple simulation runs at each step to increase the confidence of the result.
 - Application of exponential smoothing to reduce noise in the results obtained from the simulation.
 - Application of weighted moving average of the slopes to prioritise most recent trends.
- 4. Identify the optimal point by meeting the following criteria:
 - the hard constraint of wait time is met: $W_n(x-i) \le 0.01$ for $i \in \{0,1,2\}$
 - the optimisation criteria is met: $\nabla_n(x) \leq \nabla_{ref,n}$

Validation

In order to validate the optimisation module implemented in the framework, a repetitive test was performed to measure solution consistency and to validate the results. The gradient-based strategy was applied to determine the optimal number of conventional bunkering vessels required for the baseline conditions of the current market structure.

When repetitively applied to the simulation model of the conventional market, the solver yielded consistent results of an optimal bunker fleet of 20 conventional ships, which corresponds to the visual results observed in figure 3.17a from the saturation test performed in the previous section. The overlap between the visually observed saturation point and the obtained results verifies the solvers ability to interpret the simulation results correctly and return the minimal amount of bunker vessels needed to maintain similar service conditions in the simulated market conditions. Furthermore, it establishes that the model is able to determine results that are representative to current market conditions.

4

Simulation

After establishing the outlined framework, a number of various simulations are to be performed. In these simulations the projected market trends were recreated by varying the system input parameters outlined in section 3.1.

4.1. Scenario

To reflect the changing marine landscape, a transition scenario was developed based on expected trends from multiple industry sources and a literature analysis. This is due to the fact that each forecast applies a different method and produces different outcomes, as stated in section 2.1. Based on the operationally grounded segmentation established in section 2.1, the energy demand breakdown from the energy outlook of DNV was used in combination with market and fleet forecasts and created the foundation for the scenario inputs. The literature review's rule-based principles were changed to provide compatibility with different fuel types. This led to the following broad guidelines/assumptions:

- Alternative fuel uptake: 70% of alternative fuels in the energy mix by 2050 [18].
- Fleet size: 35% increase in number of vessels in the fleet by 2050 [62].
- Vessel size: 10% increase in the size of vessels [62].
- Compatibility
 - low energy demand vessels are able to adopt Biofuels and Methanol, based on the conclusion established from the supporting literature in section 2.
 - medium to large energy demand vessels are able to adopt Methanol, LNG, and ammonia.
 Based on the conclusion established from the supporting literature in section 2.

These assumptions were translated and compiled into a transition timeline of 30 years, spanning from 2020 until 2050 and having a step size of 5 years in-between each scenario, resulting in the following input parameters:

Year	Fossil [t_{fossil}]	Bio [t _{bio}]	Methanol [t_{MeOH}]	Ammonia [t_{NH_3}]	LNG [t_{LNG}]	Frequency [f]	Growth $[\vec{v}]$
2020	1.00	0.00	0.00	0.00	0.00	1.00	1.00
2025	0.93	0.02	0.02	0.00	0.03	1.06	1.03
2030	0.82	0.04	0.04	0.04	0.06	1.12	1.05
2035	0.65	0.06	0.07	0.10	0.12	1.18	1.08
2040	0.50	0.08	0.10	0.12	0.20	1.24	1.10
2045	0.38	0.10	0.12	0.15	0.25	1.29	1.13
2050	0.27	0.10	0.15	0.20	0.28	1.35	1.15

Table 4.1: Fuel transition energy share, fleet growth, and frequency over time (2020–2050)

40 4. Simulation

4.2. Scenario Analysis

The analysis of the simulation of the transition to sustainable fuels was performed by two complementary methods. An evolving analysis where the system progresses along the predetermined timeline and fixed scenarios where single parameter evaluation will be performed at specified points in the transition timeline to evaluate single supply chain performance and resilience.

Evolving Scenario Evaluation

In order to comprehend how the bunker supply chain must adapt during the transition to more sustainable fuels within the maritime supply chain, an evolving scenario analysis was conducted. This analysis spans the full 30-year timeline, incorporating gradual shifts in fuel-types, vessel sizes and fleet composition.

At each time step, the model determines the optimal bunker fleet composition, aiming to minimise both the number of required bunker vessels and the turnaround time per fuel while tracking the following key performance indicators:

- · fuel-specific turnaround time
- downtime percentages per bunker vessels

· tank utilisation rates

· total demand per fuel type

This system wide evaluation should provide insight into how the bunker ecosystem evolves under increasing alternative fuel uptake and quantifies the assets and resources required to maintain consistent system performance.

Single Scenario Evaluation

After establishing the global trends in the transition, it is equally important to assess the robustness of individual supply chains at various points in the transition timeline. These scenarios offer a snapshot of system performance under specific conditions and test sensitivity to isolated parameter changes. The years 2020,2030,2040 and 2050 in the transition timeline were selected for evaluation with the single scenario analysis to evaluate how each system responds to variations in:

- vessel frequency: which will be exposed to an additional 15% in frequency from the projected scenario.
- vessel size: which will be exposed to an additional 10% in growth in vessel size from the projected scenario.

The 2020 scenario serves as the conventional baseline, while the subsequent scenarios correspond to intermediate and advanced stages of fuel diversification. In each analysis the number of bunker vessels in operation was fixed based on the results for the optimal fleet composition obtained from the evolving scenario analysis. This method allows for evaluating each system's resilience and flexibility, especially for deviations from projected market trends.

Scenario	Growth $[\vec{v}]$	Frequency [f]	Conventional	Bio	Methanol	LNG	Ammonia
2020	1.00 - 1.10	1.00 - 1.15	25	0	0	0	0
2030	1.05 - 1.15	1.12 - 1.27	20	8	8	5	5
2040	1.10 - 1.20	1.24 - 1.39	15	8	8	8	8
2050	1.15 - 1.25	1.35 - 1.50	10	10	10	15	8

Implementing this methodology should enable a deeper understanding of fuel-specific supply chain responses to stress, if there is inter supply chain interaction and possibly aid in identifying potential bottlenecks.

4.3. Results

4.3. Results

Implementing the proposed transition timeline into the simulation, the following results were obtained for the evolving scenario and the single scenario analysis.

4.3.1. Evolving Scenarios

When implementing the proposed timeline of the transition into the model, aiming to achieve the 70% uptake of alternatives in the energy mix by 2050, the following results were obtained in terms of optimal bunker fleet composition, demand and service times projections in the bunker ecosystem.

Bunker Fleet Evolution

Evaluating the results of the solver for optimal fleet composition, a clear increase in the number and types of bunker vessels required to sustain comparable service levels is to be observed, as the fleet size is projected to increase with 230% and significantly diversify as conventional bunker vessels are projected to reduce by 83% in fleet share by the end of the transition period in 2050.

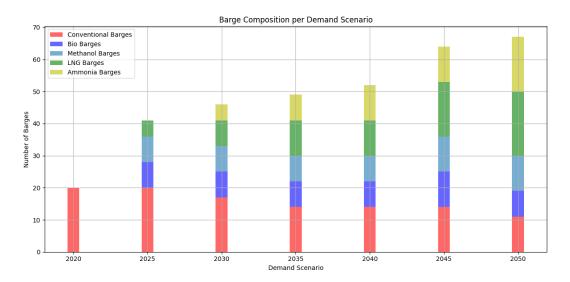


Figure 4.1: Optimal fleet composition

However, the most significant change to note is the shift in required bunker vessels that can be observed in figure 4.1 when transitioning to the first step in the timeline of the energy transition. Showcasing the significant influence of the diversification fuel demand on the fleet composition, resulting in double the number of bunker vessels needed in operation while the total fuel uptake does not significantly shift in figure 4.2 over the first time step. Highlighting that the initial fleet growth of bunker vessels is not driven by an increase in demand but by diversification of demand. This is to be explained by the introduction of new product types and the different set of requirements for bunker vessels in order to be able to supply the corresponding product, highlighting the potential challenges that the segmentation of the fuel demand introduces.

Year	Conventional vessel	Bio vessel	Methanol vessel	LNG vessel	Ammonia vessel	Total vessels
2020	20	0	0	0	0	20
2025	20	8	5	8	0	41
2030	17	8	8	8	5	46
2035	14	8	8	10	9	49
2040	14	8	8	10	12	52
2045	14	10	12	16	12	64
2050	11	8	10	20	17	66

Table 4.3: Barge fleet composition by fuel type (2020-2050)

42 4. Simulation

Fuel Demand Evolution

The projected fuel demand within the simulated system showcases substantial growth throughout the modelled scenario of a transition to more sustainable fuels, as can be observed in figure 4.2. Total fuel demand is projected to increase from 5 million tonnes in 2020 to 16.3 million tonnes by 2050, representing a 226% increase over the complete timeline of the transition period. The growth trajectory in the figure exhibits acceleration over time, with demand already reaching 9.7 million tons by 2035, indicating a 94% increase from the baseline within the first 15 years of the transition. The growth rate becomes more pronounced in the latter stages of the timeline, with demand increasing by 68% between 2035 and 2050, from 9.7 million to 16.3 million tonnes, representing a 40% increase in growth rate compared to the first 15 years of the transition period.

