Decision support system for control of emissions from ships in port areas, based on machine learning and optimisation methods

Thesis for the degree of Doctor of Philosophy

FILIP BOJIĆ

University of Split
Faculty of Maritime Studies

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Preface

This thesis is submitted for partial fulfilment of the requirements for the degree of Doctor of Philosophy (Ph.D.) in Technical Sciences (UDC 62), at the University of Split - Faculty of Maritime Studies.

This doctoral work has been performed between November 2019 and November 2025 at the Nautical Engineering Department of University of Split - Faculty of Maritime Studies in Split, Croatia, with Professor Rino Bošnjak as the main supervisor and Professor Anita Gudelj as co-supervisor.

Abstract

Air pollution from maritime transport presents a growing environmental and public health challenge, particularly in densely populated port cities. Despite the shipping industry's critical role in global trade, ship-sourced emissions, especially during port operations, are often underestimated in both regulatory frameworks and emission reduction strategies. Ports, as multimodal hubs of economic activity, experience high concentrations of pollutants such as nitrogen oxides (NO_x), sulphur oxides (SO_x), particulate matter (PM), and greenhouse gases (GHGs), which are released during key operational phases including cruising, manoeuvring, and hoteling. The lack of high-resolution, operationally grounded, and scalable methods for quantifying and managing these emissions has hindered both policy formulation and effective mitigation at the local level.

This research is motivated by the increasing need for intelligent, data-driven tools that align with the development of smart ports and the wider adoption of Internet of Things (IoT)-based technologies. The concept integrates real-time data flows, vessel tracking systems, and machine learning analytics into a structured and flexible system that can support emission management and strategic decision-making in seaports. In response to this need, the Port-related Emissions Prediction, Analytics and Risk Evaluation (PrE-PARE) Decision Support System (DSS) was developed. The system enables the quantification, prediction, evaluation, and optimisation of ship-based emissions by integrating extensive technical and operational datasets within a modular framework.

The PrE-PARE DSS comprises four interlinked modules. The Module 1 focuses on emissions estimation through a bottom-up, trajectory-based approach, utilising Automatic Identification System (AIS) data and vessel technical specifications to produce high-resolution inventories across all operating modes. The Module 2 incorporates a supervised machine learning model Multivariate Adaptive Regression Splines (MARS) to forecast emissions and identify key emission-influencing variables, with strong predictive accuracy even for previously unseen vessels. The Module 3 introduces a set of novel metrics and classification methods, including VAPOR (emission efficiency metric), SHAPE (scaling against a standardised baseline), SEIL (voyage-level ranking), PERIL (temporal risk classification), and SEPI/EOP (performance and optimisation potential). These tools enable standardised evaluation and ranking of ships based on emission efficiency and impact. The Module 4 - final module, dedicated to optimisation, applies rule-based logic and performance metrics to recommend targeted corrective measures based on available operational levers such as time at berth or engine load.

The system was applied to the Port of Split as a case study, where it demonstrated the ability to deliver actionable insights under real-world operational constraints. Across various modules, it produced meaningful outputs including a complete annual emission inventory, daily emissions forecasting, risk classification of high-emission periods, and optimisation scenarios that demonstrated a potential reduction of up to 55% on a critical day based on historical data. The research not only bridges the methodological gap between academic inventory models and applied port management but also supports long-term regulatory planning, emissions based tariffs, and data-sharing frameworks between maritime stakeholders.

In summary, the PrE-PARE DSS offers a flexible, scalable, and analytically robust solution for the management of ship-based air pollution in port areas. Its integration of machine learning, novel metric systems, and IoT-compatible datasets positions it as a significant contributor to the evolution toward smart and sustainable port operations.

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Hvala svima!

List of Publications

The following papers are included as part of this thesis:

PAPER 1

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PAPER 2

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PAPER 3

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List of Abbreviations

AE: Auxiliary Engine

AER: Annual Efficiency Ratio

AIS: Automatic Identification System

APS: Air Pollutant Substances

B-MARS: Boosting Multivariate Adaptive Regression Splines

BC: Black Carbon

CF: Correction Factor

CH_4: Methane

CII: Carbon Intensity Indicator

CIMIS: Croatian Integrated Maritime Information System

CO: Carbon Monoxide

CO_2: Carbon Dioxide

CRS: Croatian Register of Shipping

CSV: Comma-Separated Values

DCS: Data Collection System

DF: Dual Fuel

DSS: Decision Support System

E: Emissions (in mass)

ECA: Emission Control Area

EEA: European Environment Agency

EEDI: Energy Efficiency Design Index

EEOI: Energy Efficiency Operational Indicator

EEXI: Energy Efficiency Existing Ship Index

EF: Emission Factor

ENTEC: UK-based environmental consultancy firm

EO: Energy Output

EOP: Emission Optimisation Potential

ESPO: European Sea Ports Organisation

EU: European Union

FC: Fuel Consumption

GCV: Gross Calorific Value

GHG: Greenhouse Gases

GT: Gross Tonnage

GTU: Gas Turbine Unit

HFO: Heavy Fuel Oil

HSD: High-Speed Diesel

ICCT: International Council on Clean Transportation

IMO: International Maritime Organisation

IPCC: Intergovernmental Panel on Climate Change

LF: Load Factor

LNG: Liquefied Natural Gas

MAE: Mean Absolute Error

MARPOL: International Convention for the Prevention of Pollution from Ships

MARS: Multivariate Adaptive Regression Splines

MCR: Maximum Continuous Rating Speed

MDO: Marine Diesel Oil

ME: Main Engine

MGO: Marine Gas Oil

MMSI: Maritime Mobile Service Identity

MRV: Monitoring, Reporting, and Verification

MS D: Medium-Speed Diesel

N_2O: Nitrous Oxide

NAEI: National Atmospheric Emissions Inventory

NM: Nautical Mile

NMEA: National Marine Electronics Association

NMVOC: Non-Methane Volatile Organic Compounds

NO_x: Nitrogen Oxides

O_3: Ozone

OE: Operational Efficiency

P: Power (engine)

PERIL: Port Emissions Risk Level

PM: Particulate Matter

PME: Power of Main Engine

POLA/POLB: Port of Los Angeles / Port of Long Beach

PrE-PARE DSS: Port-related Emissions Prediction, Analytics and Risk Evaluation Decision Support System

PRISMA: Preferred Reporting Items for Systematic Reviews and Meta-Analyses

R^2: Coefficient of Determination

RMSE: Root Mean Squared Error

Ro-Ro: Roll-on/Roll-off

S_A: Actual Ship Speed

SECA: Sulphur Emission Control Area

SEEMP: Ship Energy Efficiency Management Plan

SEIL: Ship Emissions Impact Level

SEPI: Ship Emissions Performance Indicator

SHAPE: Ship Air Pollution Efficiency

S_M: Maximum Continuous Speed

SMED/IVL: Swedish Environmental Emission Data / Swedish Environmental Research Institute

SO_x: Sulphur Oxides

SS D: Slow Speed Diesel

S-EI: Ship Emission Intensity

S-EI-a/b: Ship Emission Intensity actual/baseline

ST-EI: Ship Type Emissions Intensity

STU: Steam Turbine

T: Time

US EPA: United States Environmental Protection Agency

VAPOR: Vessel Air Pollution Operational Rate

VAPOR-c/b: Vessel Air Pollution Operational Rate calculated/baseline

VOC: Volatile Organic Compounds

Terminology

Annual Efficiency Ratio	The AER indicates how much carbon dioxide a vessel emits for each tonne of cargo carried per nautical mile sailed over the course of a year – g CO_2 / deadweight tonne NM.
Boosting Multivariate Adaptive Regression Splines	An ensemble learning technique that improves model accuracy by sequentially combining multiple weak models (in this case, MARS models).
Bottom-up	The bottom-up approach in ship emissions quantification refers to a method that starts from the individual vessel level, calculating emissions based on detailed ship-specific operational data. This includes operational (activity) data and technical specifications, fuel type used, and specific emission factors for each pollutant. The emissions for each ship are calculated for every operational phase (cruising, manoeuvring, hoteling), and then aggregated to obtain detailed emissions for the port, region, or timeframe of interest.
Carbon Intensity Indicator	CII is a mandatory measure for assessing and monitoring the energy efficiency and carbon emissions of ships during operation. It calculates the amount of CO_2 emitted per unit of transport work over a year – g CO_2 / deadweight tonne NM.
Coefficient of Determination Validation	R^2 validation refers to the statistical measure used to evaluate how well a predictive model explains the variance of the observed outcomes during model validation. It quantifies the proportion of variability in the dependent variable that can be explained by the independent variables in the model. $R^2 = 1$ means perfect prediction.
Cruising mode	Cruising mode refers to the phase of a ship's voyage when it sails at a steady speed and power output. In this research, cruising mode is defined as the period when the ship's main engines operate at LF exceeding 20%, while the auxiliary engines provide energy for onboard services at a constant LF.
Emission factor	EF depends on both static data about engine function, engine type and fuel type and dynamic information about the characteristics of the ship's activities. Expresses the mass of pollutant released per unit of fuel burned or engine output – g of pollutant / g fuel or g of pollutant / kWh
Emission Optimisation Potential	EOP is a performance indicator introduced in this research that quantifies the extent to which a ship's emissions can be reduced compared to its own historical baseline. It reflects the difference between the ship's actual emission intensity during a specific voyage and its previously recorded average performance.
Energy Efficiency Existing Ship Index	EEXI is a technical efficiency standard for addressing the energy efficiency of existing ships – g CO_2 / deadweight tonne NM.
Energy Efficiency Operational Indicator	EEOI is a performance metric for assessing the actual operational energy efficiency of ships by considering fuel consumption, distance

	sailed, and actual cargo carried – g CO_2 / cargo carried × distance travelled.
Energy Output	EO refers to the total amount of energy delivered by a ship's propulsion and auxiliary systems over a defined period of operation. It represents the useful mechanical or electrical energy generated to perform work during a voyage or a particular operational mode (e.g. cruising, manoeuvring, or hoteling).
Energy-Based	The energy-based method is a calculation approach that estimates ship emissions by combining the amount of energy output by ship engines to corresponding emission factors and time in each operating mode.
Fuel-Based	The fuel-based method is a calculation approach that estimates ship emissions by multiplying the amount of fuel consumed with pollutant-specific emission factors. It assumes a direct link between fuel quantity burned and the amount of pollutants emitted, without detailed consideration of engine load or operational modes.
Generalised Cross Validation	GCV is a statistical method used to estimate the predictive performance of a model while controlling for overfitting.
Hoteling mode	Hotelling mode refers to the phase when a ship is stationary at anchorage or berth while loading, unloading, or waiting, with ME turned off. In this research, only auxiliary engines operate to supply energy for onboard services, hotel load, and cargo operations, running at constant LF.
Load Factor	LF is a dimensionless parameter used to express the ratio between the actual energy output of an engine and its maximum rated energy output (MCR). It indicates the proportion of engine capacity being utilised at any given moment. In emissions estimation, LF helps determine how much energy the engine produces under different operating modes (e.g., cruising, manoeuvring, hoteling), which directly influences EF and emission levels.
Manoeuvring mode	Manoeuvring mode refers to the phase when a ship is navigating at low speeds near ports, during docking, undocking, or pilotage. In this research, manoeuvring mode means that the main engines operate at LF below 20%, while auxiliary engines provide energy for onboard services at a constant LF.
Multivariate Adaptive Regression Splines	MARS is a flexible, non-parametric regression method used in machine learning and statistics to model complex, non-linear relationships between variables. It automatically detects interactions and non-linearities in the data without requiring a predefined functional form.
Operating mode/Activity	Operating mode, or activity, refers to the specific phase of a ship's voyage that directly affects engine usage and emissions. Typical modes include cruising, manoeuvring, and hoteling. Each operating mode is characterised by different power demands on ship engines, which are expressed through the LF.
Operational Efficiency	OE, as defined in this research, is the ability of a ship to complete a

	voyage on schedule with minimal energy consumption per unit of time. OE is used for evaluating ship emission efficiency within metrics developed in this thesis like VAPOR, SHAPE, and SEPI, where both technical design and real operational behaviour are assessed to understand and improve air pollution performance in ports.
Port Emissions Risk Level	PERIL is a classification algorithm developed in this research to assess and categorise the overall air pollution risk in port areas based on daily ship-sourced emissions. Daily total emissions are segmented into five classes (e.g., Very Low, Low, Moderate, High, and Very High), depending on how far they deviate from the average daily emissions.
Preferred Reporting Items for Systematic Reviews and Meta-Analyses	PRISMA is a widely used evidence-based reporting guideline designed to improve the transparency, clarity, and completeness of systematic reviews and meta-analyses. It provides a standardised checklist and flow diagram to ensure that all key aspects of the review process, including study selection, data extraction, and synthesis, are fully documented and reproducible.
Propeller Law	Propeller Law describes the relationship between a ship's speed and the power required by its main engines, stating that power demand increases approximately with the cube of the vessel's speed. This principle is applied exclusively to propulsion systems, as it reflects how propeller-driven thrust relates to vessel movement, revealing LF at specific time.
Root Mean Square Error	RMSE is a statistical metric to evaluate the accuracy of predictive models. It measures the average magnitude of the errors between predicted and actual values, with larger errors having a greater influence due to squaring. Lower RMSE indicates better predictive performance.
SHAPE	SHAPE is a standardised metric introduced in this research to evaluate and compare the emission efficiency of ships by scaling their actual emissions against a baseline reference for similar ship types and operational modes. It compares VAPOR-c (calculated hourly emissions per unit of work capacity) to VAPOR-b (baseline average hourly emissions for the same ship type and mode).
Ship Emission Intensity	S-EI is a metric introduced in this research that quantifies the total amount of emissions produced by a ship during an entire voyage relative to the work capacity of that vessel. It allows for assessing the overall emission output for a complete port visit or operational cycle, while accounting for the specific capabilities of the ship.
Ship Emissions Impact Level	SEIL is a simplified and intuitive metric introduced in this research to evaluate and compare the emissions impact of individual ships during their port visits. It enables clear visualisation and ranking of ships based on their total emissions per port call.
Ship Emissions Performance Indicator	SEPI is an advanced performance indicator introduced in this research to assess and rank the overall emissions performance of

	individual ships, with a goal of optimisation. It integrates both efficiency and optimisation potential into a single, balanced metric.
Ship Type Emission Intensity	ST-EI is a normalised metric introduced in this research that quantifies and compares the average emission output per voyage of a specific ship type relative to the entire fleet's average in a given timeframe. It is used to assess how much a particular group of ships contributes to total port emissions, considering both the number of voyages and total emissions.
Top-Down	in the context of ship emissions refers to a method where the total volume of exhaust gases is first calculated on wide level (reginal, national or port), rather than starting from individual vessel data. The method uses available statistics (traffic, fuel sales) relevant to area, and corresponding EF, often giving generalised results.
VAPOR (a/b)	VAPOR is a central emission metric introduced in this research that measures the emission efficiency by comparing the average hourly rate of exhaust gas production relative to a ship’s work capacity in each operational mode. By incorporating available operational data it enables the standardised efficiency evaluation and comparison.
Voyage	In the context of this research, a voyage includes arrival, stay, and departure, encompassing cruising, manoeuvring, and hoteling as three operational modes, ensuring a comprehensive assessment of the vessel’s operational profile.

CHAPTER 1

1. Introduction

Although maritime shipping is considered as the most environmentally efficient mode of transportation, primarily due to its capacity to transfer massive volumes of cargo in a single voyage, it is also heavily dependent on marine fuels [1–3]. A variety of harmful substances are released as a by-product of the combustion process in the propulsion and auxiliary systems of ships. These include both greenhouse gases (GHGs), such as carbon dioxide (CO_2), methane (CH_4), and nitrous oxide (N_2O), and air pollutant substances (APSs) like sulphur oxides (SO_x), nitrogen oxides (NO_x), particulate matter (PM), carbon monoxide (CO), and non-methane / volatile organic compounds (NM / VOCs) [4–6].

As maritime transport accounts for approximately 70 % to 80 % of global trade by volume, its contribution to anthropogenic CO_2 emissions is considerable, representing around 3 % of total global emissions [3,7–9]. While GHGs are known for their contribution to global warming, the other pollutants generated during fuel combustion are particularly concerning for their direct and localised health impacts, especially in coastal urban areas and port cities [2,6,10]. Inhalation of fine $PM_{2.5}$, SO_x, NO_x, CO, and VOCs has been linked to severe health effects including respiratory illnesses, cardiovascular conditions, and increased risk of premature death [10–12].

The consequences of exposure, both short-term and long-term, are especially acute with pollutants like PM, ozone (O_3), CO, NO_x, and SO_x [12,13]. In this context, port cities are particularly vulnerable, as shipping emissions occur near populated areas. The environmental burden is often most intense in coastal regions and seaports, where marine traffic is dense [6,14]. Within the European context, this issue is amplified by the fact that nearly 90% of ports are spatially integrated with cities, significantly increasing the exposure of residents to degraded air quality [14].

These facts make it clear that addressing air pollution from ships requires not only international coordination but also sound local and regional air pollution control strategies focused on the urban port environment. Although a number of global and regional regulatory measures are already active, and air pollution in seaports is increasingly monitored by conducting exhaust gas inventories, there are still large gaps in terms of standardised approach to ship efficiency and emission control.

1.1. Global Context and Regulatory Background of Ship Emissions

To address growing concerns about emissions from the shipping sector, the International Maritime Organisation (IMO) introduced Annex VI to the International Convention for the Prevention of Pollution from Ships (MARPOL) in 1997, focusing on the Prevention of Air Pollution from Ships [15]. This regulatory framework targets both APSs and GHGs, and its development over time has resulted in a set of technical and operational measures aimed at reducing the environmental footprint of global maritime transport on atmosphere [16]. In this context, the Initial Strategy on the reduction of GHG has most recently been revised, adopting a significantly more ambitious target aimed at achieving full decarbonisation of ships by or around 2050 [17,18].

1.1.1. Technical Measures

The first major technical control introduced under Annex VI was the Global Sulphur Cap, which took effect globally in January 2020. This regulation limits the sulphur content in marine fuels to 0.50% mass by mass percent (% m/m), while designated Emission Control Areas (ECAs) enforce an even stricter limit of 0.10% m/m [19]. This measure targets SO_x emissions, a primary contributor to acid rain and respiratory illness.

In parallel, the IMO established NO_x emission limits through a three-tiered approach. Tier I, applicable to ships built between 2000 and 2010, set the initial standard [20]. Tier II, for ships constructed from 2011 onwards, required approximately a 20% reduction in NO_x compared to Tier I levels [20]. In the European context, Tier III requirements have applied since 1 January 2021 for ships operating in newly designated NECA zones, including the North Sea and the Baltic Sea. Compliance with Tier III often requires the use of advanced emission control technologies such as Selective Catalytic Reduction systems or Exhaust Gas Recirculation.