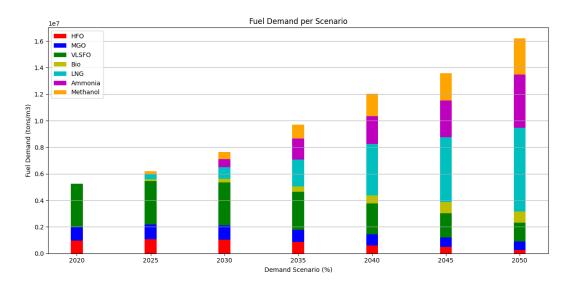


Figure 4.2: absolute demand over time

These increases in demand highlight the challenge that alternative fuels introduce into the simulated system in terms of demand, due to their lower volumetric energy density compared to conventional marine fuels. This becomes apparent when examining the overall demand relative to the required energy share demanded in the system, see table 4.1 and 4.4.

Demand Shares

Breaking down the demand into individual components, the most significant share is to be attributed to LNG, followed suit by Ammonia and Methanol. Observing graph 4.2 and table 4.4 the conclusion can be drawn that these new fuels are driving the increase in total demand, as they contribute to 78% of the demanded tonnage in 2050. This is mostly to be explained by either the lower energy density or fuel handling requirements of the newly introduced fuels, ultimately resulting in larger shares in terms of tonnes to deliver the same energy in the system.

Year	HFO	MGO	VLSFO	Bio	LNG	Ammonia	Methanol	Total Demand in tonnes
2020	1,000,000	1,000,000	3,000,000	0	0	0	0	5,000,000
2025	1,000,000	1,000,000	3,500,000	200,000	200,000	0	200,000	6,100,000
2030	1,000,000	1,000,000	3,200,000	500,000	800,000	500,000	500,000	7,500,000
2035	800,000	1,000,000	2,700,000	700,000	2,000,000	1,300,000	1,200,000	9,700,000
2040	500,000	1,000,000	2,200,000	1,000,000	3,000,000	2,000,000	1,800,000	11,500,000
2045	300,000	700,000	1,600,000	1,300,000	4,000,000	2,800,000	2,800,000	13,500,000
2050	200,000	500,000	1,300,000	1,500,000	4,300,000	4,000,000	4,500,000	16,300,000

Table 4.4: Fuel demand composition by fuel type (2020-2050) in metric tonnes

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Turnaround Evolution

The results obtained from the model in terms of turnaround time throughout the transition timeline show-case systematic changes. As presented in table 4.5, the global average turnaround time increases from 9.5 hours in 2020 to 13.9 hours by 2050 per operation, representing a 46% increase from baseline system performance. The progression showcases consistent increases across the modelled time frame, with a change of rate in 2030 when alternative fuels achieve greater market penetration.

Evaluating fuel specific turnaround times, illustrated in figure 4.3, great variation can be observed between fuel types. Gas-type fuels demonstrate the longest operational periods, as the average turnaround times for LNG and ammonia are projected at 25 and 20 hours respectively by 2050. Both fuels showcase substantial time variability, with standard deviations ranging from ± 7 to ± 8.5 hours, indicating considerable variation in duration of individual operations.

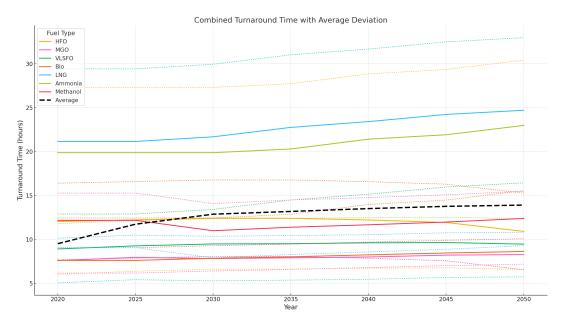


Figure 4.3: turnaround time and deviation per type

Alternative liquid fuels present different operational characteristics. Methanol bunkering operations as described in table 4.5, require around 12 hours throughout the transition period. These projected durations remain below gas-type fuel requirements while exceeding all conventional fuels, despite similar handling characteristics. Further establishing the influence of the lower energy density of these alternative fuels, requiring larger bunker quantities as already established in the demand analysis

Year	HFO	MGO	VLSFO	Bio	LNG	Ammonia	Methanol	Average Turnaround
2020	12.0 ± 4.6	7.6 ± 2.2	8.9 ± 3.0	-	-	-	-	9.50
2025	12.2 ± 4.6	7.9 ± 2.3	9.3 ± 3.1	7.6 ± 1.3	21.2 ± 7.9	-	12.2 ± 4.6	11.72
2030	12.4 ± 4.6	7.8 ± 2.6	9.5 ± 3.3	7.8 ± 1.4	21.7 ± 8.5	19.9 ± 7.3	11.0 ± 2.7	12.87
2035	12.4 ± 4.4	7.9 ± 2.7	9.5 ± 3.1	8.0 ± 1.3	22.8 ± 8.1	20.3 ± 7.3	11.4 ± 2.7	13.18
2040	12.2 ± 4.4	8.0 ± 2.6	9.6 ± 2.9	8.2 ± 1.4	23.4 ± 8.2	21.4 ± 7.2	11.7 ± 2.8	13.50
2045	11.9 ± 4.2	8.2 ± 2.8	9.6 ± 2.5	8.4 ± 1.6	24.2 ± 8.4	21.9 ± 8.0	12.0 ± 2.8	13.76
2050	10.9 ± 3.8	8.3 ± 2.5	9.5 ± 2.4	8.6 ± 1.6	24.7 ± 8.5	23.0 ± 7.5	12.4 ± 3.0	13.90

Table 4.5: Evolution of turnaround times (2020–2050) with average standard deviation (in hours)

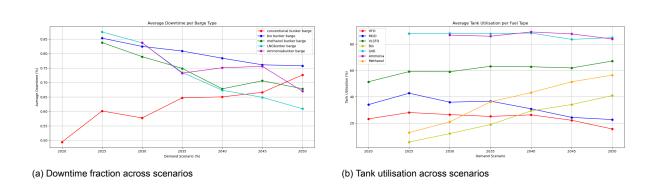
Lastly, the impact of the shift in vessel sizes can be observed, as the data indicates systematic increases in turnaround time across all fuel types, with the rate of change varying considerably by fuel type. The global increase in turnaround time is aligns with the fuel transition patterns observed in the changes in demand, where gas-type fuels become increasingly more dominant in the system's fuel mix.

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Bunker Vessel Utilisation

The operational efficiency of bunker vessels showcases varying performance across different fuel types throughout the transition period, as can be observed in figure 4.4a. Conventional bunker barges showcase an upward trend for the downtime fraction increasing from approximately 49% in 2020 to 72% by 2050, indicating declining operational efficiency for traditional bunkering vessels over the modelled transition period.

Alternative fuel bunker vessels present unique utilisation trends. LNG bunker barges showcase the lowest initial utilisation with a downtime of 87% in 2025, followed by a consistent downward trend reaching 61% by 2050. Methanol bunker vessels display more variable performance, with downtime fluctuating across various scenarios, though generally declining from peak levels observed around 2025-2030 to 67% by 2050. Ammonia bunker vessels demonstrate moderate variability in downtime, demonstrating an initial 84% downtime percentage in 2030 and declining with variations to 67% by 2050. Bio bunker vessels maintain relatively stable decrease, starting off at 85% in 2025 and decreasing to 76% by 2050. Resulting in the projection that bio barges will face the highest downtime at the end of the energy transition.



Tank utilisation varies considerably across fuel types, as presented in figure 4.4b. Among conventional fuels VLSFO demonstrates the highest utilisation rates, increasing from 52% in 2020 to 67% by 2050. In contrast to VLSFO, MGO showcases a a declining pattern, decreasing from 34% in 2020 to 22% by 2050. HFO maintains a relatively low and stable utilisation between 15% and 27% throughout the period.

Alternative fuels achieve notably higher tank utilisation rates compared to all conventional fuels, in particular the gaseous fuels. LNG maintains consistently high utilisation rates above 80% across the transition period with minor variations. Ammonia showcases similarly high utilisation, remaining above 85% throughout most of the modelled transition. Highlighting the efficient storage and refuelling these gas-bunkering vessels achieve, despite the additional challenge of managing boil-off gases. Methanol utilisation rates showcase significant improvements across the modelled scenario, increasing from 13% in 2025 to 56% by 2050. This increase in efficiency is to be attributed to the increase in methanol adoption in the system, serving a wider range of vessels. Bio fuels follow a similar growth pattern progressing from 6% in 2025 to 41% by 2050, reflecting the gradual integration of biofuels into the bunkering system.