In 2013, the IMO introduced the Energy Efficiency Design Index (EEDI), a performance-based regulation requiring new ships of 400 gross tonnage (GT) or more to meet minimum design efficiency standards [4,21]. The EEDI is calculated based on parameters such as engine power, fuel consumption, and ship capacity. The first implementation phase mandated a 10% reduction in CO_2 emissions per tonne-mile compared to a baseline derived from ships built between 2000 and 2010 [22]. This requirement becomes progressively stricter in subsequent phases introduced every 5 years.[4,21,22]

In 2023, the IMO extended technical regulations to cover existing vessels through the Energy Efficiency Existing Ship Index (EEXI) [4,23]. Like the EEDI, the EEXI uses design characteristics to calculate energy efficiency, but it applies to ships already in service. Ships of 400 GT and above must demonstrate compliance with required efficiency thresholds, which vary by ship type and size class [24]. The EEXI framework is aligned with EEDI principles but uses limited operational data and focuses on design modifications or technical adjustments such as engine power limitation or propulsion upgrades to meet compliance targets [21].

1.1.2. Operational Measures

Operational measures were introduced alongside technical requirements to address emissions during active use. The Ship Energy Efficiency Management Plan (SEEMP) was first implemented in 2013 [4,25]. It obliges ship operators to establish structured plans for improving fuel efficiency through measures such as hull and propeller maintenance, speed optimisation, weather routing, and energy management [4,25,26]. The updated SEEMP framework includes three parts: an efficiency improvement plan, fuel consumption monitoring, and a methodology for assessing carbon intensity [26].

In 2018, the IMO launched the Data Collection System (DCS), requiring ships of 5,000 GT and above to report annual fuel oil consumption [27]. This reporting system supports performance assessment and informs regulatory development.

Beginning in 2024, ships of 5,000 GT and above must also comply with the Carbon Intensity Indicator (CII) regulation [23,28]. The CII is a metric that evaluates the operational energy efficiency of a vessel by calculating the mass of CO_2 emitted per transport work (e.g., grams of CO_2 per deadweight-tonne nautical mile). Each ship receives an annual rating from A (best) to E (worst) [25,29]. Ships falling into categories D or E for 3 consecutive years may be subject to corrective action plans under SEEMP [29].

For CII assessment, emissions are calculated using the fuel-based method [30]. Fuel consumption is multiplied by its carbon content, while transport work is derived from operational data. To standardise performance measurement, the IMO has endorsed various efficiency indicators such as the Annual Efficiency Ratio (AER), cargo gross distance (cgDIST), and Energy Efficiency Operational Indicator (EEOI) [9,25,30]. The AER assesses carbon intensity by dividing the total CO_2 emissions by the total distance travelled and the carrying capacity of the ship over the course of a year, thus providing an annual overview of operational efficiency. Similarly, the cgDIST shows the amount of carbon emissions released by comparing the distance travelled when transporting cargo. In the EEOI, the fuel consumption and carbon factor for each fuel type, together with the amount of cargo transported on each voyage and the distance travelled with the transported freight, are used to indicate the energy efficiency of ship.

1.2. Regional Context and Monitoring Background of Ship Emissions in Ports

1.2.1. European Union Operational and Monitoring Measures

While global maritime emissions remain a significant concern, increasing attention is being directed to the regional and local domains, where environmental and public health effects are more immediate and measurable. Although air pollution from port activities represents a relatively small fraction of global shipping emissions, their impact at the local level is disproportionally significant, due to both the high frequency of ship movements and the close proximity of ports to residential areas [31–33]. Reflecting broader awareness of these regional issues, the European Sea Ports Organisation (ESPO) has identified air quality, climate change, and energy efficiency as core environmental priorities within the European Union (EU) port sector [14].

To address these gaps, the EU has introduced several additional regulatory instruments that target maritime emissions more specifically. One of the most notable is the Sulphur Directive (Directive (EU) 2016/802), which limits the maximum sulphur content in marine fuels used by ships operating in EU waters [34]. Since 2020, this limit has been set at 0.50% in general, consistent with the IMO's global cap, and 0.10% in designated Sulphur Emission Control Areas (SECAs) [35]. The directive applies not only to vessels at sea but also to those at berth, requiring the use of cleaner fuels or equivalent abatement technologies while moored in EU ports.

Complementing this directive is the EU Monitoring, Reporting and Verification (MRV) Regulation (Regulation (EU) 2015/757) [36]. It obliges ships of 5,000 GT and above to report verified annual data on CO_2 emissions, fuel consumption, and cargo activity on voyages to, from, and between EU ports. Unlike the IMO's DCS, which is non-public and global in scope, MRV data are accessible to the public and tailored to support regional climate policy, including integration with the EU Emissions Trading System from 2024 onwards [37].

In terms of wider emissions controlling within the EU, all member states are required to submit national GHG inventories to the European Environment Agency (EEA), following Intergovernmental Panel on Climate Change (IPCC) guidelines [38–40]. However, these inventories are primarily focused on GHGs and do not systematically mandate detailed reporting of emissions from maritime transport, particularly in port areas, where the concentration of pollutants poses a heightened risk to local communities.

Therefore, despite the mentioned monitoring mechanism and the supplementary directives, data concerning emissions from ships operating in and around ports remains inconsistently collected or reported across member states. For example, Croatia's national GHG inventory relies on the Tier 1 methodology based on overall fuel consumption without any spatial or temporal breakdown [41]. This is especially concerning given Croatia's 1,777 km Adriatic coastline and six international ports, which recorded over 359,000 vessel arrivals in 2019 [41–43]. Without high-resolution data that captures the complexity of port traffic and its environmental implications, the design of effective mitigation strategies remains limited.

1.2.2. Concept of Emission Inventories as Monitoring Tools for Ship-Sourced Air Pollution in Ports

Given the practical necessity of better understanding air pollution associated with maritime activities, both port authorities and academic researchers acknowledge the importance of compiling dedicated shipping emission inventories for seaports. These inventories are typically based on either a top-down or bottom-up approach, used in combination with fuel- or energy-based estimation methods, to calculate the volume of emissions produced over a defined time period.

In the top-down method, emissions are commonly estimated using a fuel-based technique. This involves utilising fuel sales statistics to determine the total fuel consumption (FC) of the fleet within a defined geographic area during a specific time frame. The FC data are then multiplied by an emission factor (EF), which represents the mass of pollutant emitted per tonne of fuel consumed. The resulting value gives the total quantity of emissions (E), as shown in the following equation [44]:

$$E = FC \times EF \tag{1}$$

This fuel-based approach is advantageous in that it requires minimal data inputs. Generalised data describing average fleet activity, fuel usage, and emission characteristics can be sufficient, making the method suitable when detailed traffic information is unavailable [44]. However, this simplicity comes with drawbacks. The generalisation of data introduces uncertainty, and the EFs are usually broad estimates that fail to reflect specific operating conditions or temporal variations in emission intensity [45]. Furthermore, discrepancies have been observed between bunker fuel sales and the actual FC of global fleets, which undermines the method's accuracy when assessing emissions from specific maritime activities [45,46]. This issue becomes especially pronounced in smaller-scale contexts such as individual ports, where aggregated fuel statistics provide limited resolution. For this reason, top-down approaches are more commonly used in regional or local emission inventories where data precision is secondary to broader coverage.

In contrast, the bottom-up approach is preferred when detailed vessel-specific movement data and technical specifications are accessible. This technique, which is activity-based and data-intensive, can generate high-resolution emission estimates for individual vessels, capturing emissions over time and space with significant accuracy [44,45]. Within this framework, emissions from each activity type, such as hoteling, manoeuvring, or cruising, are calculated using combinations of engine energy output (EO), FC, EF, and operational time (T) [47,48]. To compute the total emissions for a given region or time span, these individual estimates are aggregated for all voyages [44].

Both energy-based and fuel-based variants of the bottom-up method exist. Equations (2) and (3) describe the energy-based model, while Equation (4) illustrates the fuel-based calculation [44,48]:

$$E = EO \times EF \times T \tag{2}$$

$$EO = P \times LF \tag{3}$$

$$E = FC \times LF \times EF \times T \tag{4}$$

In these expressions, EO is derived from the rated engine power (P) multiplied by the load factor (LF), which represents the proportion of maximum engine capacity being used. The EF in this case is defined per unit of energy output, making the method more sensitive to operational variations.

Due to the extensive data requirements, bottom-up methods are predominantly used for smaller-scale inventories, such as those focusing on specific regions or port areas. One of the primary data sources for this method is the AIS, which provides near real-time information on a vessel's location, speed, and course [49]. Mentioned data is essential for modelling ship behaviour and estimating emissions accurately. AIS records enable experts to generate vessel-specific operation profiles, including average speeds and travel durations between defined waypoints, typically at short time intervals. These movement profiles can be used to reconstruct ship routes and assess emission patterns [44,50].

Although AIS equipment is mandatory for all commercial vessels of 300 GT or more and for all passenger ships under IMO regulations, a portion of maritime traffic still remains untracked due to non-compliance or technological limitations [51]. Therefore, in order to improve the accuracy of emission inventories, AIS data should ideally be supplemented with other sources of maritime traffic information.

1.3. Limitations in Existing Approaches

1.3.1. Policy Context Limitations

Despite continuous advancements of both international and regional policies for control of ship emissions, several limitations persist [52,53]. Although IMO's Fourth GHG Study confirmed a reduction in carbon intensity-based on AER, other analyses, such as those from CE Delft, have suggested that this decline was influenced more by external economic factors (e.g., fuel costs and freight rates) than by regulatory success [9,54]. Fluctuations in market conditions impact the rate of newbuild orders, the application of energy efficient technologies and fuel consumption [54].

Moreover, estimates by the International Council on Clean Transportation (ICCT) indicate that the EEXI may reduce CO_2 emissions from the 2030 global fleet by as little as 0.7% to 1.3%, given that many ships already operate below the speed thresholds used in compliance calculations [55]. This calls into question the practical impact of technical measures like EEDI and EEXI when applied to fleets not operating at design speeds. Their real-world effectiveness, therefore, depends heavily on how ships are operated, not just how they are designed [55–58].

There are also concerns about the accuracy and completeness of the CII. While it incorporates annual fuel use, it overlooks emissions released during hoteling or anchorage, particularly relevant for vessel types like Cruise Ships, Ro-Ro Ferries, and containerships that frequently remain in port environments [59]. Additionally, current metrics primarily focus on CO_2 and do not account for other climate-relevant pollutants. Gases such as CH_4, N_2O, and black carbon (BC), all of which have far greater warming potential over short timescales, remain outside the scope of the current regulatory framework [17,22,25]. For example, methane has a global warming potential 84 times higher than CO_2 over a 20-year period, underscoring the need to broaden the scope of future IMO strategies to include these short-lived climate pollutants [60,61].

While the EU regulatory framework shows a clear intent to address maritime emissions, its practical implementation remains fragmented. Both MRV and EEA regulations are also focused on monitoring of CO_2 emissions, overlooking other greenhouse gases and short-lived climate pollutants that contribute significantly to atmospheric warming and localised air quality degradation [37,39,40]. CH_4, NOx, and BC are not currently included, despite their well-documented climate relevance and public health implications [62]. These regulations also fail to address other ambient air pollutants that pose significant health risks from both short- and long-term exposure, particularly when ships are berthed near populated areas. Mentioned lack of relevant types of emissions and spatial analysis is particularly problematic given the concentration of shipping activity in EU ports and the potential for localised pollution hotspots. In countries such as Croatia, where the national inventory still relies on Tier 1 estimation methods, the absence of detailed temporal and spatial data prevents accurate assessments of port-related emissions and hampers the development of targeted air quality policies.

1.3.2. Limitations of Emission Inventories

To enable a more detailed examination of ship-generated emissions in seaports involving multiple air pollutants and variations by vessel type, time, and location, detailed emission inventories are increasingly being developed [44]. Although these inventories rely on large volumes of emission-related data, the systematic review presented in Paper 1 demonstrated that such efforts tend to support only generalised recommendations for emissions control within examined area. The findings of these inventories are constrained by their spatial and temporal specificity, and do not facilitate comparative evaluation across different vessels or port contexts.

Further evidence from Paper 2, which introduced an analytical modelling approach, reinforced the conclusions drawn in Paper 1. It showed that the emission profiles and pollutant compositions reported across various studies were not directly comparable, either between ports or within the same port at different times. This inconsistency stems from significant variation in the pollutants selected for analysis, differences in the technical and movement-related parameters used, and divergences in the time frames or spatial boundaries applied in each study.

Additionally, emission inventories that focus solely on reporting estimated emission volumes lack the depth needed to assess pollution intensity across vessels or over time. Without a structured scaling framework and relevant reference values, it becomes difficult to evaluate whether a particular ship, fleet segment, or entire port is performing efficiently or contributing disproportionately to local air pollution.

A more holistic and standardised method is therefore essential for meaningful pollution evaluation and risk prediction. However, implementing such a system would require processing extensive datasets and examining complex interdependencies between multiple operational and technical factors, making the task computationally intensive. Based on the findings of Papers 1 and 2, there is a clear need for a unified, scalable assessment method that can improve the transparency, comparability, and effectiveness of ship and port-level emission evaluations.

CHAPTER 2

2. Research Objective and Questions

To address the mentioned constraints, the main objective of this research was to develop an adaptable, context-sensitive, and efficient DSS that quantifies, predicts, and evaluates ship-related emissions while also delivering feasible measures for effective air pollution control in port environments. This system integrates existing emissions inventory methodologies with novel air pollution performance indicators and advanced machine learning models based on extensive technical and operational emission-related data. The goal was to enhance the spatial and temporal evaluation of maritime emissions both at ship and at the port levels while supporting policy implementation, information sharing and environmental management through data-driven, comparable, and operationally realistic emission insights. To achieve this objective, the research was guided by the hypothesis that machine learning techniques can be used to analyse ship activity data and identify the most influential factors affecting gas emissions. By combining these findings with an optimisation algorithm, the system can predict emissions and propose effective measures for controlling air pollution in ports.

This thesis addresses the current lack of standardised frameworks for evaluating the risk and intensity of ship emissions in port environments and aims to bridge the gap between academic emission inventory modelling and practical decision-making needs. The research builds upon a systematic review of existing studies and incorporates the development of an analytical emission quantification module, a predictive algorithm based on machine learning techniques, novel metric frameworks, and an optimisation system, all integrated within the PrE-PARE DSS.

However, to conceptualise and develop such a system, several key research questions needed to be formulated and addressed throughout this thesis. Thus, the research questions and relevant explanations are summarised below, while Figure 1 shows their connection to the papers produced throughout the research process.

> **RQ1:** What are the methodological limitations and data inconsistencies in current ship emission inventories used in port areas, and how do these limitations hinder comparability and decision-making?

This question explores the deficiencies in existing inventory methods, particularly their lack of standardisation, variation in input data quality, and inconsistent pollutant coverage. Understanding these issues is essential to identifying the barriers to effective policy development and benchmarking of ship emissions at the port-level.

> **RQ2:** How can analytical modelling approaches be used to enhance the accuracy and interpretability of port-level shipping emission estimates?

This question focuses on the development of an analytical model that improves transparency and replicability in emission estimation. It considers how combining technical ship data with activity-based parameters can produce realistic and context-specific emission outputs.

> **RQ3:** What indicators or metrics can be formulated to standardise the evaluation of emission efficiency and intensities across different ships and port areas?

This question addresses the need for robust performance indicators that enable consistent evaluation of ship-related emissions. The emphasis is placed on developing a scalable method for assessing emission efficiency, intensity, and optimisation potential by correlating baseline values to those observed within defined period. The aim is to facilitate the temporal classification of air pollution performance and to provide clearer insights into emission behaviour during specific operational windows. While primarily intended for temporal assessment within a single port environment, the approach is also adaptable for comparisons between individual vessels on international level and across ports using harmonised metrics.

> **RQ4:** How can machine learning methods improve predictive modelling of ship emissions in port operations?

This question investigates the role of supervised machine learning in improving the predictive accuracy of emission models by capturing complex, non-linear relationships between integrated parameters of ships in different operational modes and pollutant outputs. Beyond forecasting, machine learning is also applied to evaluate and weigh the influence of various operational and technical factors on emissions, thereby informing the optimisation module. This enables the identification of the most impactful mitigation measures, supporting the development of targeted strategies for emission control under varying port conditions.

> **RQ5:** What are the practical implications of the developed PrE-PARE DSS for port management, shipping industry, environmental monitoring agencies, maritime policy stakeholders, and the wider public?

This question addresses the real-world applicability of the PrE-PARE DSS. It explores how the system can support regulatory compliance, inform decision-making, and guide local emission reduction strategies. Additionally, it considers the potential for sharing clear, accessible emissions data with the general public to increase transparency and stimulate environmental awareness in port communities.

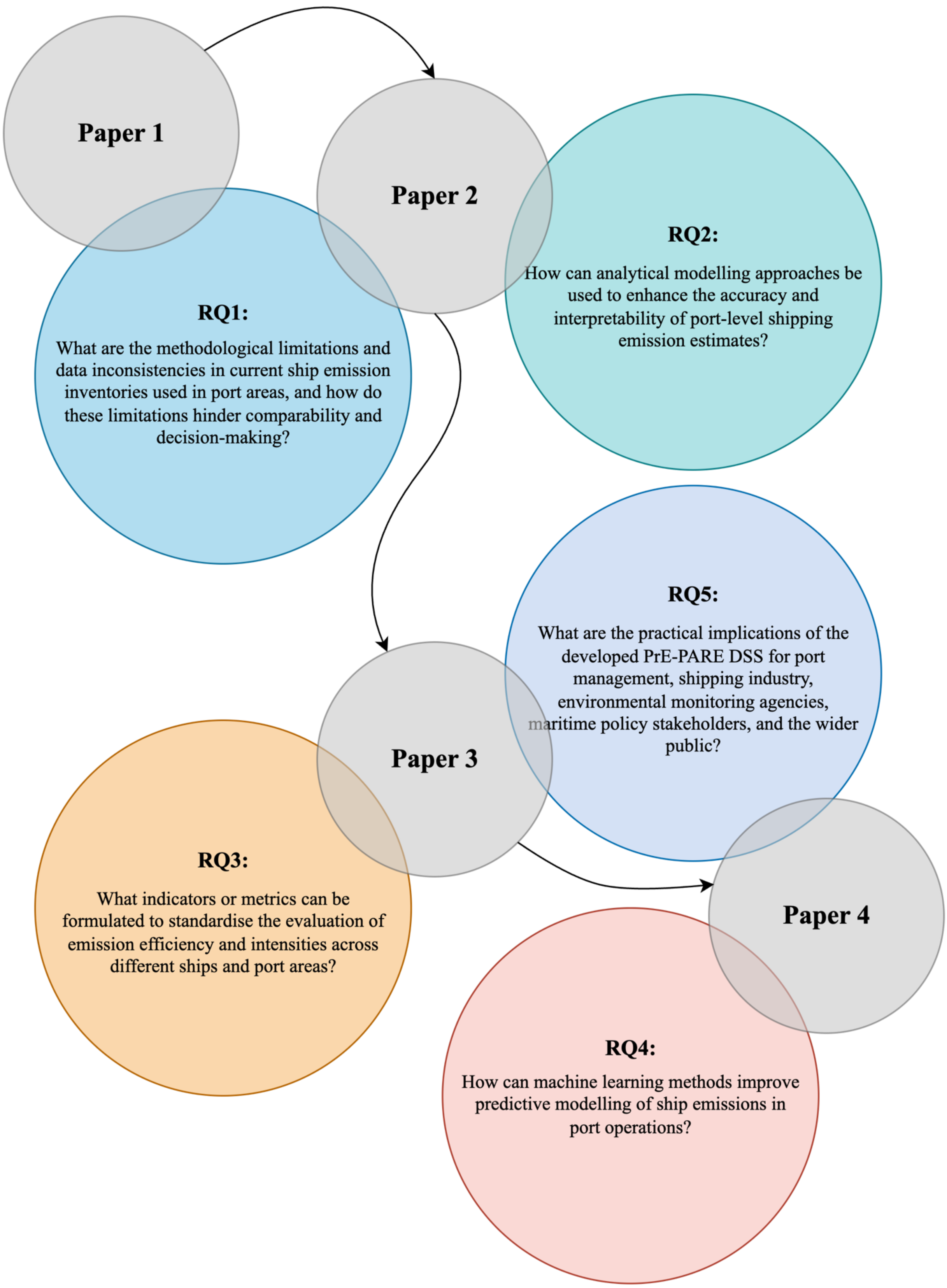


Figure 1. Research questions and their relation to the papers contributing to this doctoral research.

3. Motivation

Although seaports operate under specific jurisdictions and regulations, in many cases they are physically and functionally integrated into the urban fabric, serving as natural extensions of coastal cities towards the sea. This is particularly evident across numerous European port cities, where port infrastructure is closely interwoven with the economic, social, and transport systems of the surrounding community. Given their locational specificity, economic importance, and functional complexity, ports must not only prioritise commercial efficiency but also acknowledge their environmental footprint and social responsibility.

In this context, the protection of the surrounding environment becomes essential, especially when considering the external effects of maritime transport. Air pollution, marine litter, ballast water discharge, noise, oil spills, chemicals, and microplastics from antifouling paints are well known by-products of the shipping industry. However, among these, air pollution is particularly critical due to its immediate and long-term impacts on both public health and ecological systems. Exhaust gases released during port operations contribute to the degradation of local air quality and the intensification of greenhouse effects. These emissions are not only pervasive and persistent, but also capable of deeply penetrating human respiratory systems, often leading to severe, irreversible health outcomes.

Ports, as dynamic logistical nodes, attract concentrated maritime activity which amplifies emissions, pushing the limits of localised air pollution. This cause-effect relationship underlines a critical problem, namely the lack of clearly defined regulatory thresholds for air pollution from ships, especially in port environments.

Although indices such as the European Air Quality Index provide general standards for ambient air quality, there are currently no equivalent frameworks for categorising ship-based emissions in port areas [63,64]. Existing metrics developed by the IMO, such as the EEOI or the CII, focus solely on CO_2 and neglect key variables such as operational mode, temporal dynamics, and spatial distribution [9]. The example based on modern Cruise Ships illustrates the importance of this challenge. These vessels commonly operate with an installed power ranging from 5.5 to 7.5 megawatts (MW) [65]. Operating continuously for just one hour can consume over 6,500 kilowatt-hours (kWh) of energy, equivalent to the average annual electricity usage of nearly two European households [66,67]. The corresponding CO_2 emissions from such activity emphasise the disproportionate environmental impact even a single vessel can impose during one port call. The ongoing the continuous traffic growth and corresponding pollution motivated the formulation of the following questions:

What constitutes a high and unacceptable level of emissions for a specific port?

How can ships be objectively evaluated for emission efficiency based on their type and capacity?

Which vessels should be prioritised for operational optimisation?

To pursue data-driven and quantifiable answers, avoiding arbitrary appraisals, this research was inspired by the principles of smart port development and the potential of IoT technologies. The premise was to develop a user-friendly system that applies machine learning techniques and a novel emissions metric to large-scale technical and operational datasets. This would enable a comprehensive decision support platform focused on quantification, assessment, and ultimately optimisation of ship-sourced emissions in port areas. This logic is illustrated in Figure 2, which outlines the concept of the system. AIS-transmitted vessel movement data is integrated with technical ship specifications enabling emissions calculation and temporal mapping of air pollution contribution of each and overall marine traffic in port area. These results are then evaluated and classified into risk levels, which can be openly communicated to the public to raise awareness and support community engagement. When a high-risk level is identified, the system initiates a decision support loop by recommending targeted corrective measures to reduce emissions, thereby closing the optimisation cycle.

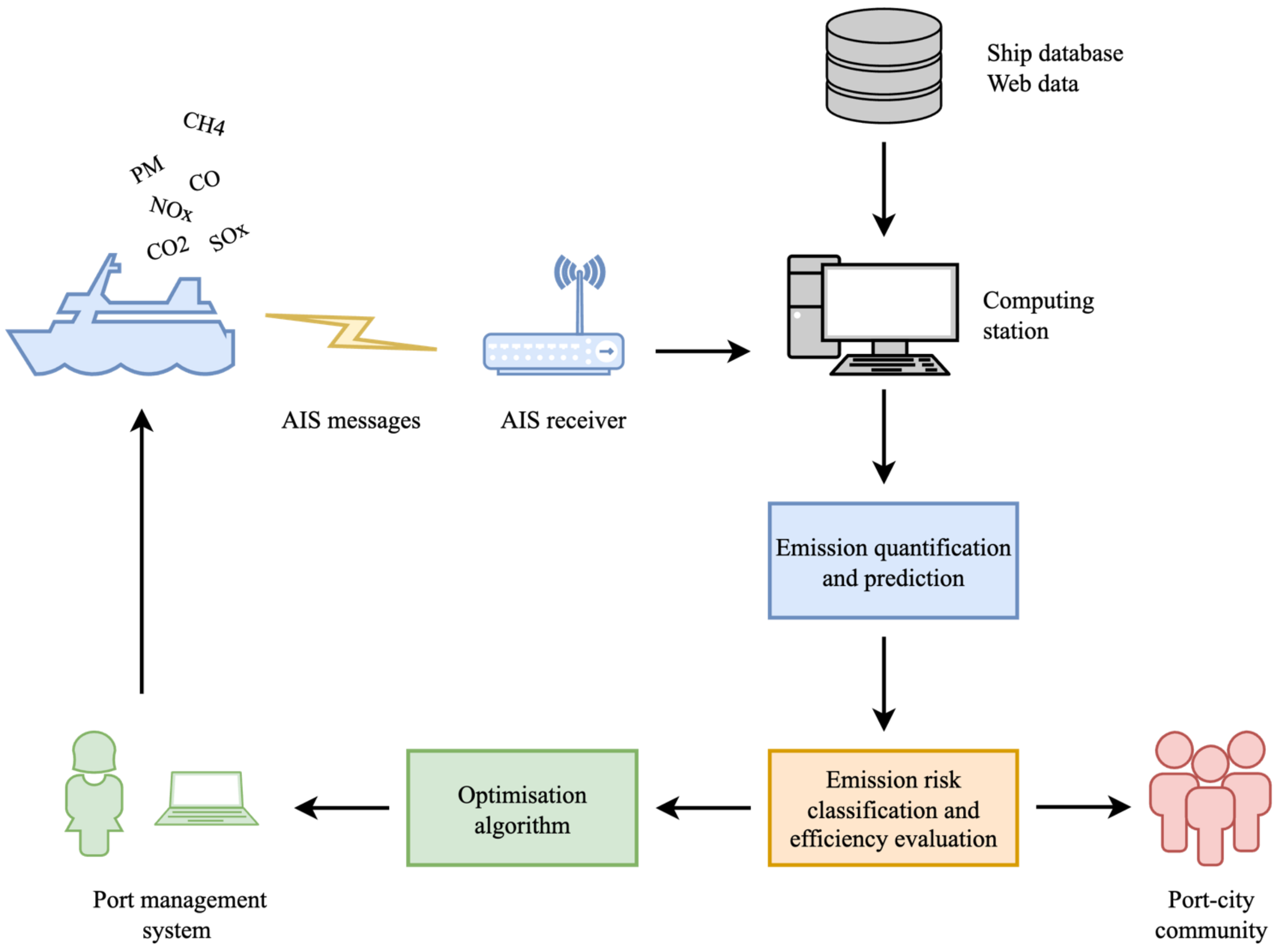


Figure 2. Conceptual overview of a ship emissions control framework for seaports based on IoT-enabled data integration and decision logic.

4. Research Structure, Strategy and Scope

4.1. Research Structure and Strategy

This compilation thesis is structured around a modular research framework, designed to progressively develop and integrate key components of the PrE-PARE DSS. These components collectively address the research questions (RQ1–RQ5) introduced in Section 2, and each paper contributes to one or more stages of the system's development. The process follows a stepwise logic, where earlier outputs provide the empirical and conceptual basis for subsequent stages, culminating in a comprehensive, scalable tool for supporting air pollution control in port areas.

The research began with a systematic literature review presented in Paper 1, where 32 original papers and 28 large-scale studies focused on port-related ship emissions were analysed. Using the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) approach and a bottom-up multi-layer analysis, the review identified prevailing methods, data inputs, and key challenges in emission quantification. Also, the analysis revealed a critical gap: existing approaches lack scalability and comparability, which obstructs meaningful evaluation of emission contributions across ports, ships, and time periods. These findings motivated the need for a more transparent, interpretable, and standardised framework that combines quantification and metric system, laying the methodological foundation for the entire research and justifying the development of the PrE-PARE DSS.

Building upon those findings, Paper 2 introduced a fully operational analytical model designed to quantify ship-sourced emissions at high temporal and spatial resolution. Using the data types and methodological structure identified in Paper 1, the model integrated technical and movement datasets to produce a detailed emissions inventory for the passenger basin of Port of Split in 2019. For acquisition of ship technical details, the Croatian Registry of Shipping (CRS), the Croatian Integrated Maritime Information System (CIMIS), and relevant web databases where used. AIS data, provided by the Faculty of Maritime Studies in Split, were filtered and converted to ensure high-resolution coverage. Therefore, the research strategy at this stage involved completing the full data preparation process to ensure accurate production of outputs throughout the research. This contribution constituted Module 1 – Quantification and analysis, materialising the methodology from Paper 1. While it enabled detailed emissions analysis, the results also confirmed the limitations noted earlier: the inability to systematically evaluate emission efficiency or pollution risk over time or in different operational scenarios without an appropriate scaling framework, even within the same area.

To address the identified limitations, Paper 3 extended the model by incorporating a novel metric framework alongside predictive modelling component. This phase of the research corresponds to Module 2 – Predictive module and Module 3 – Ship emissions metric, scaling, classification and ranking module. Building on the inventory results produced in Paper 2, a MARS method was applied within the predictive module. This supervised machine learning technique was selected as the most appropriate for analysing the processed datasets, with the objective of identifying emission-influencing factors and forecasting ship emissions under varying operational scenarios.

By relying on the same extensive database, a novel system for scaling, classification, and risk evaluation was proposed to evaluate the emission performance of individual ships and the overall temporal pollution load within the port area as main task of Module 3. This allowed for an efficient, standardised, comparable and coherent characterisation of air pollution profiles that could be used in both operational monitoring and regulatory evaluation.

Finally, the Paper 4 (in preparation) focuses on the integration of Module 4 – Optimisation, as the last component encircling DSS for ship-based emission control in port areas. This module uses the outputs from previous papers as input parameters for evaluating feasible mitigation scenarios and selecting appropriate pollution control measures based on available operational conditions. The resulting tool not only supports high-resolution predictive forecasting and performance evaluation but also delivers actionable insights to support regulatory planning and port-level decision-making.

In summary, the modularity of the research structure enables a logical progression from conceptual review to operational modelling, predictive analytics, and finally decision-oriented optimisation. Each module corresponds to a dedicated research paper, while the integrated framework constitutes the PrE-PARE DSS. Figure 3 provides the overview of the thesis structure and relation between the research objectives and papers in which they were achieved and presented.

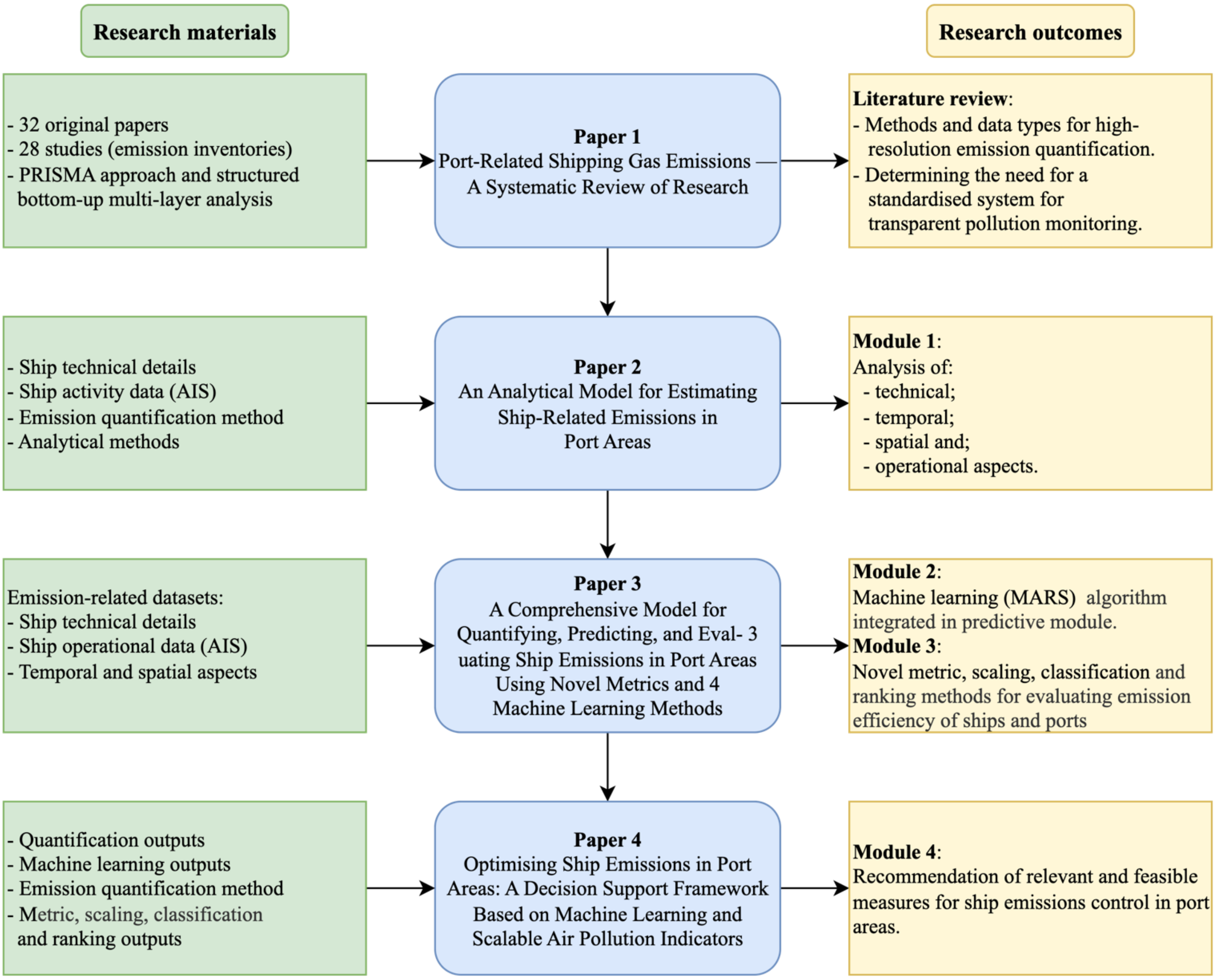


Figure 3. Overview of the thesis structure summarising the relations between with main research materials, relevant papers and outcomes.

4.2. Research Scope and Limitations

This thesis introduces a modular DSS designed to quantify, evaluate, predict, and optimise ship-related emissions in port environments. While the modularity of the framework enables the integration of additional datasets and diverse methodological perspectives in future research, the current study is delimited to specific environmental, geographical, and technical contexts.

The scope of this research includes the development of a scalable emission quantification methodology, forecasting algorithms based on machine learning, performance metric systems, and an optimisation module. Together, these modules aim to provide insight into the temporal and operational dynamics of ship-based emissions, offering guidance for mitigation strategies under existing port conditions.

The delimitations of this thesis include:

- The study is focused exclusively on ship-sourced air pollutants (e.g., CO_2, NO_x, SO_x, PM, CH_4, NMVOC, CO) in port environments. Other contributors to air pollution in port areas, such as road traffic and port-related industrial activities, are not considered in this study. Emissions of NMVOC from cargo handling and bunkering operations are also excluded due to their minor scale and negligible contribution in the context of overall ship-related emissions. In addition, other environmental issues, such as underwater noise, marine litter, and ballast water discharge are beyond the scope of this research.
- The emissions were quantified by combining the energy-based calculation method with bottom-up logic, selected as the most exhaustive approach. Consequently, alternative monitoring techniques, such as direct air sampling via sensors or remote sensing through satellite observations, were not prioritised in this research. These methods, while valuable for certain applications, fall outside the scope of the methodological focus adopted in this study.
- The analysis is restricted to port operations and does not cover emissions generated during open-sea navigation. The results, although scalable, are derived from case-specific data obtained from the Port of Split and may not directly generalise to ports with significantly different vessel traffic or regulatory frameworks.
- While several air pollution mitigation strategies are acknowledged, the optimisation module primarily addresses feasible operational measures (e.g., turnaround optimisation, berth scheduling, speed reduction). The analysis does not model technological transitions such as fuel switching, shore power, or engine retrofitting due to current infrastructural and regulatory limitations in the research area.
- Broader socio-economic and policy implications of emission reduction strategies are mentioned but not systematically analysed. The primary focus remains on technical and environmental parameters.