Comparing the data for downtime and tank utilisation across all fuel types, an interesting pattern emerges. Conventional bunker vessels, while experiencing lower downtime compared to most alternative fuels, correspond to the fuel types with the lowest tank utilisation rates. In contrast, alternative fuel bunker vessels experience higher downtime percentages, yet make more efficient use of tanks and thus refuelling opportunities. This suggests that operational efficiency does not necessarily correlate with storage efficiency, indicating potentially different operational dynamics. Reflecting on the tank capacity of these vessels, higher utilisation rates may be achieved by a more optimal capacity matched for the specific demand in their segment.

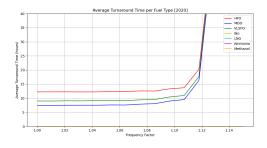
4.3. Results 45

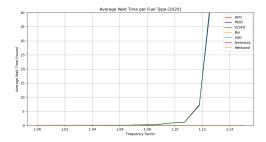
4.3.2. Single Scenario

After obtaining the projections for the global trends in the modelled timeline, unique system performance should be evaluated by applying various single parameter variations. This in order to develop an understanding of how all of the individual supply chains respond to unforeseen stress in the timeline.

Scenario 2020

The frequency sensitivity test for the 2020 scenario, evaluated inter-arrival time scaling factors f in the range of 1.0 to 1.15, with the results illustrated in figures 4.5a-4.7b. The analysis showcases that the existing bunker fleet demonstrates limited adaptability to increased frequency of arriving vessels. A critical threshold emerges at an increase of 10%, where figure 4.5a shows a sharp rise in turnaround times for all fuel types, while figure 4.5b showcases corresponding increases in wait times, indicating that the system is under capacitated at this point.

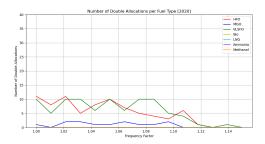




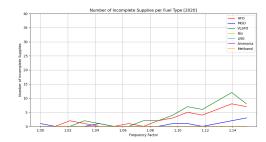
(a) turnaround time vs. frequency

(b) wait time vs. frequency

The results for double allocations and incomplete supplies reveal various operational challenges. Figure 4.6a showcases that double allocations occur even under baseline conditions despite no system growth, suggesting capacity limitations in the current fleet of bunker vessels. As frequency increases, figure 4.6a shows a gradual decrease in double allocations, while figure 4.6b shows a corresponding increase in incomplete supplies beginning at 8% above baseline frequency. This inverse relationship confirms the system's capacity limitations and indicates a transition from resource redundancy to service deficiency as demand intensifies.



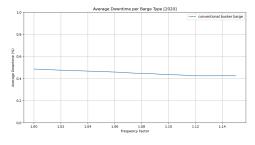
(a) double allocations vs. frequency

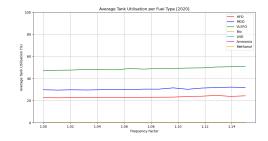


(b) incomplete supplies vs. frequency

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The downtime metric provides further insight into system performance under varying frequency. Figure 4.7a illustrates a relatively stable downtime across all frequency factors, decreasing marginally from 0.48 to 0.42 at maximum frequency. This consistent downtime performance indicates that individual vessel availability is not a limiting factor in the system's capacity constraints. The fuel-specific tank utilisation metrics shown in figure 4.7b showcase individual performance characteristics across the three types a conventional bunker vessels carries. All three fuel types showcase relatively stable utilisation rates across frequency variations, this is to be explained by the fact that the demand proportions remain consistent despite overall increased system load.

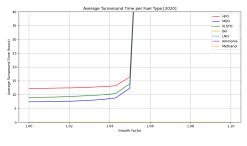


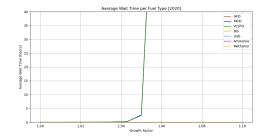


(a) downtime vs. frequency

(b) tank utilisation vs. frequency

The growth sensitivity test evaluated vessel scaling factors \vec{v} from the range of 1.0 to 1.10, obtaining the following results illustrated in figure 4.8a-4.8b. The results from the analysis showcase significant capacity thresholds within the modelled system to an increase in vessel sizes. Evaluating figures 4.8a-4.8b, a drastic increase in both turnaround and waiting times is to be observed at only an increase of 6% of the vessel sizes, highlighting the potential constraint capacity versus demanded quantities imposes on the current system.

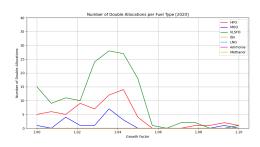




(a) turnaround time vs. growth

(b) wait time vs. growth

Evaluating the metrics for double allocation a drastic increase is to be observed from a 2% increase for all fuel types in figure 4.9a. From an increase of 4% the double allocations decrease, while figure 4.9b showcases a drastic increase. This transition demonstrates how the system initially attempts to accommodate larger vessel fuel demands through resource redundancy, but ultimately shifts from multiple vessel assignments to service failure as the larger individual bunker requirements of growing vessels exceed available capacity. This highlights the constraint of bunker vessel capacity.

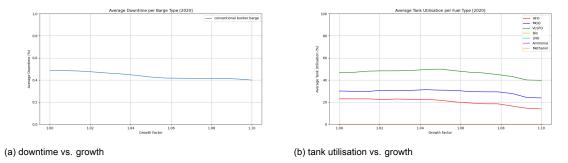


(a) double allocations vs. growth

(b) incomplete supplies vs. growth

4.3. Results

The downtime metric showcases in figure 4.10a a positive response to the growth factor up to a 4% increase showcasing a 5% improvement, reducing initial system redundancy. Past the point of 4% growth the downtime factor stops to improve, which coincides with the observations made in figure 4.9b as the system in unable to perform complete supplies at that point.



Evaluating the tank utilisation of all fuel types during this scenario, an improvement of 5% is to be observed in figure 4.10b over the growth test. This further establishes the limiting factor of the determined capacity of a bunker vessel on system performance.

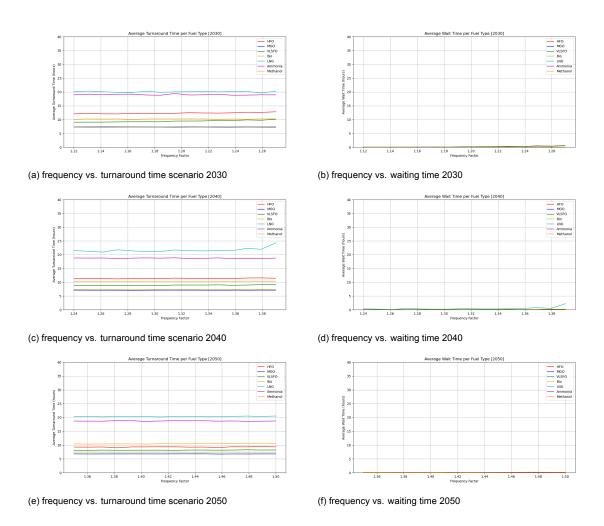
48 4. Simulation

Scenarios 2030-2050

For the alternative scenarios the results were consolidated into a single overview, as all scenarios include all types of required supply chains at various points in time, yet at a different scale of operation. Therefore, consolidating the results from all three different scenarios would provide the most complete insights into the sensitivity, resilience and characteristics of each individual supply chain.

The frequency sensitivity tests performed for the 2030, 2040 and 2050 scenario evaluated the same additional stress as the 2020 scenario for the inter-arrival scaling factor f, evaluating the range of 1.12 to 1.27, 1.24 to 1.38 and 1.35 to 1.50 respectively, with the results illustrated in 4.11a-4.13f. The analysis showcases notably different results from the baseline 2020 scenario in response to the frequency increase for all scenarios.

The turnaround and wait time results demonstrate vastly different results to the characteristics demonstrated in the 2020 baseline. In contrast to the 2020 scenario where a significant response was observed at increases above 10%, figures 4.11a-4.11f illustrates stable results across all frequency factors for the conventional and newly introduced LNG, ammonia and methanol supply chains. This performance consistency suggests that the system, obtained from the solver, possesses substantially different capacity margins than the threshold-sensitive 2020 scenario.



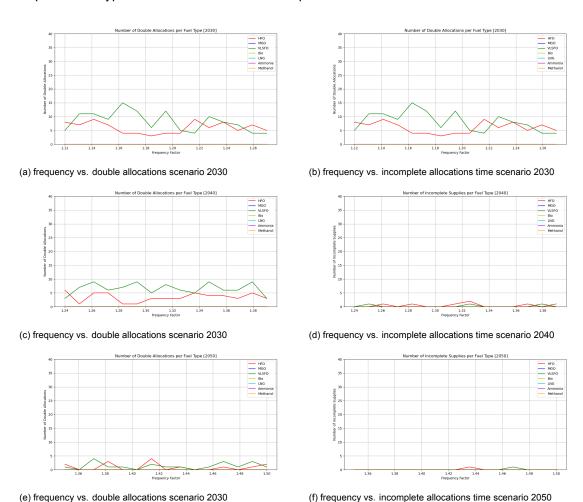
The stable performance across variations in frequency indicates that future supply chain configurations possess adequate capacity buffers to absorb demand volatility without compromising service levels within the system. This additional buffer represents an improvement over the baseline system where increases in frequency resulted in waiting times and service degradation.