The limitations of this study refer to factors beyond the researcher's control that may influence the accuracy or generalisability of the results:

- AIS Data Coverage: Not all vessels are required to use AIS under IMO regulations. As a result, smaller vessels, though less impactful in terms of emissions, may not be fully accounted for. Additionally, transmission errors and missing AIS signals required filtering and cross-verification with national shipping statistics.
- Load Factor Estimation: LFs for main engines were derived using propeller law, but generator (AE) workloads lacked direct data. Instead, static values from compatible studies were applied based on ship type and operating context.
- Fuel Composition Uncertainty: Fuel composition can vary between deliveries even within the same type. Estimates were made based on applicable regulations and engine types, introducing some assumptions.
- Emission Factor Variability: EFs are influenced by multiple parameters including engine condition, fuel type, and operating mode. Since no specific EF data were available for vessels in the study area, values were derived using standardised methods and datasets, with a recognised degree of uncertainty.
- Weather and Environmental Conditions: The effect of meteorological conditions such as wind,

sea state, and ambient temperature on fuel consumption was not directly modelled. However, seasonal fluctuations in temperature were considered, especially for auxiliary systems of passenger ships. Broader integration of meteorological data is recommended for future research.

By acknowledging these delimitations and limitations, the research clarifies the contexts within which the findings are valid, while outlining opportunities for further development and enhancement of the DSS.

CHAPTER 3

5. Research Summary

5.1. Literature Review

Although already discussed in Introduction, particularly Section 1.2.2. (Concept of Emission Inventories as Monitoring Tools for Ship-Sourced Air Pollution in Ports) and Section 1.3.2. (Limitations of Emission Inventories), this segment of the thesis presents a focused summary of the methodological framework and outcomes derived from Paper 1. The study provides a comprehensive systematic review of existing port-related ship emission research and is central to establishing the research foundation for the development of the PrE-PARE DSS.

5.1.1. Objectives and Motivation

The main objective of Paper 1 was to analyse existing research methodologies and types of data related to ship emissions in port areas, identify knowledge gaps, and propose a suitable structure for a scalable and standardised emission estimation model. The motivation stemmed from the diverse and inconsistent methodologies applied in literature, which hinder the comparability and standardisation of emission data across ports. Therefore, this review aimed to synthesise the most reliable practices into an aggregated and applicable approach.

5.1.2. Review Methodology Overview

5.1.2.1. Systematic Review Approach

The review was conducted using a bottom-up, multi-layer analytical approach developed specifically for this research, which integrates four sequential analytical layers, depicted in Figure 4 [68].

- The first layer involved conducting an analytical review of the methodologies and datasets employed in scientific papers and large-scale studies (inventories) addressing port-related ship emissions, using a bottom-up approach guided by the PRISMA framework [68,69]. Subsequently, the methodological foundations of each selected publication were carefully analysed and traced back to their original sources.
- In the second layer, the identified methodological sources were subjected to an exclusion process, then compiled and quantified to determine the most frequently applied techniques within the reviewed body of literature.
- In the third layer, the focus was on evaluating and comparing the methodologies and data used in the most commonly cited studies.
- Based on this evaluation, the final layer presented a recommended methodology for quantifying ship emissions in port areas, with a detailed explanation of all relevant factors.

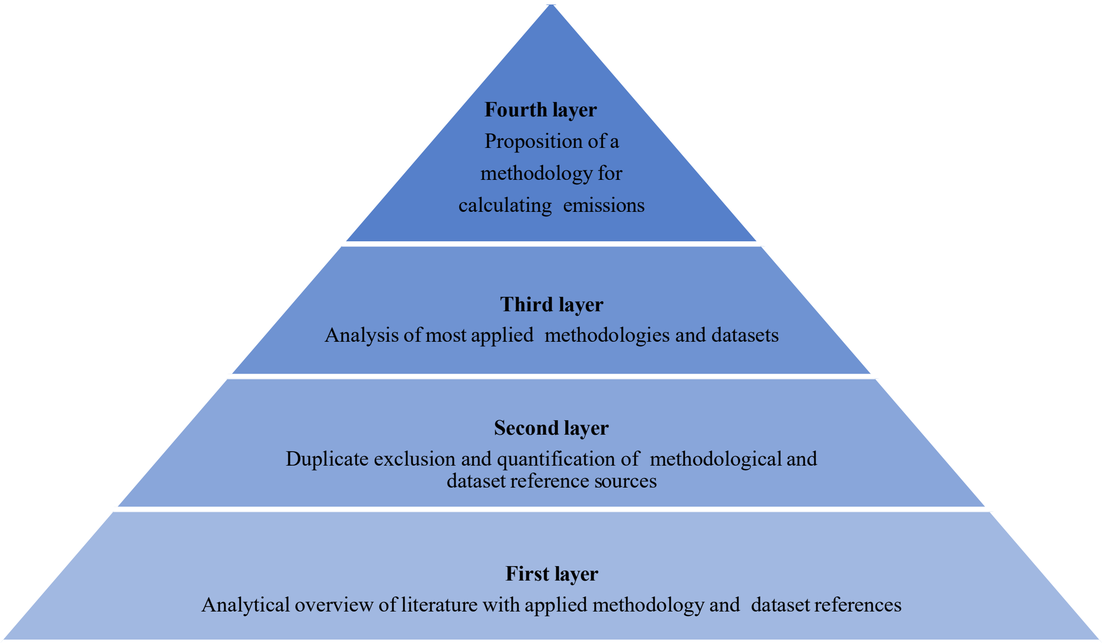


Figure 4. Bottom-up multi-layered analysis approach presented in the Paper 1.

5.1.2.2. Literature Search

The review process began with a keyword-based search across the Web of Science Core Collection, Scopus, and Google Scholar, using combinations of terms such as port, ship, emissions, inventory, gas, pollution, quantification, and method. After initial screening, selected documents were further examined to extract references related to methodologies and datasets. These references were then used to conduct a secondary review, which extended the search to institutional and organisational websites cited in the original literature. By combining keyword and reference-based searches, the methodological approaches and datasets used in each paper were traced back to their original sources. Ultimately, 32 original scientific papers and 28 large-scale emission inventories were analysed, covering over 80 ports globally within the 2008–2021 timeframe [3,6,8,31–33,45,48,70–121]. This completed the first layer of the analysis, as illustrated in Figure 5.

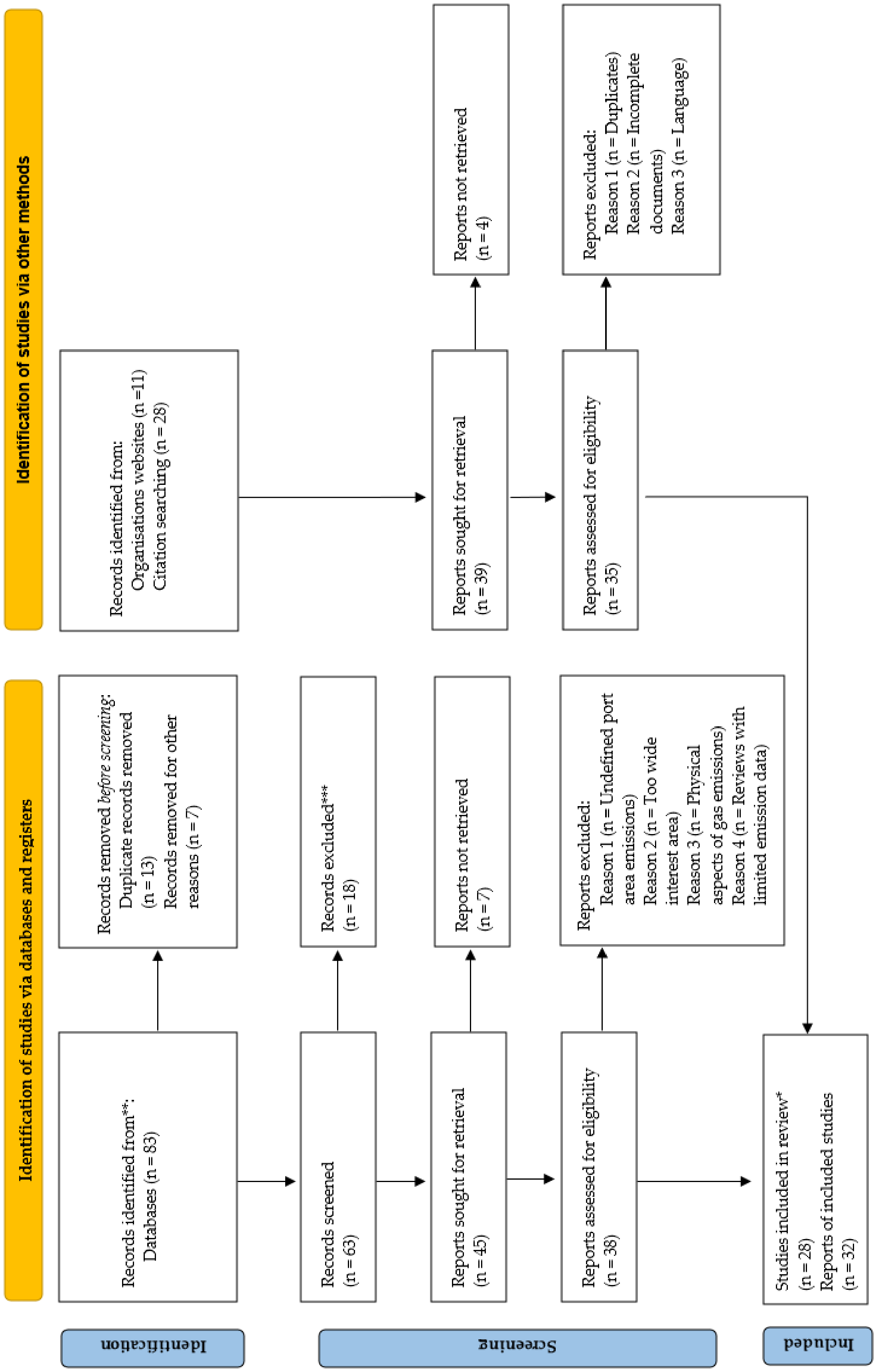


Figure 5. PRISMA 2020 analysis flow diagram for systematic reviews which included searches of databases, registers and other sources from the Paper 1.

5.1.2.3. Key Findings by Layer

- First Layer: Analytical Overview

The majority of the studies reviewed utilised a bottom-up methodology, specifically favouring energy-based approaches due to their localised and high-resolution advantages. Top-down or fuel-based methods were generally restricted to macro-scale inventories. The most commonly used activity data source was AIS with technical specifications obtained from a combination of ship registries and global (web) databases.

- Second Layer: Reference Quantification

This stage involved the removal of duplicates, narrowing down to ten unique methodological references and sixteen primary datasets. Frequently cited sources included:

- US EPA (2006, 2009)
- ENTEC (2002–2010)
- EEA (2009–2020)
- POLA/POLB (Port of Los Angeles/Port of Long Beach)
- SMED/IVL (Swedish Environmental Emission Data / Swedish Environmental Research Institute)

These references contributed EFs, LFs, and operational assumptions crucial to the reviewed studies.

- Third Layer: Methodological Comparison

The following models were explored in detail:

- ENTEC/NAEI: Provided a UK-based framework using fuel type, engine power, and abatement technologies.
- US EPA: Introduced a rigorous bottom-up, energy-based structure segmented by voyage activity.
- POLA/POLB: Developed a comprehensive local emissions inventory based on AIS data.
- EEA Tier 3: Supported tiered inventory development, with Tier 3 designed for data-extensive port-level emissions.
- SMED/IVL: Swedish models offering current EFs and context-specific data.

Each of these models incorporates a unique combination of static inputs (e.g., ship dimensions and engine configurations), dynamic inputs (e.g., activity durations and voyage speeds), definitions of operating modes and EF values.

- Fourth Layer: Proposed Estimation Approach

A consolidated bottom-up energy-based methodology was developed, integrating best practices across the reviewed studies. This method employs a combination of technical details, ship activity data and EFs. Static technical data detailing ship and engine specifications, such as main and auxiliary engine power (PME/AE), engine function, engine type, and fuel type, serve as the basis for emission calculations. Dynamic data is characterised by ships actual voyage speed, course, position and corresponding timesteps derived from AIS. These datasets are used to categorise ship operational modes (activities) defined by the percentage of main engine (ME) and AE load, expressed as LF. Since engine workload directly influences emission levels, the time spent in different operational phases, cruising, manoeuvring, and hoteling, must be considered in the analysis. As the essential and most complex part of the emissions quantification process, the emission factor (EF) relies on a combination of static data, such as engine function, speed, engine type, and fuel type, and dynamic data reflecting the ship's operational characteristics.

Accordingly, the bottom-up, energy-based methodology outlined in Equation (5) which incorporates key factors identified through a systematic review is applied in the emission quantification module developed as part of this research (Paper 2 and Paper 3).

$$E = (PME \times LF \times EFME + PAE \times LF \times EFAE) \times T \times CF \quad (5)$$

Where:

E: Emissions quantity by mode for each ship call – in grams (g);

PME/AE: total power of main engines/auxiliary engines – kilowatts (kW);

LF: load factor expressed as actual engine work output – as a percentage of engine power (%);

EFME/AE: emission factors of different pollutants in regard to engine function, engine type, fuel type, and installation year – in grams per kilowatt hour (g/kWh);

T: time spent in a certain movement activity – in hours (h);

CF: correction factor for emission reduction technologies – constant.

Along with determining data and methodological approach, through its systematic, multi-layered analysis, Paper 1 identified substantial inconsistencies in both methodological approaches and data application in the reviewed studies. These differences pose a limitation to standardisation and prevent the comparability of emission inventories between ports and periods, thereby directly addressing RQ1.

5.2. Methodology - Structure of the PrE-PARE DSS

Upon defining the base parameters and methodological foundation for quantifying ship emissions and identifying key limitations and inconsistencies in inventory practices through the systematic review presented in Paper 1 it became possible to construct a modular framework for comprehensive emission control. The structure of the PrE-PARE DSS, illustrated in Figure 6, comprises four interlinked modules, each sequentially developed based on the methodologies and outputs presented in the preceding research papers.

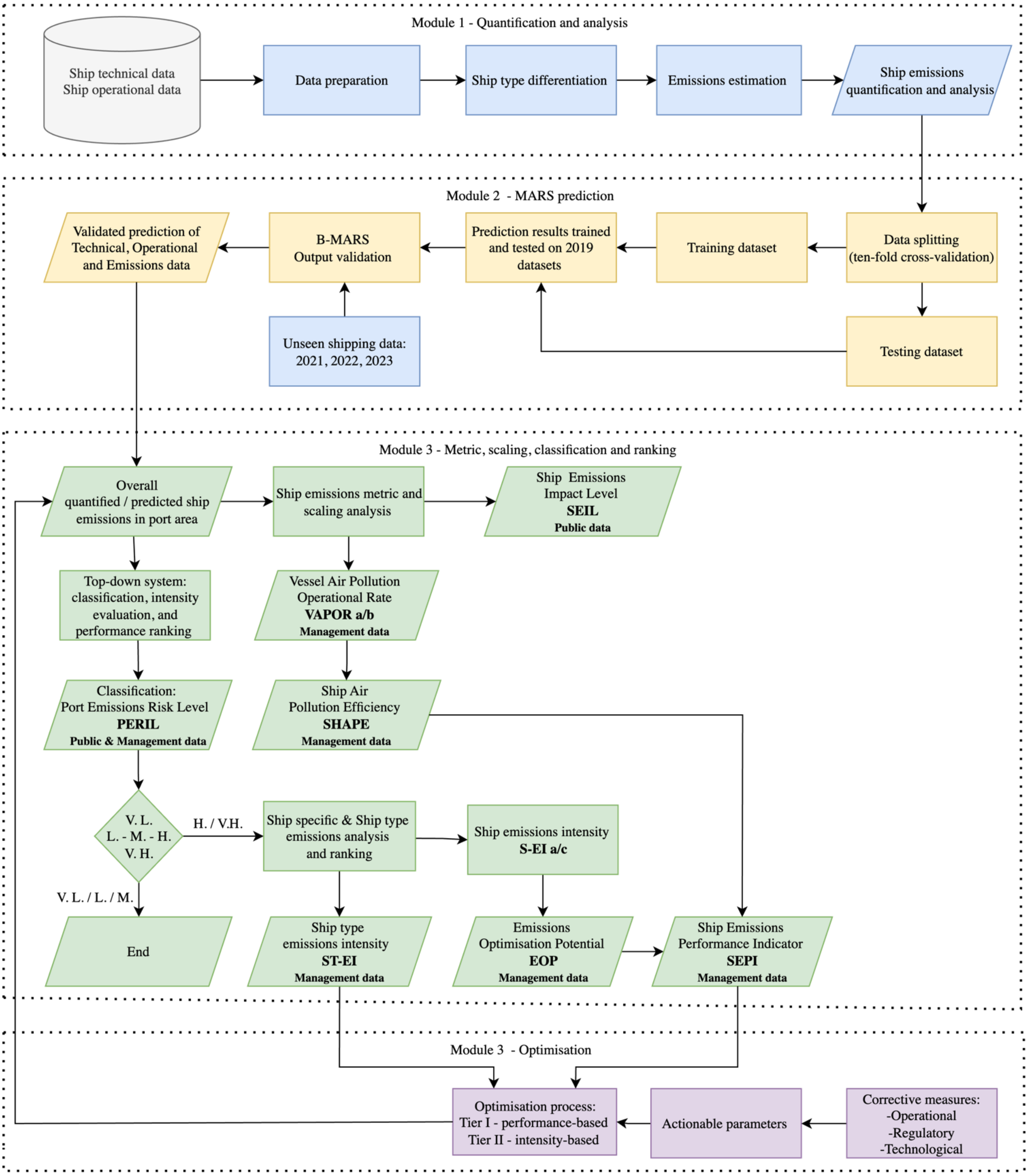


Figure 6. Conceptual flow diagram of the PrE-PARE DSS, adapted and expanded from the version originally introduced in Paper 3.

The first module dedicated for the quantification and analysis of emissions was introduced in Paper 2 and subsequently applied in Paper 3. Here, technical and movement data are prepared to reconstruct full voyage trajectories for each ship arrival, stay, and departure. Based on this reconstruction, emissions are calculated with high temporal and spatial resolution, providing a robust dataset for further predictive analysis.

In the second module, developed within Paper 3, machine learning algorithms are introduced to model emission trends and project future outputs. Since each vessel's operational trajectory is treated as a complex data cluster containing numerous influencing variables, the MARS method was identified as the most suitable modelling technique. It enables both the quantification of influence among factors and the prediction of emissions under varying operational scenarios. To verify its performance, ten-fold cross-validation was conducted, along with additional validation using independent datasets not included in the training process.