4.3. Results 49

However, evaluating the results for the double and incomplete allocations reveals the fundamental issue of redundancy-based system design. Figures 4.6a-4.12e show persistent double allocations for the conventional supply chain across all frequency variations, indicating that the solver relied on resource redundancy to meet turnaround and waiting time criteria. Meanwhile the persistent incomplete allocations shown in figures 4.12b-4.12f demonstrate that systematic over-provisioning with limited individual bunker vessel capacity fails to guarantee service reliability.

This pattern reveals a critical limitation in conventional system scaling. Despite deploying additional vessels to maintain service standards, the rigid constraint of individual vessel capacity creates persistent operational failures. The decreasing frequency of these failures across the simulated scenarios reflects reduced demand for conventional fuels rather than improved system performance, highlighting the importance of bunker vessel design.

Alternative supply chains for LNG, ammonia, and methanol show different results, with no double or incomplete allocations across all frequency ranges and scenarios. This absence of operational failures indicates a fundamental architectural advantage: purpose-built vessels with optimised capacity for specific fuel types eliminate the multi-fuel compromise constraints.

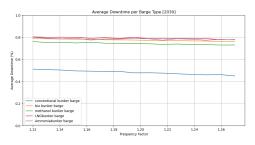


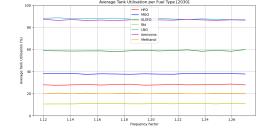
The results illustrate the effect of individual capacity of bunker vessels on scalability and performance when comparing the conventional supply chain with the alternatives. The continued presence across all simulated scenarios for incomplete allocation demonstrates that the elimination of critical frequency thresholds has been achieved by systematic over-capacitated system design, rather than capacity optimisation. Despite the additional resources implemented in the system, the supply chain fails to eliminate incomplete allocations, establishing that under capacitated systems cannot achieve reliability through fleet expansion alone.

50 4. Simulation

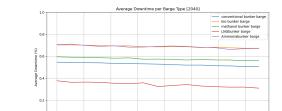
The downtime analysis confirms the redundancy-based capacity across all scenarios. Figures 4.13a-4.13e showcase the conventional bunker vessels maintaining similar levels of downtime across all modelled scenarios, while LNG, ammonia and methanol bunker vessels display various downtime factors. These availability patterns remain relatively stable across variations in frequency factors, in contrast to the 2020 scenario where availability decreased under operational pressure, confirming the deliberate over-capacitated fleet.

The tank utilisation metrics, to be observed in figure 4.13b-4.13f, demonstrate the efficiency implications of the implemented strategy to maintain operational levels, as for conventional bunker vessels the most dominant fuel type achieves the highest utilisation rate, while other fuel types achieve significantly lower utilisation rates. Ammonia and LNG operations achieve high utilisation rates, unused capacity persists across other conventional fuel types throughout all scenarios. This systematic under-utilisation of capacity, occurring in combination with the incomplete allocations, highlights the fundamental flaw of the redundancy-based system design.

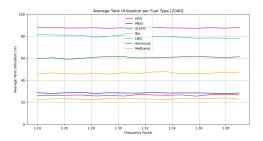




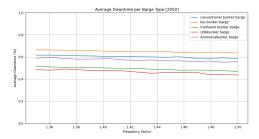
(a) frequency vs. down time scenario 2030



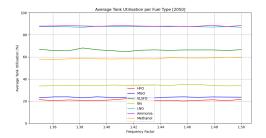
(b) frequency vs. tank utilisation scenario 2030



(c) frequency vs. down time scenario 2040



(d) frequency vs. tank utilisation scenario 2040



(e) frequency vs. down time scenario 2050

(f) frequency vs. tank utilisation scenario 2050

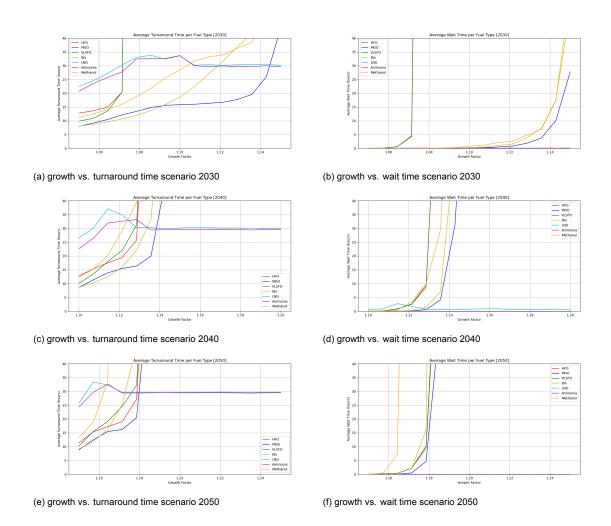
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The growth sensitivity tests for the simulated scenarios evaluated growth factors in the range of 1.05 to 1.15 for 2030, 1.10 to 1.20 and 1.15 to 1.25 for 2050, with results visualised in figures 4.14a-4.16f. In contrast to the frequency sensitivity tests which demonstrated smooth operational curves and resilience to additional stress introduced in the system by increasing the frequency, the growth scenarios display threshold effects similar to those observed in the 2020 baseline.

The turnaround and wait time metrics reveal threshold-driven performance degradation across all scenarios for liquid type bunker vessels. In 2030, illustrated by figures 4.14a-4.14b, the system demonstrates stable results for liquid type bunkers up to 7% growth. Bio and methanol bunker vessels display a more gradual resilience to simulated growth, introducing waiting time in the system from 10% additional growth. In 2040 and 2050 (figures 4.14c-4.14f) this threshold is further compressed.

The progressive threshold reduction reveals that the redundancy-based approach becomes less effective over time. As demand grows, capacity limitations of liquid bunker vessels become more binding, creating increasingly more vulnerable supply chains.

In contrast to the liquid type bunkers, the gas type bunkers display vastly different results. Figures 4.14a-4.14e display an initial increase to growth, yet stabilise across further growth. Furthermore, across all scenarios no waiting time is introduced into the system. This stability showcases the greater scalability potential of these bunker vessels as capacity constraints are less binding in system operation.

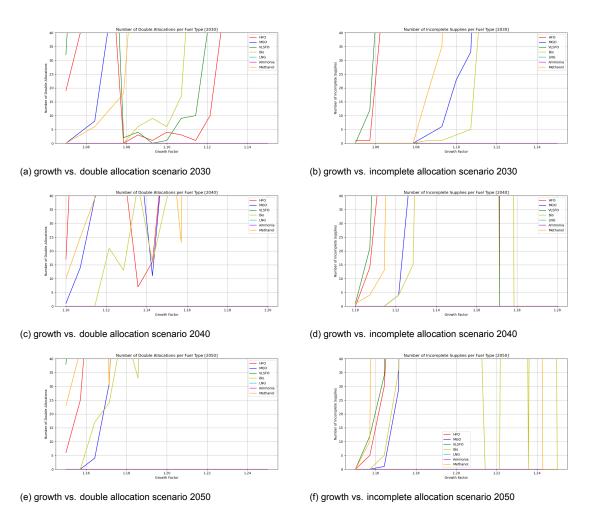


52 4. Simulation

The analysis of the results for double and incomplete allocations provide the complete breakdown of the redundancy-based approach under unexpected growth pressures. In the 2030 scenario, illustrated in figure 4.15a and 4.15b, double allocations initially increase with growth factors for all liquid bunker fuels, reaching peaks of 15-40 occurrences before rapidly dropping to zero as the system rapidly transitions to incomplete allocations, demonstrating complete depletion of system redundancy for the methanol, bio and fossil fuel supply chains.

Under growth pressure, the systems redundancy reserves are rapidly depleted, leading to an instant transition from resource over-allocation to unmaintainable and failed service levels. The 2040 and 2050 scenarios (figures 4.15c-4.15f) exhibit similar but more compressed and extreme failure patterns, with critical transitions occurring at lower growth thresholds.

The binary transition of double to incomplete allocations demonstrates that growth drive demand increases expose flaws in the redundancy-based solution space. Unlike frequency variations which can be observed through over-capacitated systems, sustained growth requires individual capacity expansion which the system is unable to accommodate. This limitation highlights once more that system scaling cannot be achieved by fleet expansion strategies alone, instead requiring optimisation of vessel capacity.