The third module, also presented in Paper 3, builds upon these results to deliver comprehensive evaluation of emissions performance. This is achieved through the introduction of several novel metrics that enable scaling, classification, and ranking of emissions from individual ships, groups of vessels, and entire port operations. The framework supports transparent comparisons and allows for systematic tracking of air pollution risks and efficiency outcomes over time. Importantly, the PrE-PARE DSS incorporates not only CO_2, but also other greenhouse gases such as CH_4, and a full spectrum of APSs (SO_x, NO_x, PM_{10}, $PM_{2.5}$, NMVOC, CO). This allows for a holistic assessment of ship emissions that extends beyond what is currently offered in most regulatory reporting tools.

The fourth and final module, currently presented in this thesis and is part of Paper 4 (in preparation), represents the optimisation layer. It builds on the results generated in previous modules to assess risk, identify inefficiencies, and propose actionable mitigation measures. Depending on the severity of the emissions classified by the system (e.g. high or very high category), corrective actions are proposed at either the ship or ship type level. These recommendations may include operational interventions such as adjusting berth duration, speed reduction, or coordination of manoeuvring procedures, as well as broader strategies for scheduling and prioritisation. The optimisation process continues in an iterative cycle until emissions are reduced to acceptable levels, using performance-based indicators to guide decision-making.

Because the system is constructed using universal emission-related parameters and open-source processing, it is not limited to a specific case study and can be adapted to other ports or regions. Furthermore, its modular design enables continuous upgrading, including the integration of new emission types, external data streams, or regulatory factors. All algorithms and data-handling were developed using the RStudio 2023.09.1+494 software package, ensuring transparency and reproducibility.

Therefore, the present section summarises the overall structure of the PrE-PARE DSS, outlining the logical interrelation of the modules and the systemic flow of data. Detailed explanation of each module, including methods for data acquisition, preparation, modelling, and application, is provided in the following subsections.

5.2.1. Defining Input Databases – Technical and Operational Data

The majority of data used in this research was obtained during the development of Module 1, as detailed in Paper 2, with supplementary datasets acquired later to support the validation of the predictive module introduced in Paper 3. Since the passenger basin of the Port of Split was selected as the case study area, this section outlines both the spatial and operational characteristics of the port, as well as the specific technical and movement-related databases that were utilised as input parameters throughout the PrE-PARE DSS framework.

5.2.1.1. Context of the Case Study Area – Maritime Traffic Characteristics and Spatio-Temporal Specifications of the Port of Split

The methodologies within this research were applied with a focus on the Port of Split, specifically its passenger basin, as the primary case study, with data corresponding to the 2019 calendar year. This period was selected as it marked a peak in port activity at a time when this part of the research was conducted, offering a representative operational context for analysis.

The Port of Split stands as one of the busiest passenger and vehicle ports in the Mediterranean. In 2019, it handled more than 5.6 million passengers and over 829,000 vehicles [122]. In contrast, cargo throughput remained of local significance, with approximately 2.9 million tonnes recorded [122]. As a result, port traffic was dominated by passenger-focused vessel types, primarily Ro-Ro Ferries, High Speed Craft, Cruise Ships, and leisure vessels. Collectively, these categories accounted for nearly 90% of all vessel arrivals.

Geographically, the port is divided into two distinct zones by the urban structure of the city of Split. The northern section, known as the North Port, is situated on the peninsula's northern coastline and predominantly serves cargo vessels. The southern part, referred to as the City Port basin, is oriented towards passenger services and accommodates the vast majority, around 90%, of the port's maritime traffic. Its close integration with the historical and commercial centre of Split results in a dense overlap between port operations and the urban environment. This spatial configuration, illustrated in Figure 7, highlights the potential for port-related air pollution to pose significant risks to public health, especially given Split's status as Croatia's second-most populous city. Moreover, the port's strategic role as a transport gateway to the Adriatic islands and the Italian coast, alongside its growing popularity as a cruise destination, underscores the urgency for enhanced emission monitoring and control. Accordingly, the present study narrowed its analytical scope to the passenger basin, where shipping activity and environmental exposure are most intense. The defined research area, along with its geographical coordinates, is visualised in Figure 8.

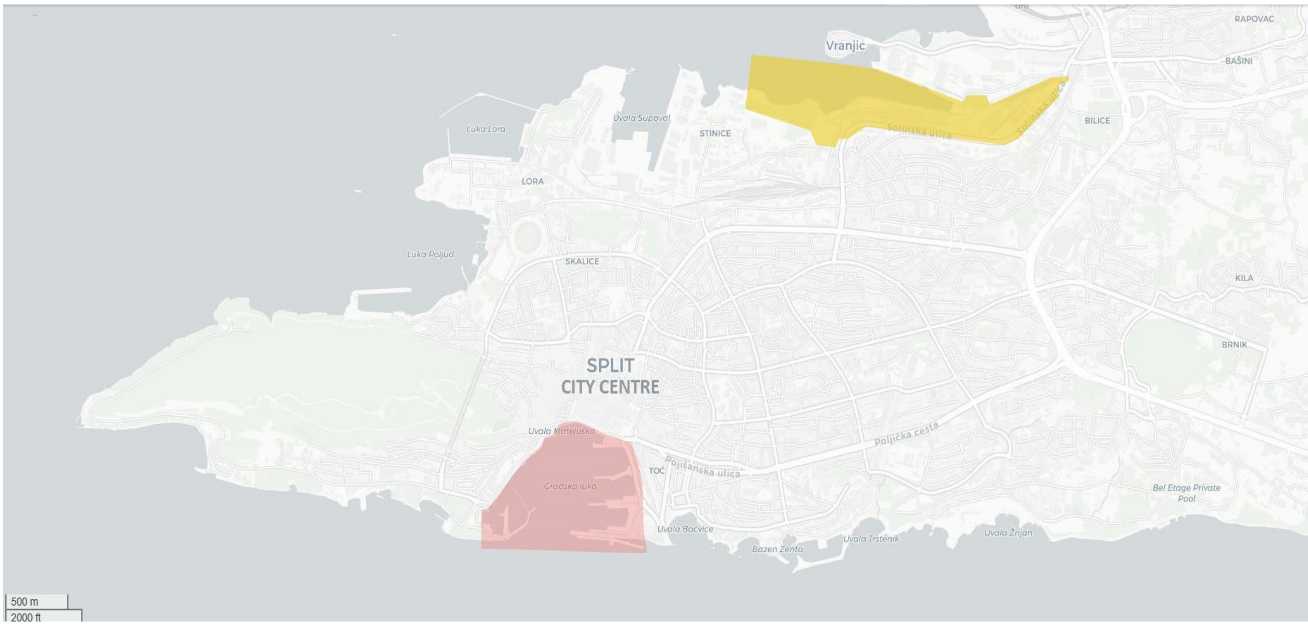


Figure 7. Spatial layout of the Port of Split, highlighting the North Port (yellow) and City Port basin (red), in direct proximity to the Split city centre. The integration of the City Port into the urban core is of relevance for air quality assessment. Originally presented in Paper 2.

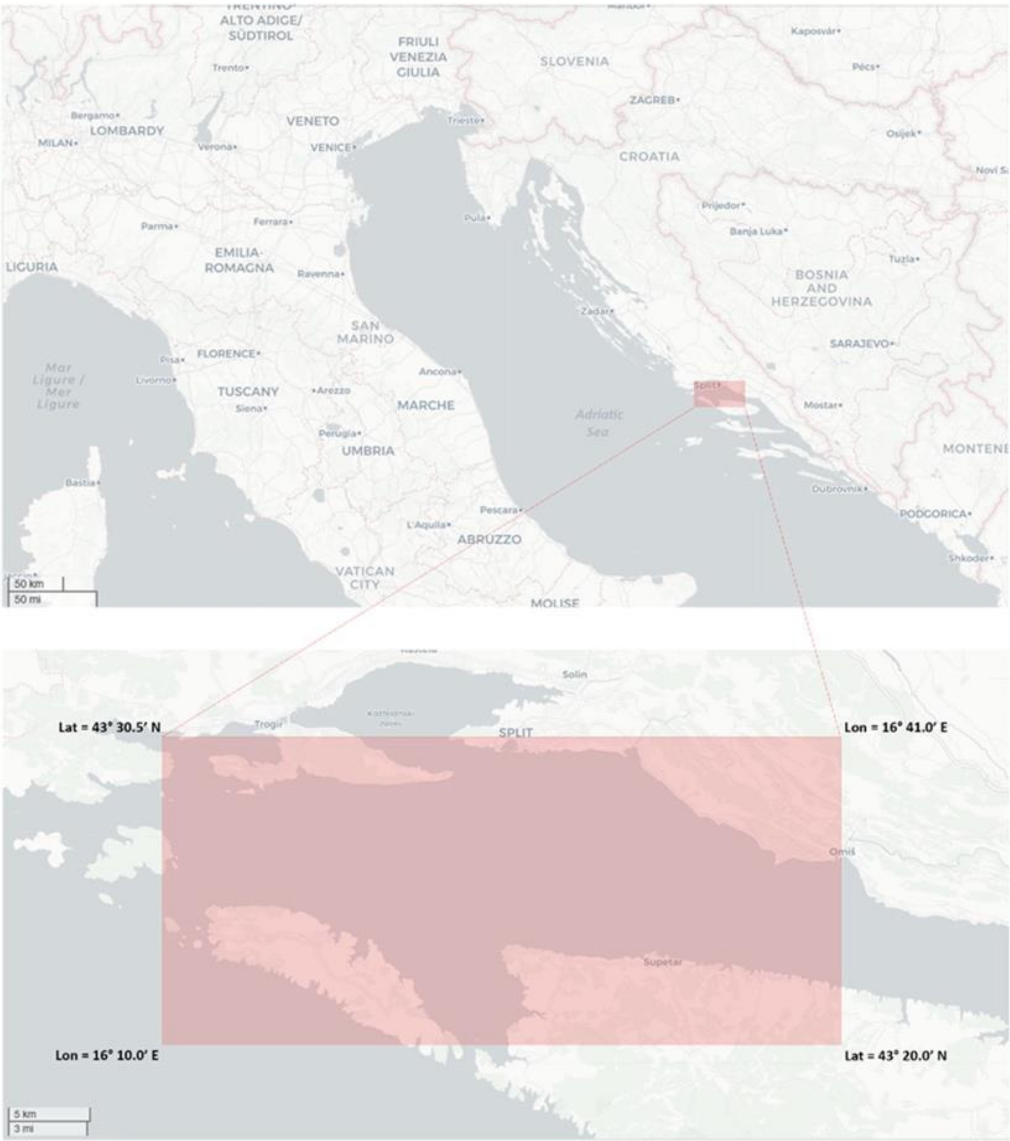


Figure 8. Geographic location of the research area with reference to the Adriatic region. The lower panel provides a magnified view of the defined port activity zone used for emission modelling. Originally presented in Paper 2.

5.2.1.2. Data Acquisition and Integration: Technical Specifications and AIS Movement Records

To compile a comprehensive dataset for emission quantification, prediction and evaluation, a detailed technical database was created by linking ship identifiers, specifically name, type, and Maritime Mobile Service Identity (MMSI) number, to multiple information sources. These included the CRS, the CIMIS, and verified online resources from ship operators and public registries. The compiled technical parameters encompassed GT, vessel length and breadth, year of build, ME and AE power, engine type and speed, fuel type, maximum ship speed at maximum continuous rating (MCR), and installed emission reduction technologies. Where discrepancies or redundancies were encountered, data from the CRS was treated as the primary source to ensure consistency and reliability.

The AIS, while originally developed to enhance navigational safety through the real-time transmission of ship-related data to other vessels and shore stations, has become a valuable tool for operational analysis [123]. This system broadcasts both static and dynamic ship data. Static AIS data includes MMSI number, IMO number, vessel type, name, length, and call sign [124]. Dynamic AIS data, on the other hand, captures positional and navigational parameters such as geographic coordinates, timestamp, course over ground, and speed over ground [124].

For this study, a full AIS dataset was provided by the University of Split - Faculty of Maritime Studies. Given that AIS transmissions do not include engine specifications or operational LFs, critical for emission modelling, only the dynamic AIS components were used for tracking ship trajectories. The static AIS identifiers served exclusively to merge movement data with the previously constructed technical database, ensuring a seamless integration of ship characteristics and operational records across the PrE-PARE DSS.

5.2.2. Module 1: Emission Quantification and Analysis

This component, initially developed and validated in Paper 2 and later adapted in Paper 3, forms the foundational module of the PrE-PARE DSS system's modular architecture. Its core function is to generate a high-resolution inventory of ship-sourced emissions including CO_2, CH_4, NO_x, SO_x, CO, PM_{10}, $PM_{2.5}$, and NMVOC, while also providing comprehensive technical, spatial, temporal, and operational profiles of maritime traffic within port areas, fulfilling the objectives outlined in RQ2.

To fulfil this objective, a structured multi-step methodology was employed, involving the systematic collection, integration, and preprocessing of both technical and operational datasets. The process encompassed cleansing, formatting, and merging extensive dynamic AIS records with static ship technical data, enabling emissions to be estimated for each individual port call and aggregated over broader operational periods. Once the data preparation was completed, the bottom-up energy-based method was applied to every vessel that called at the Port of Split in 2019. This approach, aligned with the methodological recommendations highlighted in the Key Findings section of the Paper 1 review, allowed for emissions to be quantified with high-density and accuracy.

Together, these variables and procedures, ranging from data acquisition to preprocessing and final emissions estimation, form the core of the quantification and analysis workflow. This process is summarised in Figure 9, which illustrates the structure of Module 1. The figure presents a detailed overview of the module's design, including the integration of static and dynamic datasets, the calculation of LFs, identification of operational modes, and the application of EFs. These elements collectively underpin the bottom-up energy-based estimation model expressed in Equation (1), which has been consistently implemented throughout the PrE-PARE DSS.

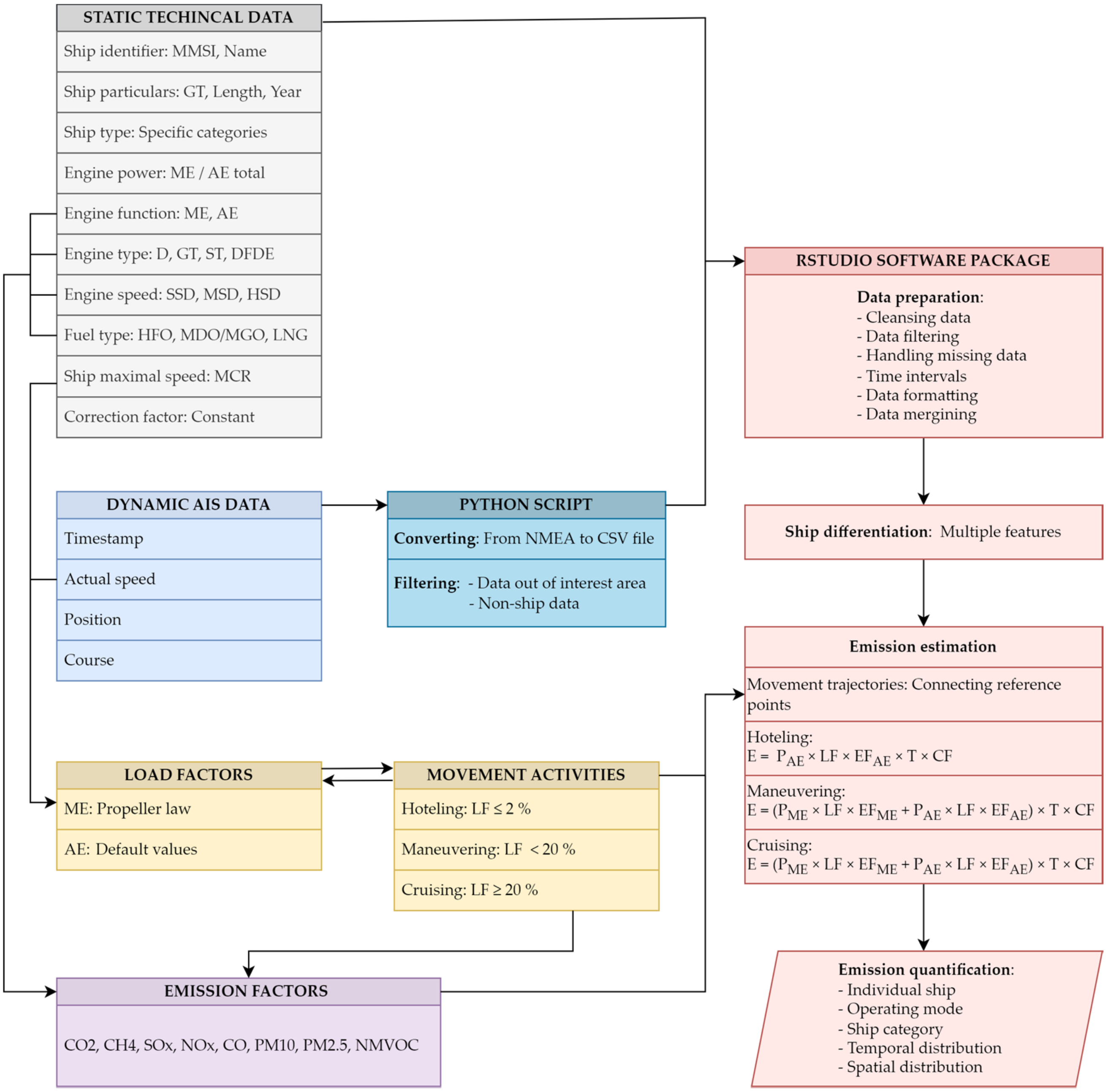


Figure 9. Flow diagram of Module 1 for quantifying ship emissions.

Within the grey box, which outlines the technical attributes used in the model, several abbreviations are applied: MMSI refers to Maritime Mobile Service Identity; GT denotes Gross Tonnage; D represents Diesel engines; GTU stands for Gas Turbine Unit; STU for Steam Turbine Unit; and DF indicates Dual-Fuel engines. Engine speed categories are marked as SS/MS/HS D, referring to Slow-, Medium-, and High-Speed Diesel engines, respectively. Common fuel types include HFO (Heavy Fuel Oil), MDO/MGO (Marine Diesel Oil/Marine Gas Oil), and LNG (Liquefied Natural Gas). MCR refers to the maximum power output tested by the engine manufacturer [94]. Typically, ships operate at a nominal continuous rating, calculated as 85% of 90% of the MCR value [107]. The dark blue box indicates the use of NMEA (National Marine Electronics Association) sentence format.