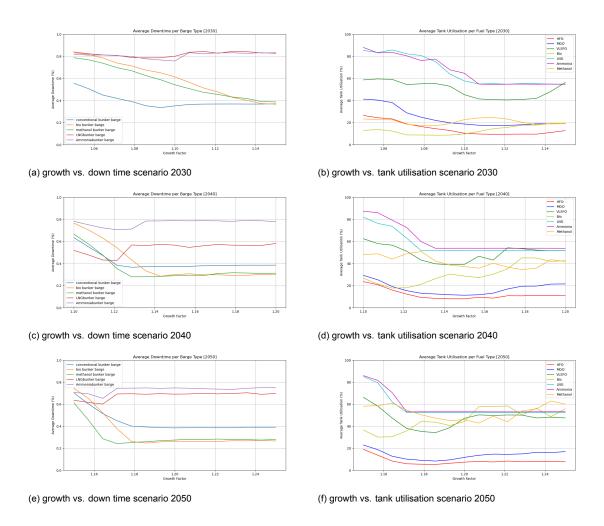


The increasingly severe failure patterns across the various scenarios indicate that the problem compounds over time. Systems that appear to be adequately capacitated in early phases of the transition become critically vulnerable as demand growth continues, suggesting that capacity planning should consider long-term scaling requirements rather than immediate operational needs.

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The results from the downtime metric confirm the complete utilisation of the available fleet capacity under the simulated growth scenarios for the liquid bunkering vessels. In 2030 (figure 4.16a), vessel downtime decreases across all vessel types carrying liquid bunkers as growth factors increase, with conventional bunker vessels improving from 55% to 38% downtime and methanol and bio matching similar downtime percentages at 14% growth. This utilisation improvement occurs at the corresponding points of failure of system performance, exposing an operational paradox that maximum fleet deployment coincides with operational failure.

Tank utilisation metrics, illustrated in figure 4.16b,4.16d and 4.16f, reveal the complete saturation of the capacity under varying growth factors. In contrast to the stable utilisation patterns observed in frequency scenarios, growth driven demand forces utilisation rates to approach or exceed 80% across multiple fuel types before system performance drastically deteriorates. The utilisation saturation, combined with the performance failures, demonstrates that the current vessels implemented in the simulation face scalability constraints.



The single scenario analysis demonstrates that growth sensitivity exposes the critical weakness of redundancy-based system optimisation employed in future scenarios. While frequency variations can be absorbed through systematic over-capacity, sustained demand growth reveals that the elimination of capacity optimisation in favour of redundancy creates systems that appear stable under a vast amount of different operational scenarios, yet fail under scaling requirements. This highlights the importance of individual bunker vessel capacity over number of bunker vessels deployed in a system. Furthermore, it establishes that under-capacitated systems cannot be scaled through introducing additional assets, only through scaling individual assets.

Discussion and Conclusion

The discrete-event simulation of the bunker supply chain in the Strait of Gibraltar has revealed various insights into how the maritime industry's transition to sustainable fuels will reshape bunker operations. This chapter discusses the implications of the results and places the findings in a broader context of the maritime industry, besides the bunker industry.

5.1. Discussion

The Scale of Transformation: Beyond Fuel Substitution

The simulation results show that the shift to sustainable fuels would entail substantial changes in bunker operations, fundamentally altering the industry's notion of what exactly constitutes as a 'fuel transition.' The projected 230% increase in bunker fleet size from 20 conventional vessels for a single integrated supply chain in 2020 to 66 vessels over 5 unique supply chains by 2050 illustrates that this transformation will go well beyond simple fuel substitution to include a expansive restructuring of operational infrastructure and models.

The observation that the fleet is required to double in the initial transition stage (2020-2025), when just 7% of the total energy mix moves to alternatives, emphasises that diversification, rather than volume growth drives the first phases of infrastructure investment. This conclusion challenges the fundamental assumption about gradual transition impacts that have supported industry planning. The assumption that moderate alternative fuel uptake will necessitate correspondingly small infrastructure changes proves incorrect - even little diversification necessitates large infrastructure requirements.

The underlying driver of this step-change lies in the incompatibility between current multi-fuel operational requirements and alternative fuel requirements. The demand for purpose-built, fuel-specific bunker vessels, as illustrated by the transition from a single multi-fuel supply chain to five unique supply chains, introduces capacity constraints that cannot be addressed via gradual modifications. Each new fuel type necessitates the development of a new supply chain, including specialised vessels, fuel specific operational processes and dedicated storage infrastructure.

This realisation has consequences for the transition strategy in place by the industry and investment timing. These findings highlight that the traditional method of building infrastructure in stages may be misaligned with the actual industry requirements of alternative fuel adoption. Instead, the industry faces a binary choice: maintain current infrastructure for conventional fuels while creating parallel infrastructure for alternatives, or commit to comprehensive system transformation that anticipates the full scale of necessary change.

The scale of this transition is further illustrated by the projected 226% rise in overall fuel demand from 5 million tons in 2020 to 16.3 million tons by 2050. This tripling of demand volumes, caused mostly by the lower energy density of alternative fuels, complicates the infrastructure challenges beyond simple fleet diversification. The simulation shows that LNG and ammonia alone will account for

78% of the total tonnage by 2050, despite being a smaller portion of the energy mix, demonstrating how differences in energy density amplify logistical complexities in ways that conventional volumetric planning approaches fail to capture.

The scale of change displayed in the results of the simulation indicate that the bunker industry will undergo significant changes beyond simple infrastructure and fuel portfolio diversification. The need for purpose-built vessels and infrastructure, combined with the capital requirements of these systems, may encourage industry consolidation as smaller market shareholders lack the resources to sustain competitive positions across several fuel types. :The simulation results further establish this as purpose-built systems displayed greater scalability compared to multi-fuel systems, suggesting that the future bunker industry may be characterised by fuel-specific operators rather than universal fuel suppliers.

Operational Performance Implications

The simulation findings show a substantial shift in operational efficiency, that extends beyond simple increases in turnaround time, altering the complexity in scheduling maritime operations and route dynamics of marine logistics. The 46% increase in average turnaround time from 9.5 hours in 2020 to 13.9 hours by 2050 suggests not only longer operations, but also significantly broader operational windows, challenging the strict scheduling on which maritime operations are based. By 2050, LNG and ammonia operations are projected to extend to 25 hours and 23 hours respectively, with significant variability ranges of ± 7 to ± 8.5 hours. This transforms bunkering from a narrow-window auxiliary operation to a wide-window scheduling constraint, requiring significantly larger time buffers.

When compared to present maritime operations the extent of this transition becomes clear. While container vessel turnaround times in major ports currently range from 24-72 hours [14], simulation results show that alternative fuel bunkering operations are approaching 30 hours for dominant fuel types, indicating that bunkering is moving from a minor port call component to a potential critical path constraint, illustrated in figure 5.1. Beyond causing operational strain, this convergence alters the critical path analysis that forms the basis of maritime scheduling. The extended duration of alternative fuel bunkering operations, combined with safety and regulatory considerations that may limit simultaneous cargo operations, creates uncertainty about whether bunkering can continue as a parallel activity alongside cargo handling or must transition to a sequential constraint that determines overall port stay duration. This operational unpredictability adds to the scheduling complexity, as port call planning must account for several different operational situations based on individual port regulations, safety measures, and infrastructural capabilities for each alternative fuel type.

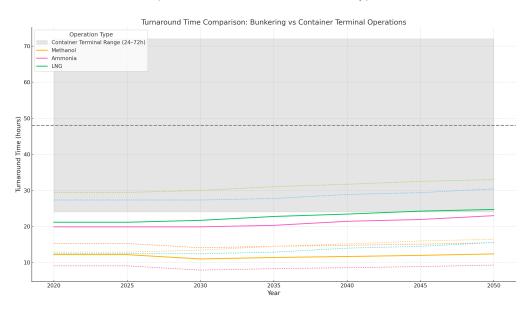


Figure 5.1: loading vs bunkering times

5.1. Discussion 57

The implications extend beyond individual vessels and have an impact on the entire shipping network efficiency. Extended and variable bunkering times reduce the effective capacity of the maritime transport system by increasing the downtime in port, just when global trade demand necessitates higher transport capacity. This capacity reduction can not be addressed by typical optimisation since the lower energy density and fuel handling requirements of alternatives fuels result in inescapable increases in operational time that persist independent of operational efficiency of bunkering operations.

The operational performance changes illustrated in the simulation create a multiplicative rather than additive effects across maritime networks, having an impact that extends beyond bunkering operations. Extended bunkering times at major bunkering hubs like Gibraltar cause accumulating delays across marine networks, particularly for line services that operate on set schedules and rely on predictable port call scheduling. The concentration of fuel demand in these bunker hubs compounds these impacts, potentially resulting in congestion bottlenecks that degrade overall system reliability.