5.2.2.1. Data Preprocessing Workflow

The preprocessing phase began with the handling of dynamic AIS datasets. However, as AIS transmits signals in the NMEA sentence structure, which is not directly compatible with RStudio software, a dedicated Python script was developed and embedded within the first module to convert the raw AIS data into a readable CSV (Comma Separated Value) format [125]. During the subsequent preprocessing stage, all non-ship and erroneous entries were excluded, resulting in a cleaned dataset comprising 49,540,895 valid records for vessels operating in 2019 within the research area. These entries served as the basis for emission estimations within the quantification module and were also used for training and testing in the predictive module. An equivalent procedure was later applied to collect an additional 15,930,840 AIS reference points for ships calling at the same port during 2021, 2022, and 2023. These supplementary datasets, treated as unseen data, were used to perform extended validation of the predictive model.

Once the AIS records were processed, they were merged with corresponding technical data for each vessel using unique identifiers through a dedicated script developed within the RStudio environment. Technical details of ships included GT, vessel dimensions, engine types and speed, fuel type, design speed of vessel, and any installed emission control technology. By linking each AIS point to a ship's technical profile using identifiers such as MMSI, IMO number, and vessel name, it was possible to obtain a complete operational picture of each port call in 2019.

The next step in this phase involved classifying ships into defined types. This categorisation was based on a combination of vessel function and specific technical attributes, such as size, speed, and engine specifications. In cases where certain vessel groups displayed high variability in parameters like engine power, probabilistic distribution methods were used to refine the classification further. This approach ultimately led to the identification of eleven distinct ship types:

- Large Cruise Ships
- Ro-Ro Ferries
- Large Ro-Ro Ferries
- Small Cruise Ships
- Medium Cruise Ships
- High Speed Crafts
- Excursion Ships
- Tugs
- Pleasure Craft
- Fishing Vessels
- Sailing Ships

Grouping vessels according to these multiple criteria not only enhanced the precision of imputing missing technical data but also established a foundation for the predictive modelling developed in the subsequent module.

5.2.2.2. Operating Mode Identification and LF Estimation

Once the ship trajectories were defined, each movement was further classified into specific operational modes: cruising, manoeuvring, and hoteling. This segmentation was essential for accurately estimating emissions, as engine workload and pollutant output vary considerably across these phases [9,126]. It is well established that engine load has a direct impact on combustion efficiency and, consequently, on emission levels [76]. Studies suggest that engines achieve optimal efficiency at around 80% load, with performance deteriorating at lower loads, especially below 20% load. To identify these segments, the LF of the ME was calculated using the propeller law as expressed in equation (6) [9,126]:

$$LF = (S_A/S_M)^3 \tag{6}$$

Where:

S_A: actual speed of the ship – in knots (kt);

S_M: speed of the ship at MCR – in knots (kt).

Modes were classified as follows:

- Cruising: LF > 20%
- Manoeuvring: 0% < LF ≤ 20%
- Hoteling: LF = 0%, ME off, AE in use

While the generators' workloads reflect the power demands of each operational mode, they cannot be predicted using the propeller law or comparable approaches. As a result, LFs for AEs are typically uncertain [44,107]. Due to the lack of detailed studies on AE workloads for ships operating within the study area, static LF values were adopted from several large-scale studies and publications that involve comparable traffic patterns and spatial conditions [31,40,126].

5.2.2.3. EF Assignment and Calculation

Following mode identification, appropriate EFs were assigned to each activity segment. These were not predefined in the AIS or technical datasets but were introduced at the final stage of preprocessing. EFs were selected based on engine function (main or auxiliary), engine type, fuel type, and year of installation, and derived from the IMO 3rd and 4th Greenhouse Gas Studies and the San Pedro Bay Ports Report [3,9,126]. This step ensured emissions estimation aligned with international standards while reflecting realistic engine behaviour. The types of EFs, along with the elements for identifying them, are presented in Table 1.

Table 1. Engine details, modes of operation and types of EFs incorporated in the model as present in Papers 2 and 3.

Elements for determination and types of EFs							
Engine function	**Engine type**	**Engine speed (rpm)**	**Fuel type**	**Mode & LF**		**GHG EFs**	**APS EFs**
ME	D	SS D < 300	MDO/MGO	C	LF = > 20 %	CO_2	SOx
AE	GTU	MS D 300 - 900	HFO	M	LF < 20 %	CH_4	NOx
	STU	HS D > 900	LNG	H	LF = < 2 %		$PM_{10, 2.5}$
	DF						NMVOC
	D-E						CO

5.2.3. Module 2: Predictive Module

Following the comprehensive emissions inventory generated in Module 1 where raw data was pre-processed and emissions were systematically quantified and analysed, the second component of the PrE-PARE DSS was developed as a part of Paper 3 to support emission forecasting, thereby directly addressing RQ4 related to predictive modelling. This predictive module is designed to anticipate ship-sourced emissions across a range of operational scenarios by modelling the complex, non-linear relationships between technical specifications, operational variables, and actual emission outputs. Since ship-generated pollutants are influenced by a range of interdependent variables, including engine characteristics, energy output, and voyage profiles, traditional linear models are insufficient for accurate forecasting. To address this, a non-linear modelling approach was adopted.

5.2.3.1. Multivariate Adaptive Regression Splines (MARS)

MARS was selected as the most suitable machine learning method for modelling the non-linear and interactive effects between the independent variables (e.g. engine power, fuel type, LF) and the dependent variables (emission values) [127]. MARS constructs flexible, piecewise regression models using basis functions, mathematical splines that allow the model to adapt to local variations in the data [128].

The modelling process consists of two key stages:

- Forward phase: Iteratively introduces basis functions that improve the model's fit by identifying breakpoints (knots) within the predictor variables [127,129].
- Backward (pruning) phase: Eliminates those basis functions that contribute the least to predictive accuracy, minimising overfitting [127,129]. This is guided by the Generalised Cross-Validation (GCV) criterion, which balances model complexity and error. The GCV can be expressed as follows (7) [128]:

$$\mathrm{GCV}(\mathrm{M}) = \frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}_M(x_i)^2)}{(1 - C(M)/n)^2} \tag{7}$$

To improve robustness, the study evaluated both standard MARS and Boosting MARS (B-MARS) methods, with and without log-transformed targets [130]. This resulted in four predictive variants, all trained using 2019 data derived from Module 1. Hyperparameter tuning was conducted using ten-fold cross-validation, ensuring reliable performance assessment across different data partitions.

5.2.3.2. Performance Evaluation and External Validation

To evaluate the predictive performance of the MARS models, three widely accepted statistical metrics were applied: Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and the Coefficient of Determination (R^2), as presented in Equations (8), (9), and (10) [127]. These metrics are commonly used to assess the accuracy and robustness of regression-based models in environmental and technical forecasting.

R^2: Indicates how well the model explains the variance in the target variable. Its value ranges from 0 to 1, with values closer to 1 signifying better model performance and a stronger correlation between predicted and actual values [131,132]. RMSE: Measures the square root of the average squared differences between predicted and observed values. Since it is sensitive to large errors, lower RMSE values indicate better predictive accuracy [131]. MAE: Reflects the average absolute difference between predicted and actual values. Unlike RMSE, it treats all errors equally. As with RMSE, lower MAE values represent more accurate predictions [132].

In addition to standard model evaluation metrics, this study incorporated an extended validation phase using previously unseen shipping data from the years 2021, 2022, and 2023. Emissions were first calculated based on this new dataset and then compared to the predictions generated by the model trained on 2019 data. This comparative approach provided a robust assessment of the model's forecasting accuracy and perform reliably in different operational periods.

$$\mathrm{R}^2 = 1 - \frac{\sum_{\mathrm{i=1}}^{\mathrm{n}}(\mathrm{X_i} - \mathrm{Y_i})^2}{(\sum_{\mathrm{i=1}}^{\mathrm{n}}(\bar{\mathrm{Y}} - \mathrm{Y_i})^2} \tag{8}$$

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|X_i - Y_i| \tag{9}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(X_i - Y_i)^2}{n}} \quad (10)$$

where Xi is the predicted i[th] value, and the Yi element is the actual i[th] value, while n stand for the number of samples [127,132].

5.2.4. Module 3: Ship emissions metric, scaling, classification and ranking

As the central analytical component of the PrE-PARE DSS, Module 3 was developed as a part of Paper 3, to translate complex emission data into meaningful performance metrics, with the objective of supporting port authorities and stakeholders in identifying key polluters, understanding emission dynamics, and informing optimisation strategies. While emission quantification (Module 1) and prediction (Module 2) offer high-resolution insights into actual and forecasted exhaust outputs, Module 3 focuses on interpretation, comparison, and communication of these results through novel indicators and classification systems, leading to clear explanation of the RQ3. These tools are grounded in the measured operational output of ships and aim to overcome the limitations of inventories and global carbon-centric metrics such as the IMO's EEDI, EEOI or CII, which typically overlook port-specific behaviours, non-CO_2 pollutants, and mode-specific operational distinctions [9,17].

5.2.4.1. Development of Emission Metrics and Scaling Logic

Since the core mission of maritime transport is to ensure safe and efficient service, emissions must be assessed relative to this functional objective. Thus, to enable a standardised and transparent approach for assessing the operational efficiency and environmental impact of individual ships, it was first necessary to define and measure the energy output of ships as a consistent operational outcome. This is captured by the Operational Efficiency (OE) that can be described as a ship's capacity to complete its voyage within the expected timeframe while using the least possible amount of energy, as shown in Equation (7).

$$\text{OE (kWh)} = \sum_{\text{C,M,H}} \text{Operational LF (kW)} \times \text{Operational time (h)} \quad (11)$$

In the context of port operations, a voyage is defined as the complete sequence of a ship's arrival, stay, and departure, incorporating the three key operational modes: cruising, manoeuvring, and hoteling. This segmentation enables a thorough assessment of a vessel's operational behaviour. By aligning the time required to achieve the expected OE with the vessel's operational capacity, and then comparing this to the emissions produced throughout the voyage, it becomes possible to calculate the Vessel Air Pollution Operational Rate (VAPOR) for each mode, as outlined in Equation (12). In contrast to IMO's existing metric frameworks, VAPOR utilises available operational data and emission values to assess performance across the entire voyage. It does so by calculating the average hourly emissions per unit of work capacity for each operational phase individually. This approach facilitates a more precise and standardised measure of emissions efficiency.

$$\text{VAPOR} = \frac{\text{Emissions (g)}}{\text{Work capacity} \times \text{Operational time (h)}} \quad (12)$$

To maintain consistency, interpretability, and comparability across different vessel types and operational contexts, the calculated VAPOR (VAPOR-c) for an individual ship is normalised using feature scaling. This is done by comparing it to the baseline VAPOR (VAPOR-b) representative of the relevant ship type. The resulting ratio defines the Ship Air Pollution Efficiency (SHAPE), as presented in Equation (13). The

VAPOR-b values are derived from a comprehensive emissions database built for each ship type group, previously categorised in the system's first module. SHAPE therefore serves as a benchmark indicator, showing whether a specific vessel performs better or worse in terms of emissions efficiency relative to its category average. Additionally, it allows tracking of efficiency improvements over time for individual vessels and vessel groups.

$$\text{SHAPE} = \frac{\text{VAPOR-c}}{\text{VAPOR-b}} \tag{13}$$

Furthermore, to enhance public understanding and accessibility, a simplified and intuitive metric system has been introduced to clarify the contribution of individual ships to port-related air pollution. This metric, known as the Ship Emissions Impact Level (SEIL), measures the emissions produced by a specific vessel during a single voyage in comparison to the average emissions per voyage of a typical or baseline ship over a defined period, as expressed in Equation (10). By offering a straightforward and standardised emissions impact scale, SEIL enables the broader port community to easily interpret, assess, and compare the environmental footprint of different ships during their port visits, initiating public awareness.

5.2.4.2. Classification and Prioritisation Framework

Although the emissions are quantified using a bottom-up approach, the evaluation framework progresses from a top-down perspective, beginning with an assessment of total exhaust gases emitted across the entire port area, followed by examining the relative contributions from different ship types, and concluding with the performance evaluation of individual vessels. This sequential structure ensures a comprehensive and methodical assessment, initially identifying the overall air pollution risk, then measuring the intensity of emissions across ship categories, and finally determining vessel-specific performance indicators, allowing for the optimisation-ranking of individual ships. The process also incorporates the SHAPE metric, alongside a calculation of emission optimisation potential, to support a balanced and evidence-based approach to managing ship-sourced air pollution both ship and at the port perspectives.

To support this, the Port Emissions Risk Level (PERIL) classification algorithm has been established as the first step. This algorithm assesses the overall severity of ship emissions within a given time frame by categorising emission levels into five classes: Very Low, Low, Moderate, High, and Very High. The classification is based on statistical comparisons with annual average emissions and their standard deviation, thereby offering a consistent, data-driven assessment based on observed distribution patterns rather than relying on subjective threshold values. Once these thresholds are defined, the system automatically classifies emissions data. If the total emissions are found to exceed the high-risk category, the framework proceeds to the second analytical stage, where the contributions of ship type groups to the port's total emissions are examined in greater detail.

If the total quantified emissions surpass the defined high-risk threshold, the analysis advances to a second phase that focuses on identifying the specific contributions of individual ship groups. This involves applying the Ship Type Emission Intensity (ST-EI) metric, which compares the average emissions per voyage of each ship type against the overall fleet average within a defined time frame, as shown in Equation (14). This comparative approach allows for the creation of a ranked emissions contribution scale, supporting the prioritisation of certain ship categories for targeted emission reduction measures.

In the final analytical phase, the system evaluates the potential for emission reduction on a per-vessel basis. This is achieved through the calculation of the Emission Optimisation Potential (EOP), which assesses a ship's actual emission performance, expressed as the Ship Emission Intensity (S-EI), relative to a baseline reference value for each operational mode, as outlined in Equation (15). If a ship's S-EI exceeds the baseline (EOP > 1), it indicates excess emissions and a higher potential for optimisation; values below 1 suggest more efficient performance. These baseline values are derived from historical records processed in the Module 1. In cases where no previous data exists, such as during a vessel's first recorded port visit, the system relies on the predictive module to estimate emissions based on the ship's type, configuration, and movement data.

However, not all ships will have the same level of improvement potential. Some vessels may already be performing efficiently, leaving minimal room for further optimisation. To ensure fairness in evaluating and ranking vessels, the Ship Emissions Performance Indicator (SEPI) is introduced. This composite metric combines the SHAPE value (which measures emission efficiency) with the EOP value (indicating optimisation potential) to provide a comprehensive performance score, as can be seen in Equation (16). SEPI thus facilitates a balanced and prioritised emissions ranking, ensuring that vessels with the greatest potential for improvement are highlighted for corrective action.

$$\text{ST-EI} = \frac{E_{st} \times V_{tot}}{V_{st} \times E_{tot}} \tag{14}$$

$$\text{EOP} = \frac{\text{S-EI a}}{\text{S-EI b}} \tag{15}$$

$$\text{SEPI} = \text{SHAPE} \times \text{EOP} \tag{16}$$

Where:

ST-EI: Ship Type Emission Intensity – normalised value (dimensionless);

Est: Total emissions for a specific ship type – in kilograms (kg);

Vst: Number of voyages for that ship type – dimensionless value

Etot: Total emissions for all ship types in the period – in kilograms (kg)

Vtot: Total voyages for all ship types in the period – dimensionless value

EOP: Emission Optimisation Potential – normalised value (dimensionless)

S-EI a/b: Ship Emission Intensity actual/baseline – as emissions mass in entire voyage per units of work capacity (kg/wcu)

5.2.5. Module 4: Ship emissions optimisation module

Since the top-down evaluation system introduced in this research enables data-driven classification of air pollution risk in entire port areas, as well as emissions performance assessment for ship types and individual vessel, the final module of the PrE-PARE DSS was developed to support targeted operational improvement and emissions optimisation actions. This optimisation module, which forms the core of Paper 4 (currently in preparation) and directly responds to RQ5 by delivering actionable recommendations for enhancing port operational efficiency. It functions as a DSS that proposes targeted emission control solutions adapted to specific ships, operational modes, and emission scenarios based on quantified and evaluated performance data within the observed period.

The optimisation process is structured into two tiers: a first-tier performance-based optimisation and a second-tier intensity-based optimisation. Both tiers operate under a rule-based logic system that integrates data from all previous modules, including machine learning-based emissions influence analysis, quantification results, and emissions ranking metrics such as SEPI, EOP, and ST-EI.

The initial phase begins by identifying ships and operational modes with above-average emission indicators, particularly those with an EOP greater than 1. These values indicate operational phases where emissions exceed expected baselines. The priority for recommending optimisation actions is initially based on the SEPI, which reflects both the overall efficiency, and the extent of operational improvement required. The principle is to improve emissions performance at the individual level before escalating to systemic or group-level interventions. These performance-based recommendations are directed at the operational level and involve targeted strategies to reduce time and engine load in the relevant mode.

In cases where optimisation based on high EOP values is not sufficient to reduce the total port-level emissions to an acceptable range, particularly when the PERIL is classified as High or Very High, the system initiates a second-tier optimisation. In this phase, the system considers the average emission performance of ship groups using the ST-EI. If the ST-EI value for a group exceeds 1, further optimisation recommendations are extended to other vessels within that group, starting with ones having highest SEPI values. Here, optimisation is applied specifically to voyage sequences (modes) where emissions are most concentrated, either to the ME or AE operations based on their dominant share of total output. This broader scope ensures that even if individual performance improvements are insufficient, adjustments based on intensity can still bring overall emissions within acceptable thresholds.

This iterative cycle continues until total emissions for the evaluated period are expected to fall within the Moderate PERIL threshold. The optimisation mechanism follows a set of conditional rules. The logic governing these optimisation decisions can be formalised as follows in equations (17), (18) and (19):

$$\text{IF } EOP_{i,m} > 1 \Rightarrow \text{Recommend } \{O, R, T\}_{i,m} \tag{17}$$

$$\text{IF } ST\text{-}EI_j > 1 \Rightarrow \text{Recommend } \{O, R, T\}_{i \in j} \tag{18}$$

$$\text{Repeat until } PERIL_t \leq \text{Moderate} \tag{19}$$

Where:

$EOP_{i,m}$: Emission Optimisation Potential of ship i in mode m,

$ST\text{-}EI_j$: the average emissions per voyage for ship type j relative to the reference value,

$\{O, R, T\}_{i,m}$: the set of operational (O), regulatory (R), and technological (T) recommendations relevant for ship i and mode m,

$PERIL_t$: the emissions risk classification for time period t.

The recommendations are based on key influencing parameters identified by the B-MARS predictive module. Since this component integrates both technical and operational characteristics of each vessel, it specifies the most impactful variables contributing to emissions, which are then used to suggest viable emission reduction options.