These effects across the network suggest that the transition to alternative fuels may need/introduce changes in maritime network design and operating philosophy. Traditional operating models that prioritise transit time and fuel economy may be insufficient when bunkering activities become more time consuming and variable. The industry may require new network designs that can handle stochastic rather than deterministic bunkering processes, which could necessitate more distributed infrastructure or alternate service patterns that reduce reliance on main bunker hubs.

The extended bunkering operations would necessitate increased collaboration among bunker suppliers, terminal operators and port authorities to manage this new operational reality. Port authorities face the problem of restructuring locations for bunkering operations, which may require alternative fuel bunkering areas in order to mitigate prolonged berth allocations that conflict with the high utilisation patterns of modern ports. Terminal operators must include lengthier, more variable bunkering operations into cargo handling schedules, which may necessitate additional safety protocols and system that allow for simultaneous operations with alternative fuels.

Supply Chain Resilience and Vulnerability Patterns

The sensitivity analysis displays that the industry's redundancy-based optimisation creates systematic vulnerabilities in both conventional and alternative fuel supply chains, with these flaws becoming increasingly more amplified in future systems due to the higher individual capacity requirements. The baseline system already demonstrates the limitations of the current optimisation philosophy, operating within narrow margins that displayed performance degradation at an 8% increase in vessel frequency and system failure at 10% growth in individual vessel demand. These results highlight that the existing approach of prioritising vessel quantities over individual capacity, creates supply chains that lack operational buffers needed for reliable service under modest demand fluctuations.

When the same redundancy-based approach is applied to future energy transition scenarios, the underlying design flaws are magnified, resulting in even more sensitive supply chains with lower thresholds. The solver's consistent response of adding more vessels rather than deploying more capable vessels, becomes inevitably more inadequate as individual demand increases to exceed single vessel capabilities. This fundamental mismatch between optimisation philosophy and operational reality results in the various asymmetric risk profiles seen across the simulated scenarios.

The 2030-2050 scenarios show how these optimisation flaws manifest in the conventional, methanol and biofuel systems: while they can accommodate significant increases in vessel frequency (up to an additional 15% in tolerance) using the redundancy-based approach of adding more vessels, they fail when individual vessels require moderately larger fuel quantities (as little as a 2% increase in growth). This asymmetric pattern is a direct result of using quantity-over-capability optimisation on systems. As a result, systems appear over-resourced under typical conditions yet become inadequate as energy demands rise - a more extreme version of the baseline system's already narrow margins.

The persistent presence of double allocations across future scenarios, occurring simultaneously with incomplete allocations, demonstrates how redundancy-based optimisation errors worsen rather than improve through system scaling. While baseline supply chains show gradual performance degradation under load, future scenarios go from apparent overcapacity to service failure. This transition from progressive to binary failure modes highlights the limitation of redundancy-based solutions to increasingly complex operational requirements. This pattern highlights that the optimisation strategy requires a revision to address individual capacity over minimising assets.

The analysis finds significant performance variations across fuel types that have implications for system scaling and risk management. Gas-based systems (LNG and ammonia) are more resilient to both frequency and growth variations, with no double or incomplete allocations across all scenarios due to their purpose-built design philosophy with increased individual capacity. In contrast, liquid fuel systems (conventional, methanol and biofuels), often based on conventional small tanker designs, exhibit threshold effects and binary failure modes, suggesting that individual vessel capacity is the primary constraint creating the observed vulnerabilities.

The better resilience of gas-type systems supports the key strategic takeaway from the single scenario analyses: in order to develop reliable and future proof supply chains, expansion strategies must prioritise individual capacity over vessel count. The complete absence of operational problems in LNG and ammonia systems, together with favourable resilience to system growth, illustrates that larger capacitated purpose-built vessels overcome optimisation flaws from quantity-based methods. These results suggest that bunker suppliers should avoid deploying a large number of smaller vessels in favour of fewer, larger, purpose-built vessels matched to long term operational requirements.

The capacity focused approach represents a shift from minimising capital investment and risk through vessel count minimisation to maximising operational reliability through capability optimisation. While this strategy will necessitate higher individual capital expenditure, the results show that the operational benefits justify the additional capital through improved long term reliability and reduced operational risk. The strategic imperative is clear: sustainable fuel implementation necessitates purpose-built vessels with capacity as the fundamental design criterion, with fleet size defined by capacity needs rather than asset minimisation.

Infrastructure and Capacity Challenges

The results of the simulation consistently indicate that individual vessel capacity is the key constraint limiting system performance and scalability in bunker supply chains, which challenges the strategy behind present industry practices and regulatory regulatory frameworks. The analysis directly confronts the widespread strategy of employing vessels under 4,999 GT to avoid pollution frameworks such as EU-ETS, Fuel EU and IMO Net-Zero, demonstrating that these avoiding tactics result in an imbalance between compliance and operational optimisation. The sensitivity analysis demonstrates that capacity constraints cannot be addressed just through fleet expansion, they necessitate individual scaling of assets, requiring to prioritise capability over number and compliance cost.

The comparison between liquid and gas-type bunkering illustrates the implications of this capacity constraint. While conventional bunker vessels serving multiple fuels achieve utilisation rates of 20-70%, constrained by the operational complexity of managing diverse fuel requirements, purpose built vessels gas-type vessels achieve 80% utilisation rates on average. This higher utilisation, combined with the absence of operational capacity shortage, suggests that larger single-fuel purpose-built vessels are a better platform to scale, despite the need for a larger more diversified fleet.

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The failure of redundancy-based scaling through the constraint-driven behaviour patterns of the optimisation solver in the research identifies a key shortcoming in the conventional capacity management in the industry. When confronted with capacity shortages, the solver responds systematically by adding additional vessels rather than deploying vessels with larger individual capacity, not by choice, but by the limitations imposed by the fixed vessel specifications based on current vessel designs. This constraint reflects the inadequacy of design requirements imagined by bunker suppliers for alternative fuel operations, in which individual fuel demands exceed the capacities of current bunker vessel layouts. The end result is a redundancy-based scaling approach, that prioritises vessel count over capacity, resulting in systems that appear to be over-resourced in terms of vessel count while essentially underdesigned for actual operating requirements.

The effects of these design constraints are demonstrated by the frequent occurrence of double and incomplete allocations across all simulated scenarios. The combination highlights the basic shortcomings of current design proposals when applied to future scenarios, as it necessitates multiple assets for individual deliveries while simultaneously failing to service other enquiries. The binary transition patterns observed under growth stress, in which systems go from apparent over-capacity to service failure, show that current vessel designs in combination with redundancy-based scaling create fragile systems that conceal fundamental deficiencies until operational thresholds are exceeded. The results obtained from the solver demonstrates that the fault lies in the limited underlying vessel designs that determine capacity possibilities.

The demand projections suggest significant imbalances that could entail changes in sourcing strategies and potentially storage strategies. The difference between the expected methanol demand and announced regional production capacity illustrates these difficulties. The aggregate production capacity of one confirmed and two conceptual methanol plants around Gibraltar is set to deliver 687, 000 tons per year by 2035 [41], yet the simulation projects regional methanol demand to reach 1.2 million tons by the same year, suggesting a supply gap approaching 2:1 even in the near future.

This regional imbalance despite worldwide methanol production capacity forecasts of 14 million tons by 2035 [41], demonstrates the localised nature of bunker supply chain networks and the difference between the global capacity evaluation for regional operational requirements. This gap suggests that bunker suppliers will need to adopt more extensive sourcing strategies that go beyond regional suppliers, possibly requiring proactive storage in order to meet demand that exceeds local production by quite a margin.

These supply-demand imbalances suggest that bunker supply chains will face the challenge of a significant restructuring, potentially including greater storage facilities, long-distance sourcing and pro-active inventory management strategies that differ significantly from current real-time inventory availability models. The need to source alternative fuels from distant production facilities introduces new forms of supply chain risk, including transportation delays, quality variations and supply chain disruptions.

Strategic Implications for Bunker Suppliers

The transition from a single integrated supply chain to five distinct supply chains represents a significant shift in business model that will challenge all aspects of current suppliers operational models. The results suggest that bunker suppliers could face a strategic choice between diversification across multiple fuel types and increased operation complexity versus specialisation in specific fuel segments that allow for concentrated optimisation and risk management. The operational complexity suggested by the simulation for managing diverse fuel portfolios, compared to the efficiency demonstrated by single supply chains, could indicate that the traditional universal supplier model may become economically unviable.

The efficiency differences between approaches further provide evidence for the specialisation strategies. Purpose-built systems demonstrate higher utilisation rates, better resilience across stress scenarios and better long term operational viability. However, specialisation introduces the risk of market concentration and reduced diversification that must be weighed against the operational benefits.