However, while B-MARS provides insight into what causes differences, the energy-based bottom-up calculations used in the quantification module, offer a complementary view by quantifying the absolute contribution of each emission source. Therefore, the optimisation module integrates both perspectives: B-MARS results identify actionable parameters, while energy-based shares determine emission impact potential. These measures are grouped into the following categories, all applicable from a port management perspective:

Operational measures include managing vessel activity through improved berth allocation, synchronised tug assistance, and arrival/departure slot optimisation to reduce idling and related emissions, minimised turnaround times, zones with reduced approach speed and load optimisation at berth.

Regulatory actions are aligned with ship emissions metric, scaling, classification and ranking module.

They involve emission caps derived from PERIL or ST-EI thresholds, port-level policy instruments, tariff schemes for high SHAPE vessels, mandatory shore power use where infrastructure exists, priority berthing for low-emission or high-efficiency ships and onboard emission-related data reporting.

Technological recommendations include provision of alternative fuels, application of available shore power infrastructure and energy provided from renewable sources.

The application of specific measures depends on the emission performance associated with each mode of operation. In cruising, the system may recommend speed limits during pilotage or optimised scheduling to reduce waiting time. In manoeuvring, solutions such as improved berth traffic management may be suggested. For hoteling, enforcement or facilitation of using shore power infrastructure and turnaround time reduction could be advised, along with rescheduling or reducing time spent at berth.

This module ensures that recommendations are neither arbitrary nor generic, but rather tied to measurable underperformance as revealed through the model's metrics. Contained measures are aligned closely with the goals of the SEEMP by offering structured strategies that ports can use to support vessels in implementing energy efficiency and emission reduction measures from the shore side. The port-based recommendations are directly actionable under SEEMP Part III, which mandates ship-specific carbon intensity reduction plans. Furthermore, the model can interface with existing port sustainability frameworks. For instance, ports such as Los Angeles, Rotterdam, and Singapore already implement Green Port Programmes or differentiated port fee schemes based on emission performance or fuel type. By integrating outputs from the PrE-PARE DSS, particularly SEPI and EOP scores, into these incentive structures, ports can promote cleaner ship operations without requiring vessel-side technological overhauls.

Thus, the optimisation module offers mitigation actions for decision-makers that support regulatory alignment and implementation under global standards.

6. Output Summary

While the primary contribution of Paper 1 was to identify the most appropriate methodological approach for calculating ship-related emissions and to expose the limitations of existing air pollution inventories in port environments, discussed in detail within the Introduction and Literature Review chapters, the outputs generated by each segment of the PrE-PARE DSS were presented progressively in subsequent papers. Paper 2 provided a comprehensive overview of the technical, temporal, spatial, and operational aspects of emissions from all ships that visited the passenger basin of the Port of Split in 2019, as estimated by Module 1. An analysis of the same features generated by Module 1, now focused on a specific day, was presented in Paper 3. This article also includes the results derived from the predictive component (Module 2), alongside the detailed implementation of novel metrics and classification techniques applied to the datasets from the selected period. As a final sequence, the implementation of corrective operational strategies is being explored in Paper 4, which is currently in preparation.

6.1. Module 1 – Emissions Quantification and Analysis

The quantification module estimated ship-related emissions by integrating key technical attributes with a dataset of 49,540,895 AIS reference points, which had previously been processed to define individual vessel trajectories, operational modes, and corresponding EFs. Utilising this bottom-up framework in combination with an energy-based method allowed for high-resolution quantification of air pollutants emitted by each ship during every port call in 2019. These emission estimates, tied to specific port visits and ship characteristics, were stored within the system, enabling the generation of various analytical outputs.

Based on the analysed AIS data, a total of 16,429 port calls were recorded in the Split City Port basin for the year 2019. This result was consistent with official port traffic statistics, confirming the accuracy of the model in representing ship movements, which are fundamental for calculating emissions. The number of port calls detected showed full or high levels of agreement with maritime traffic records for nearly all major ship categories: 100% for all Cruise Ships, 98% and 95% for the two categories of Ro-Ro Ferries, 96% for High Speed Craft, and 94% for Tugs and Fishing Vessels. However, discrepancies were observed for Excursion Ships, Pleasure Craft, and Sailing Ships, where reported figures varied significantly across different data sources. As a result, the emissions associated with these vessel types may be underestimated in the current model. A visual summary of the port call distribution by ship type, derived from the AIS dataset used in this study, is presented in Figure 10.

In all of the analysed vessels, the most frequently installed engine type is the MS D, accounting for 78% of all ships. This is followed by HS D engines, present on 22% of vessels, while LS D engines are found on just 3%. GTU, STU, and DF engines are installed on fewer than 1% of ships and thus have a negligible influence on overall emissions within the study area. Considering the engine configurations and in accordance with the EU Sulphur Directive, it is assumed that all vessels operate on MDO or MGO with a sulphur content limit of 0.1% throughout their entire stay in port.

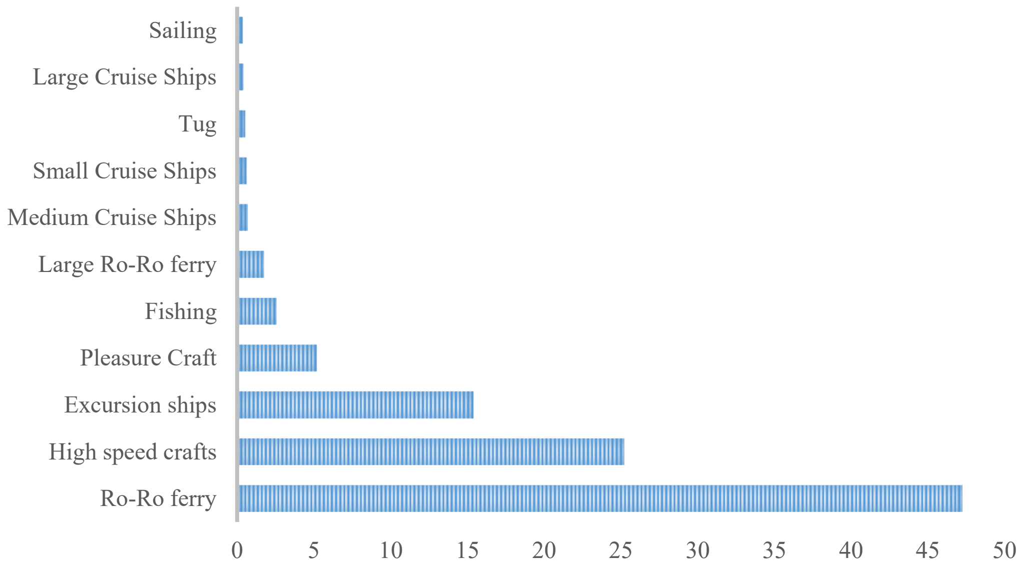


Figure 10. Share of visits to the Port of Split – passenger (City port) basin in 2019 based on AIS data, as illustrated in Paper 2.

It is important to highlight that 2019 was designated as the baseline year for this research, and the datasets from this period were used to establish reference values and operational benchmarks. To support validation and comparative analysis, an additional 15,930,840 AIS reference points, along with the corresponding technical specifications of ships visiting the port during 2021, 2022, and 2023, were also collected. These datasets were processed using Module 1 following the same methodology, enabling consistent integration and analysis throughout the whole system.

As Module 1 was employed in Paper 2 to generate emission-related results on an annual scale, and in Paper 3 to analyse emissions for a specific day, this section of the thesis is structured accordingly, with two corresponding subsections.

6.1.1. Annual Emissions Estimation and Analysis of Technical, Temporal, Spatial, and Operational Aspects

6.1.1.1. Quantification of Ship Emissions on Annual Basis

Based on the processing logic and methodological framework elaborated in the Research Summery section of this thesis, the quantification module produced a high-resolution emissions inventory for all vessels operating within the City port basin of the Port of Split during 2019. Emissions were calculated by aggregating pollutant quantities across defined voyage trajectories, first for individual ships, then grouped by vessel type, and finally summed to reflect overall port emissions.

The annual totals for both GHGs and APSs, presented in Table 2, are quantified by ship category and pollutant type. While the number of port calls was a strong indicator of emissions for Ro-Ro Ferries and High Speed Craft, noticeable deviations occurred for other ship groups. This disparity is largely attributed to variations in engine configuration and operational energy demands across vessel types.

Table 2. Annual emissions quantified by the model for the Port of Split – City port basin in 2019 expressed in mt., as shown in Paper 2.

Ship Type	GHG		APS					
	CO_2	CH_4	SOx	NOx	PM_{10}	$PM_{2.5}$	NMVOC	CO
Ro-Ro Ferry	19,734.524	0.345	11.694	297.449	6.484	5.966	16.857	12.132
High Speed Craft	5962.247	0.105	3.533	85.349	1.945	1.789	5.475	5.037
Large Ro-Ro Ferry	4697.735	0.088	2.782	86.684	1.619	1.490	4.085	0.698
Large Cruise Ships	4276.095	0.080	2.532	77.546	1.471	1.354	3.617	0.772
Medium Cruise Ships	4160.025	0.077	2.464	75.264	1.427	1.313	3.509	0.821
Excursion Ships	1431.938	0.033	0.849	26.338	0.526	0.484	1.870	0.836
Small Cruise Ships	1156.656	0.020	0.685	16.751	0.378	0.348	0.899	0.838
Pleasure Craft	525.652	0.013	0.312	11.866	0.203	0.187	0.777	0.173
Fishing	351.700	0.007	0.208	4.610	0.117	0.108	0.350	0.331
Tug	135.243	0.003	0.080	1.770	0.049	0.045	0.167	0.141
Sailing	30.074	0.001	0.018	0.739	0.011	0.010	0.038	0.007
Totals	42462	1	25	684	14	13	38	22

6.1.1.2. Operating Modes, Spatial and Temporal Distribution of Emissions

The emission inventory developed through Module 1 allowed for the segmentation of pollution by operational mode, offering a detailed understanding of when and where emissions are most pronounced. On an annual basis, the model indicated that 59% of emissions were released during cruising, 8% during manoeuvring, and 33% during hoteling. However, these proportions vary significantly across ship types, as illustrated in Figure 11.

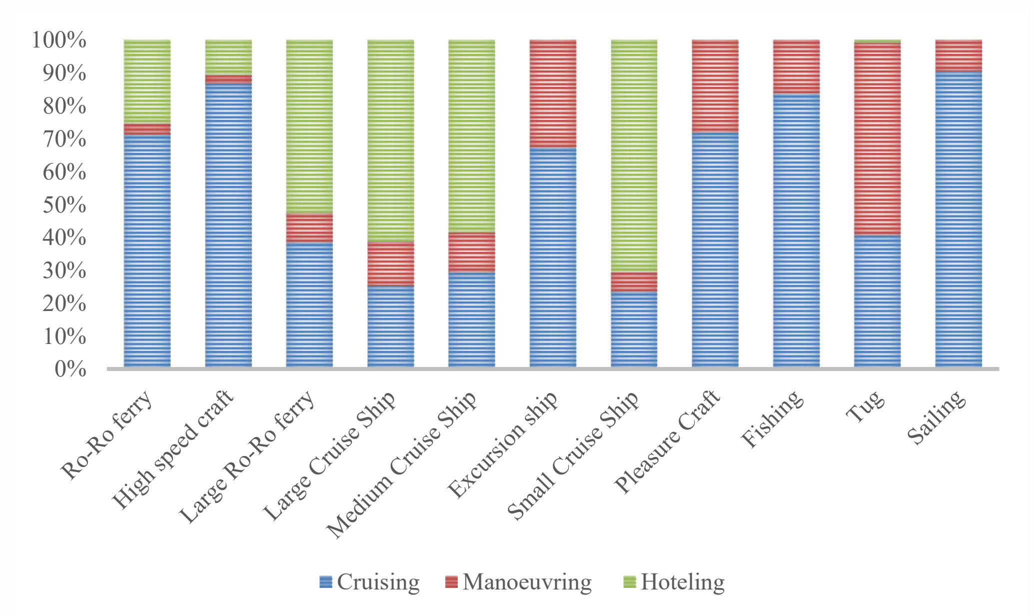


Figure 11. Proportional distribution of annual emissions by operational mode by ship type, as presented in Paper 2.

This insight is crucial for developing emission mitigation strategies, especially considering that APSs released near urban areas pose a greater risk to local air quality. To visualise the emission dispersion patterns of various ship types, the model was applied to generate a high-resolution spatial distribution of emissions according to operational activities. This annual overview, illustrated in Figure 12, highlights that approximately 59% of emissions associated with cruising (red) occurred within a 13 nautical mile **(NM)** radius from the port, whereas the remaining 41%, originating from manoeuvring (green) and hoteling (blue) operations, were predominantly concentrated within just 0.5 NM of the city centre.

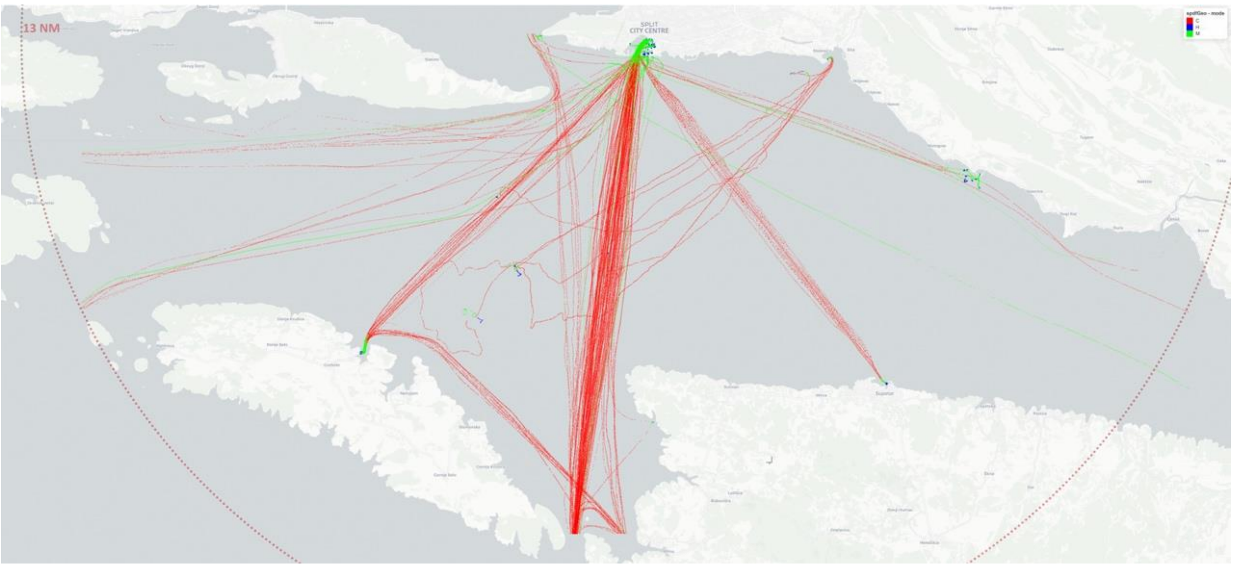
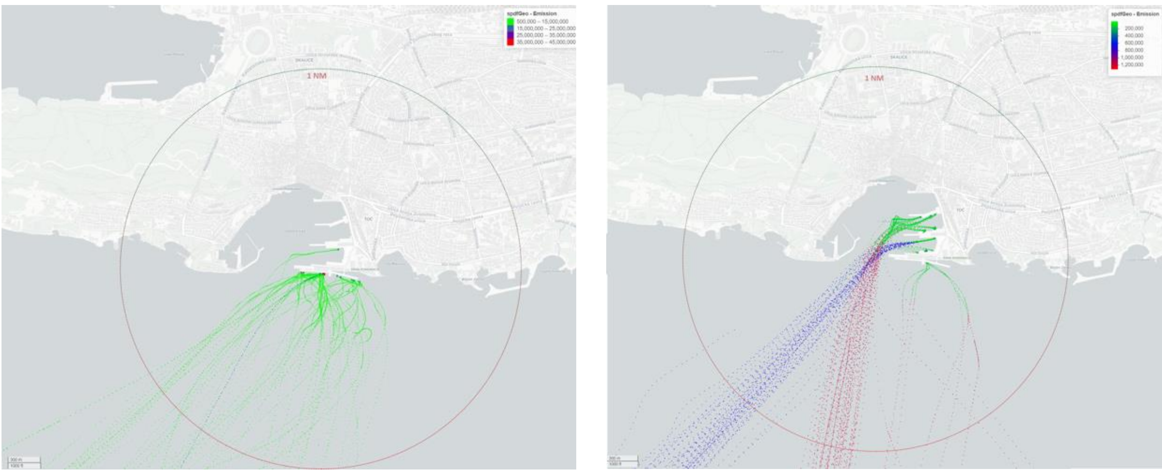


Figure 12. Spatial distribution of emissions by activity, shown in Paper 2 (cruising, manoeuvring, hoteling), illustrating distance of dispersion from city centre based on annual model output.

To further illustrate the emission hotspots by mode and ship type, detailed spatial maps were generated for large Cruise Ships and Ro-Ro Ferries. These are presented in Figure 13, which displays emission totals per port call for the month of October, colour-coded by magnitude. The map clearly shows a spatial divergence in emission patterns: large Cruise Ships concentrated the majority of their emissions near the berth during hoteling, whereas Ro-Ro Ferries primarily emitted during their approach and departure phases, consistent with cruising mode. The legend located in the upper-right section of the map indicates that large Cruise Ships emitted between 35 and 45 mt of air pollutants during hoteling operations, whereas Ro-Ro Ferries generated approximately 1.2 mt while operating in cruising mode.



(**a**) (**b**)

Figure 13. High-resolution spatial representation of emissions per port call within a 1 NM radius from peak emission points: (a) Large Cruise Ships (hoteling dominant), (b) Ro-Ro Ferries (cruising dominant). Originally presented in Paper 2.

The temporal distribution of emissions reflects the seasonality of tourism-driven maritime traffic. As shown in Figure 14, emissions peak in the summer months, particularly in July, which recorded GHG and APS levels nearly three times higher than those in winter months such as January or February. This seasonal surge highlights the need for targeted emission reduction strategies during peak periods. By distinguishing between high and low traffic seasons, port authorities can implement demand-responsive environmental controls. The alignment of GHG and APS peaks underscores the interrelated nature of emissions in a predominantly passenger-based port environment.

Figure 14. Temporal distribution of emission totals based on monthly fluctuations and the annual average for 2019 in mt, as illustrated in Paper 2.