The 230% increase in required bunker vessels, along with the need for complex fuel-specific vessels, creates a serious capital investment challenge for the bunker industry. The results from the optimisation show that this investment cannot be scaled progressively due to the step-change in infrastructure requirements driven by diversification of demand, necessitating significant upfront capital investment before demand and revenue mature. This temporary mismatch between investment requirements and revenue generation raises basic finance issues that could affect structure and ownership. Furthermore, it raises the question whether to adopt an a first mover advantage and be proactive or adopt a reactive mindset and follow demand.

The capacity constraint findings suggest that investment decisions should prioritise vessel capability over vessel quantity, contradicting the traditional cost management strategy of employing smaller, less expensive vessels. The simulation demonstrates that under-capacitated vessels cannot achieve reliability through redundancy, suggesting that investment should be targeted at fewer larger vessels over larger fleets of smaller vessels - an investment strategy that significantly influences capital allocation and fleet planning.

Model Performance and Applicability

The hybrid-modelling framework developed in this research provides a quantitative method for evaluating the operational implications on the ship-to-ship bunkering operation for transitioning to sustainable marine fuels. The main component of the model lies in the discrete-event simulation module, which enables a detailed representation of ship-to-ship bunkering operations. By simulating each process individually, the model offers a detailed analysis of how different fuel types and demand profiles influence system performance, including turnaround times, asset utilisation and gueue formation.

The integration of real-world operational data provided by Peninsula grounded the simulated behaviour, ensuring outcomes reflect practical constraints rather than theoretical abstractions/assumptions. The integration of distinguished liquid and gas-based bunkering adds value, as it is a critical requirement given the operational divide between emerging fuels. Methanol and biofuel follow conventional liquid handling procedures, whereas LNG and ammonia introduce cryogenic or pressurised conditions, requiring fundamentally different operational approached. By modelling both types based on actual process characteristics, the simulation supports data-grounded extrapolation to future fuels without relying solely on generic assumptions.

The optimisation module of the framework adds value by identifying near-optimal fleet compositions for transition scenarios through a structured search technique, which combines results from multiple simulation runs. The module effectively assessed various combinations of bunker vessels using performance measures such as turnaround time and waiting time. This enabled the module to determine not just the number of bunkering vessels required, but also the fuel configurations required to meet future demand under segmented demand conditions. The optimisation module's results revealed that diversification, rather than expansion, drives fleet growth, which has obvious consequences for fleet planning.

Modelling Assumptions

Despite these outlined strengths, the model still faces several limitation in its current implemented form that must be discussed. A key constraint lies in the behavioural rules governing agent interaction. Stakeholders are modelled with fixed decision patterns and are unable to adapt their decision making process in response to changing conditions. As a result, realistic dynamics such as supplier competition, re-routing, or reactive scheduling are not represented, limiting the models ability to capture the full dynamics between stakeholders in a bunkering hub.

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In addition, a number of parameters related to alternative fuels were derived from vessel design guidelines, limited pilot studies/projects or engineering assumptions. While some operational characteristics are based on real-world data from similar processes, large-scale bunkering of fuels such as methanol and ammonia remains untested. This introduces a certain degree of uncertainty into the outcomes of the simulation, in particular to the results obtained for service duration and infrastructure requirements. The results of should therefore be interpreted with a careful bias, especially when assessing fleet sizing and demand for future scenarios.

Operational Constraints and Scope

On an operational aspect, the simulation excludes several important real-world variables. Unplanned disruptions such as equipment failures, weather delays and human error are excluded from the performance, even though these elements often shape day-to-day bunker operations. Similarly, fuel-specific safety procedures for toxic fuels like ammonia and methanol are not explicitly accounted for in the process logic, potentially leading to an underestimation of service durations for certain fuel-specific supply chains.

Furthermore, the model does not simulate terminal operations in detail, excluding production and storage constraints, infrastructure availability and berth allocation queues. This abstraction limits the models ability to assess bottlenecks or queuing dynamics created by terminal throughput limitations. Vessel transport times are drawn from distributions rather than position based routing, which removes the influence of spatial layout and reduces the accuracy of queue dynamics.

The optimisation framework is constrained as well by its reliance on predefined vessel designs. All bunker vessels are modelled as rigid, fuel specific platforms, instead of flexible or modular configurations that are the current standard in modern bunkering operations. This limits the solution space the solver can explore for determining optimal fleet compositions and potentially under-represents the operational flexibility that could be achieved through mixed-fuel vessel strategies or adaptive deployment models. Furthermore, by optimising on each individual scenario instead of a longer duration for the transition timeline, the optimiser only obtains an temporary fleet configuration.

Lastly, the models spatial scope presents a fundamental constraint. The simulation environment is specifically calibrated for the bunkering hub of Gibraltar, using data and infrastructure parameters unique to that operating area. While this specificity enables for more realistic modelling, it also limits generalisability.

Overview Discussion

Despite all the outlined limitations, the model served its purpose. It provided a framework to quantify the influence of fuel diversification on service times, fleet performance, fleet composition and overall system pressure. It enabled a consistent evaluation of each simulated scenario using the same operational logic. Its integration of real-world data and scenario-based logic allows for meaningful comparisons across transition pathways, offering insights that are both prescriptive and grounded in plausible operational conditions.

To conclude on the results of the discussion, the transition to sustainable marine fuels will not only introduce new fuel types, but will also reshape the structure and function of bunker supply chains. This model demonstrates how fuel diversification increases systemic complexity, amplifies pressure on existing assets, and challenges the assumptions underpinning current fleet configurations. Although simplifications were necessary to enable implementation, the simulation produces results that align with projected transition dynamics. With further development of infrastructure modelling and dynamic infrastructure allocation, the model could prove to be a helpful for suppliers to understand the energy transition.

5.2. Conclusion

The maritime industry's transition toward sustainable fuels represents far more than a simple fuel substitution; it is a fundamental shift that will redefine the structure of fuel logistics, operational performance and infrastructure requirements across the bunker and maritime supply chain. This research applied a research framework for developing a case study of the Gibraltar bunkering hub to quantify the operational impact of this transition on a port-level basis. The results demonstrate how even a small transition to alternative fuels can result in large infrastructure requirements, driven mostly by the projected segmented fuel uptake. The model produces three key findings that challenge current industry assumptions on the transition to sustainable fuels:

Fleet expansion through market diversification: The shift from a single integrated supply chain to five fuel-specific supply chains may require a 230% increase in number of bunker vessels. Remarkably, fleet requirements may already double when alternative fuels represent only 7% of total energy demand. This challenges the gradual planning approaches, as infrastructure strain is caused by the segmentation effects inherent in fuel diversity, rather than by growing demand. Early-stage infrastructure constraints appear unavoidable without directed investment initiatives.

Operational Performance Under Pressure: The transition introduces challenging operational complexities that extend well beyond fuel handling. Average system turnaround times increase by 46%, while gas-based operations stretch to 23-25 hours on average with considerable variability based on the receiving vessel. These extended durations could potentially transform bunkering from a routine background operation into a critical constraint that directly impacts port planning and voyage scheduling. The effects could prove substantial as operational margins would compress across the maritime supply chain.

Rethinking Vessel Design Philosophy: Conventional approaches to vessel design and deployment prove inadequate for alternative fuel scenarios. The research demonstrates that traditional tactics that rely on redundant deployment and use a large number of vessels with limited individual capacity are vulnerable to systemic failure under operational pressure. In turn, purpose-built vessels, particularly those designed for gas-based fuel, achieve complete reliability across all scenarios when equipped with sufficient individual capacity. This suggests that future infrastructure requirements should prioritise individual vessel capability over fleet quantity.

These insights were derived from the hybrid-modelling approach applied in the case study that integrates discrete-event simulation with optimisation. The model included both liquid and gas-based fuels, enabling realistic projections for emerging fuels including methanol, ammonia and potentially hydrogen. The simulation enables a high level of detail in system analysis by modelling the operational dynamics of bunkering, including service time variability and queueing behaviour. The optimisation component identifies fuel-specific fleet configurations that can operate reliably under a variety of future demand scenarios. This dual approach provides both diagnostic insight on current limits and prescriptive direction for strategic fleet expansion and resource allocation.

The research presented here challenges market participants to reconsider incremental implementation and account for more discontinuous operational shifts in the transition to sustainable marine fuels. The findings suggest a revision of asset acquisition strategies where individual vessel capability and capacity exceed fleet size.

As the maritime sector transitions to alternative fuels, ensuring reliable bunker operations remains fundamental to ensure global trade functionality. The quantitative framework applied in this study provides initial guidance for understanding the impact of this transition and ensuring that projections align with operational practice.

The path forward necessitates significant infrastructure decisions now to support tomorrow's fuel scenario. Only by taking proactive steps can the sector avoid the operational constraints that threaten to constrain the very energy transition it seeks to achieve.

5.3. Recommendations for Future Research

The findings derived from the results highlight several critical areas requiring additional research to further develop an understanding of the bunker supply chain transition to sustainable fuels and to provide more comprehensive decision support for industry stakeholders.

Enhanced Model Complexity: Future studies should include terminal modelling to capture the interactions between bunker vessels and loading terminals, such as product and berth availability. To generate more realistic operational time predictions, future models should take into account operational inefficiencies, delays and additional safety procedures. Position-based transportation calculations and queue modelling would for a more detailed study of bunker hubs that serve multiple ports, as well as a more accurate portrayal of the transport phase in the supply chain.

Expanded Scenario and Sensitivity Analysis: The scope of research should extend beyond a single transition scenario to include various transition timelines, delayed fuel uptake, shifts in projected demand in order to challenge the results found from this research. Multi-hub dynamics and demand migration patterns between bunker hubs are significant additions that should be addresses in order to understand the implications of concentrated regional demand and availability. Shifts in regulation and their effect on vessel design requirements and in particular on operational process need to be further investigated.

Multi Parameter Optimisation: Future models should implement multi-parameter optimisation incorporating bunker vessel capacity, fuel type compatibility and asset allocation across the transition timeline rather than static five-year intervals. Cost-based optimisation integrating capital and operational expenditure and revenue would provide more realistic recommendations for commercial decision making for determining fleet composition.

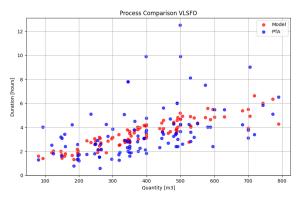
Market Dynamics: Market mechanisms such as fuel price changes, supply and demand elasticity, supplier competition and customer decision behaviour should be considered in further research. Asset lifecycle modelling, which includes vessel replacement cycles, retrofit options and mixed-generation fleet management throughout the transition scenario would further provide more accurate planning insights.

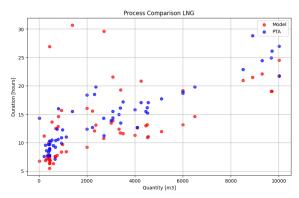
By implementing the outlined suggestions a more comprehensive picture could be created on the impact the energy transition will have on the bunker industry and what challenges they might face now or in the future.



Statistics

In figures A.1a and A.1b, the results comparing the actual and simulated operations can be observed for a set of random operations, highlighting similar grouping. Please take note that the K-S test represents the actual comparison between the distributions as the stochastic nature of the simulation misrepresents these results.





(a) PTA data vs. model VSLFO

(b) PTA data vs. model LNG

Operation	Distribution	Mathematical Formulation
Gas Mooring Connection Time	Lognormal	$X \sim \text{Lognormal}(s = 0.870, \text{ loc} = 0, \text{ scale} = 0.3150)$
Gas Mooring Time	Lognormal	$X \sim \text{Lognormal}(s = 0.820, \text{loc} = 0, \text{scale} = 1.6807)$
Gas Unmooring Time	Lognormal	$X \sim \text{Lognormal}(s = 0.820, \text{loc} = 0, \text{scale} = 1.6807)$
Gas Disconnection Time	Gamma	$X \sim \Gamma(k = 2.375, \text{ loc} = 0, \theta = 0.1762)$
Bio/Conv Mooring + Unmooring	Uniform	$X \sim \mathcal{U}(0.9, 1.1)$
Sailing Time (All Barges)	Uniform (Scaled Int)	$X = 2 \cdot \mathcal{U}_{\text{int}}(7, 13)/10$

Table A.1: Stochastic Distributions Used in Bunker Barge Operations

The following table A.2 includes the variance in results for the various simulated operations per fuel type. The scale of the variance determined the factors for the thresholds of the gradient based optimisation, higher variance meant a higher threshold factor.

Table A.2: Factors for fueltypes

Туре	HFO	MGO	VLSFO	Bio	Methanol	LNG	Ammonia	
Variance	low	low	standard	medium	medium	high	high	
Factor	0.80	0.80	1.00	1.20	1.20	1.50	1.50	

66 A. Statistics

The following distribution was drawn from the S&P data in order to determine the inter arrival time between bunkering operations performed in the Gibraltar bunkering hub. Based on the obtained distribution the lognormal distribution was fitted in order to develop the simulation component for the vessel generator. Where $\mu_a=-0.131$ and $\sigma_a=1.113$

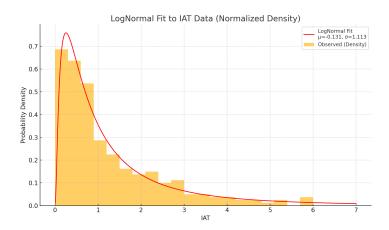


Figure A.2: Overview of drawn distribution of IAT probability (01/01/2024 - 31/12/2024)

The following two tables include the probability weights of the sizes of vessels (A.3) arriving in the Gibraltar bunkering hub and the type probabilities corresponding to the respective sizes (A.4). For confidentiality the tables for respective deal sizes for size/type and receiving rates have been excluded from the research.

size	probability
capesize	0.0509
conventional gas carrier	0.0025
general tanker	0.0417
handymax	0.0314
handysize	0.0343
kamsarmax	0.0409
large gas carrier	0.0018
large handy	0.1635
lr1 (panamax)	0.0151
lr2 (aframax)	0.0422
medium gas carrier	0.0117
mini capesize	0.0201
mr (handymax)	0.0434
new panamax	0.0128
pmax	0.0271
post panamax	0.0191
q flex	0.0048
q max	0.0001
small	0.0291
small gas carrier	0.0085
small handy	0.1047
small tanker	0.0186
suezmax	0.0389
supra	0.1278
ultramax	0.0945
very large gas carrier	0.0078
vlcc	0.0068

Figure A.3: Size Probability Vector For Gibraltar Bunkering Hub (01/01/2024 - 31/12/2024)

0.	0	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9	0	9	0	0	0	0	0	0
ro-ro	00.00	00'0	00'0	0.03	00'0	00'0	00'0	00'0	00'0	00'0	00'0	00.00	00'0	00'0	00.00	00'0	00'0	00.00	0.36	00'0	0.16	00'0	00.00	00'0	00'0	00.00	00.00
passenger cruise products tanker	0.00	0.00	0.01	0.00	90.0	0.00	0.00	0.00	0.89	0.51	00.0	0.00	0.14	00.0	0.00	0.00	00.0	0.00	0.00	00:00	0.00	0.14	0.03	0.00	0.00	0.00	0.00
passenger cruise	00.00	0.00	00'0	00.00	0.00	00.00	00.00	00.00	0.00	00.00	00'0	0.00	0.00	00'0	0.00	0.00	00'0	0.00	0.11	00'0	0.01	00'0	0.00	0.00	00'0	0.00	0.00
offshore	00.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	00.00	0.00	0.00	00.00	0.00	0.00	0.00	0.03	0.00	0.00	0.00	00.00	0.00	0.00	00.00	0.00
general cargo	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.40	0.00	0.20	0.00	0.00	0.04	0.03	0.00	0.00
gas tanker	0.00	1.00	00.00	0.00	00.00	0.00	1.00	00.00	00.00	00.00	1.00	00.00	00.00	1.00	00.00	00.00	1.00	1.00	00.00	0.99	00.00	0.00	00.00	00.00	00.00	1.00	0.00
crude oil tanker cellular container gas tanker general cargo	0.47	0.00	0.00	0.55	0.00	0.24	0.00	0.19	0.00	0.00	0.00	0.92	0.00	0.00	0.30	0.72	0.00	0.00	0.10	0.00	0.52	0.00	0.00	0.22	0.15	0.00	0.00
crude oil tanker	0.00	0.00	0.00	00.00	0.00	0.00	0.00	0.00	0.04	0.49	00.00	0.00	0.00	00.00	0.00	0.00	00.00	0.00	0.00	00.00	0.00	00.00	0.97	0.00	0.00	0.00	1.00
chemical tanker combined chemical and oil tanker	0.00	0.00	0.08	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.03	0.22	0.00	0.00	0.00	0.00	0.00
chemical tanker	0.00	0.00	0.91	0.00	0.89	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.80	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.63	0.00	0.00	0.00	0.00	0.00
bulk carrier	0.52	0.00	0.00	0.32	0.00	0.76	0.00	0.64	0.00	0.00	0.00	0.08	0.00	0.00	69.0	0.28	0.00	0.00	0.00	0.00	0.07	0.00	00.00	0.75	0.82	00.00	0.00
size/type probability	capesize	conventional gas carrier	general tanker	handymax	handysize	kamsarmax	large gas carrier	large handy	Ir1 (panamax)	Ir2 (aframax)	medium gas carrier	mini capesize	mr (handymax)	new panamax	pmax	post panamax	q flex	q max	small	small gas carrier	small handy	small tanker	suezmax	supra	ultramax	very large gas carrier	vlcc

Figure A.4: Size vs. Type Probability Matrix For Gibraltar Bunkering Hub (01/01/2024 - 31/12/2024)

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