6.1.2. Daily Emission Analysis and Overview of Technical, Temporal, Spatial, and Operational Aspects

Although Module 1 provided the capability to estimate emissions on a ship-by-ship basis and generate a comprehensive inventory encompassing various dimensions of air pollution, the analysis primarily focused on an annual timescale. As highlighted in Paper 2, emission levels and their distribution across different vessel types are not only influenced by technical characteristics of fleet and operating modes but also vary significantly with time. These temporal dynamics can considerably alter the relative contribution of different ship types to overall emissions. Consequently, the development of effective emission control strategies requires consideration of all aspects, which implies processing extensive datasets and analysing complex interactions among multiple parameters, what can be both computationally intensive and time-consuming.

Hence, the implementation of a scalable framework based on emissions inventory analysis can provide a more transparent and effective depiction of the critical characteristics of ship-sourced air pollution in port areas. Such a system offers a structured and consistent foundation for managing air quality in port communities, as demonstrated in the findings presented in Paper 3. To facilitate more informed decision-making and enhanced risk assessment, Module 1 was again employed in the aforementioned article to analyse emissions over shorter time intervals. This approach was adopted due to the identified correlation between elevated emission levels and peak seasonal traffic. Consequently, the analysis was expanded to include daily fluctuations, with a particular focus on high-traffic periods during the baseline year of 2019.

Accordingly, daily total emissions for the entire year were visualised using Module 1, as illustrated by the blue line in Figure 15. This graph not only reinforces the seasonal trends observed in the previous annual analysis but also reveals significant intra-month variability, particularly during the summer season. The deviations are especially striking when compared to the calculated annual average of 120,164 kg, marked by the yellow line. Daily emissions frequently exceeded this benchmark, with some days registering more than double the average output. Given this observed discrepancy, a detailed case analysis was undertaken for a representative peak day in July, the month identified as having the most pronounced emission spikes.

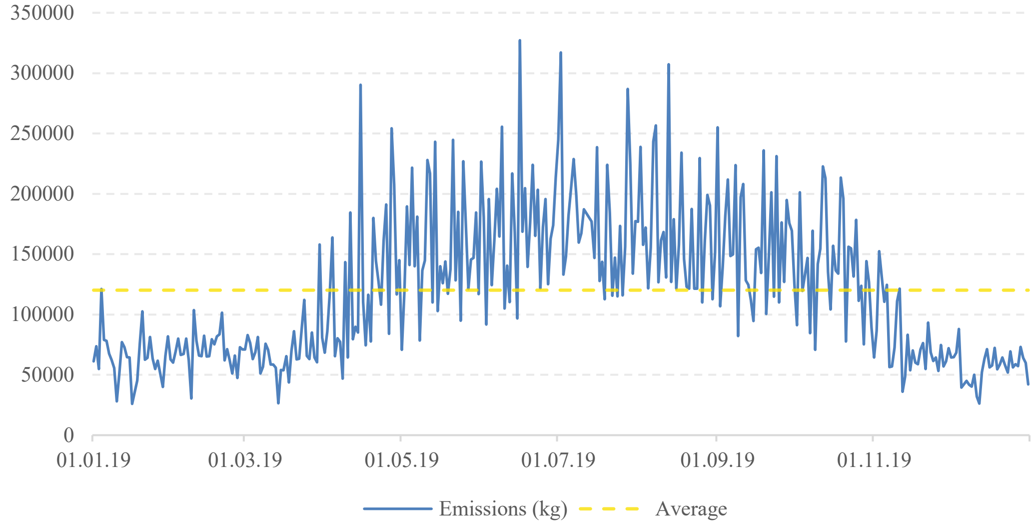


Figure 15. Distribution of daily emission totals and annual average expressed in kg, released by ships calling at the Port of Split passenger basin in 2019, as presented in Paper 3.

Table 3, thus, presents the emissions estimated by the quantification and analysis module for the passenger basin of the Port of Split on 2 July 2019, identified as the day with the highest emission levels during the selected month. The results reveal that total ship-generated emissions on this particular day exceeded the annual daily average by more than 2.5 times, underscoring the acute environmental pressure such short-term peaks can exert on densely populated urban areas. Notably, Large Cruise Ships alone accounted for approximately 37% of the emissions on that day, nearly double the contribution of Ro-Ro Ferries, the second largest source, and only slightly less than the combined emissions of all other ship types. This deviation from the annual distribution highlights the temporal variability of emission patterns and reinforces the importance of short-interval analyses for accurate impact assessment.

Table 3. Emission of GHGs, APS and ship totals in kg by different ship types for the Port of Split passenger basin on 2 July 2019, quantified by the first module in Paper 3.

Ship type	GHG		APS						SHIP TYPE
	CO_2	CH_4	SOx	NOx	PM_{10}	$PM_{2.5}$	NMVOC	CO	TOTALS
Large Cruise Ships	116,161.249	2.133	68.801	2174.880	39.936	36.741	94.975	9.674	118,588.391
Ro-Ro Ferry	63,221.461	1.102	37.466	885.589	20.553	18.908	54.663	48.716	64,288.459
Large Ro-Ro Ferry	39,378.559	0.758	23.300	733.636	13.703	12.607	36.573	3.364	40,202.501
Small Cruise Ships	35,969.292	0.642	21.315	655.656	12.220	11.242	27.581	5.751	36,703.699
Medium Cruise Ships	31,222.711	0.591	18.481	582.766	10.817	9.951	26.038	2.642	31,873.997
High Speed Crafts	19,380.975	0.346	11.486	262.921	6.312	5.807	17.733	17.273	19,702.854
Excursion Ships	21,46.156	0.051	1.272	35.847	0.783	0.720	2.849	1.456	2,189.134
Tug	14,60.308	0.028	0.865	18.785	0.480	0.442	1.324	1.413	1,483.644
Pleasure Craft	1,349.716	0.047	0.800	26.445	0.584	0.537	2.797	0.616	1,381.542
Fishing	691.295	0.021	0.410	9.374	0.272	0.250	1.081	0.765	703.468
Sailing	94.409	0.002	0.056	2.026	0.035	0.032	0.117	0.038	96.715
EMISSION TYPE TOTALS	311076.132	5.722	184.252	5387.925	105.694	97.239	265.730	91.709	317214.402

By correlating the proportion of emissions generated by individual ship types with the number of their respective voyages on 2 July 2019 as the most emission-intensive day, a pronounced imbalance becomes evident. As illustrated in Figure 16, the comparative analysis reveals that High Speed Crafts, although responsible for the highest number of port calls (37%), contributed just 6% to the day's total emissions. In contrast, Large Cruise Ships accounted for only 2% of voyages but generated an overwhelming 37% of emissions.

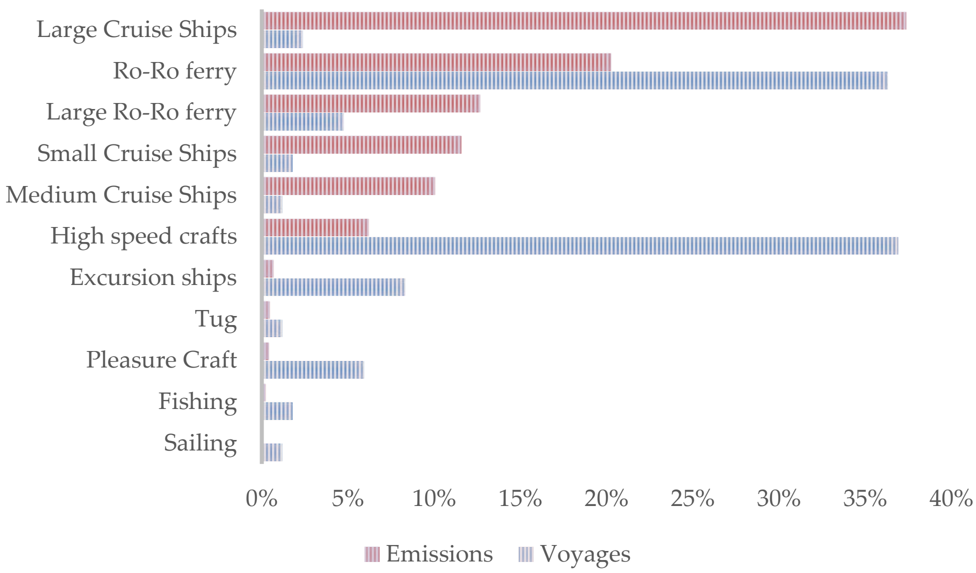


Figure 16. Share of emissions (orange) and voyages (blue) between ship types relevant in the research area on 2 July 2019, provided in Paper 3.

This disproportionate distribution highlights the importance of differentiating emission sources not solely based on frequency of operation but also by assessing underlying operational and technical characteristics. This case, in itself, illustrates the uneven contribution to total emissions and underscores the importance of conducting a detailed investigation into the operational and technical factors that lead to elevated levels of shipboard exhaust production.

In Paper 3, the emission inventory created by Module 1 was further used to analyse operational and spatial patterns, now considering a different period. Specifically, the operational mode breakdown of emissions on 2 July showed a significant shift from annual averages. Emissions were distributed as follows: 43% during cruising, 12% while manoeuvring, and 46% when hoteling. These variations reflect a unique daily operational dynamic and highlight the influence of voyage profiles on emission intensity. Figure 17 clearly demonstrates that all categories of Cruise Ships emitted the majority of their pollutants while hoteling. In contrast, Fishing and Pleasure Craft produced the most emissions during manoeuvring, while all other vessel types primarily contributed during the cruising phase.

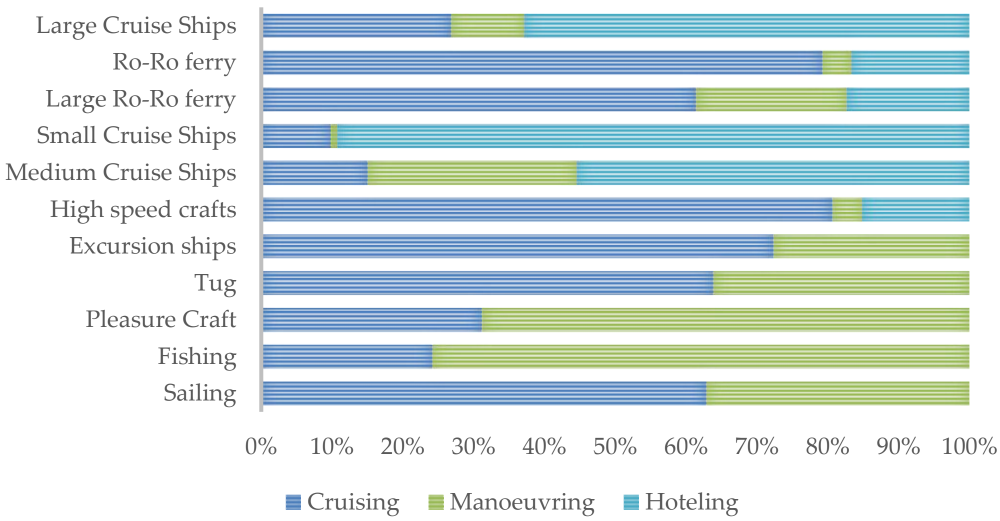


Figure17. Distribution of emissions produced in operating modes for each ship type that visited the passenger basin of Port of Split on 2 July 2019, as presented in Paper 3.

Considering that each operating mode occurs in geographically distinct zones within the port area, a high-resolution spatial emissions map was generated. Figure 18 presents the dispersion of air pollutants categorised by operating phase. The analysis revealed that nearly all emissions were released within a 12 NM radius of Split city centre. Of particular concern is the concentration of hoteling and manoeuvring emissions, constituting 58% of the total, within just 0.5 NM of the urban area. This spatial concentration of exhaust near populated zones is especially critical for air pollutants with strong local health effects, such as NOx, PM, and SOx.

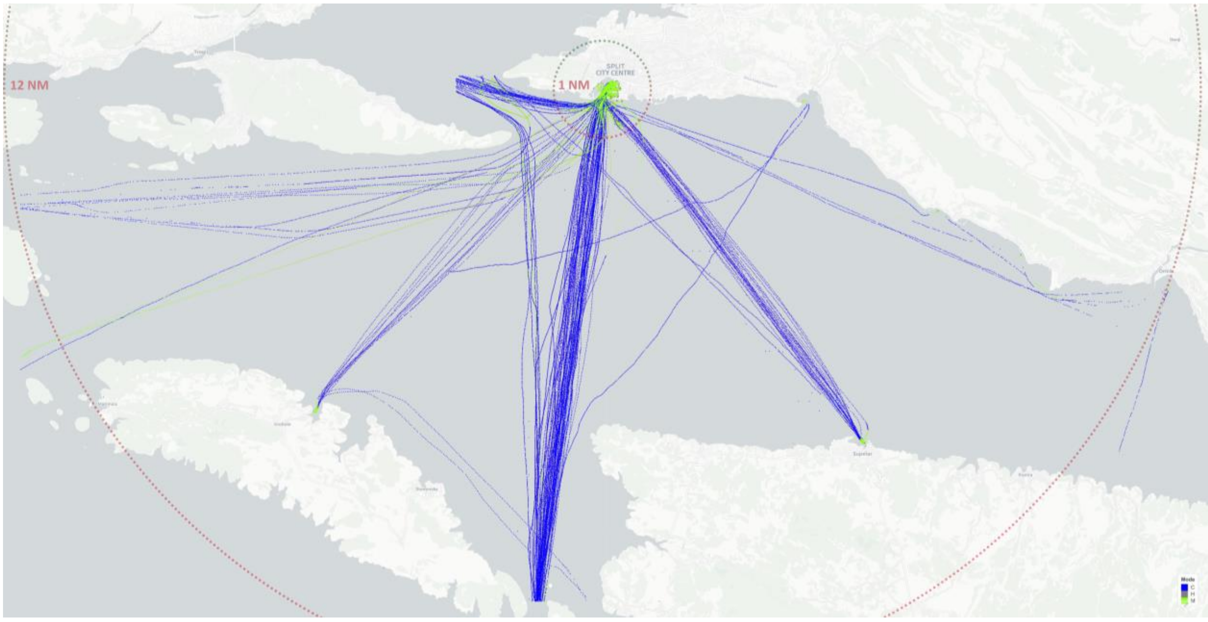


Figure 18. Spatial distribution map of ship emissions based on operating modes developed as a part of Paper 3. The reference points shown represent the individual voyages of each ship that visited the passenger basin of the Port of Split on 2 July 2019 and contain a complete set of emission-related data.

The high-density emission mapped in Paper 3 provided a crucial visual and analytical tool for understanding real-time pollution patterns. However, as observed in Figure 17, variations in ship operation and composition across time periods directly affect emission outcomes. This emphasises the limitations of relying solely on historic data overview of one period. To address this, predictive modelling, enabled by machine learning algorithms introduced in subsequent modules, must be integrated to simulate emissions under varying operational scenarios. Such an approach ensures the development of more adaptive and forward-looking mitigation strategies grounded in empirical evidence and capable of supporting dynamic port operations.

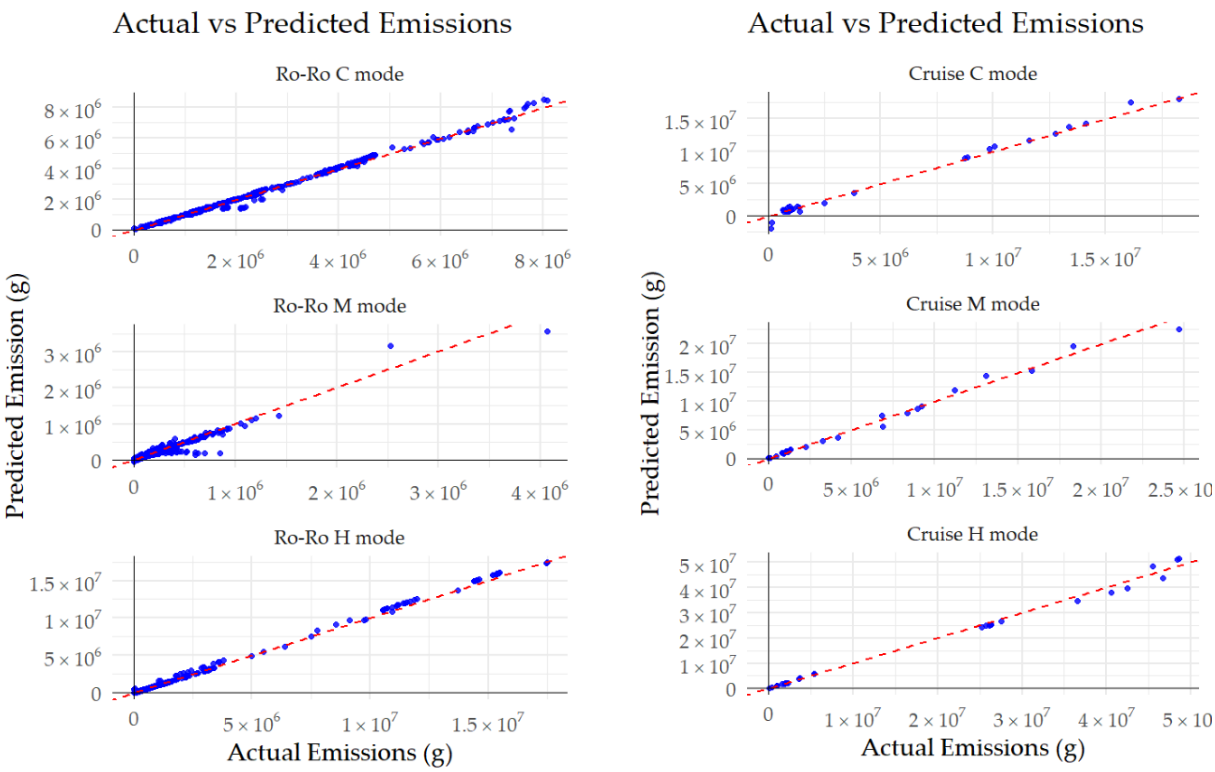
6.2. Module 2 – Emissions Prediction Based on MARS Approach

By relying on the comprehensive emission-related database and analysis of operational profiles derived from fisrt component, Module 2 of the PrE-PARE DSS applied predictive analytics to estimate exhaust gas emissions from ships using machine learning techniques. This module was implemented and evaluated in Paper 3. To capture the complex, nonlinear relationships between multiple predictors and emission outputs, four variants of MARS models were deployed: standard MARS and B-MARS, each with and without logarithmic normalisation. These models were trained using the complete 2019 dataset, which included technical details and over 49 million AIS reference points covering ship activities in the Port of Split area.

Model performance was evaluated through ten-fold cross-validation to ensure robust generalisation. Each fold randomly assigned 90% of data for training and 10% for testing, rotating through all iterations. For each run, RMSE, MAE, and R^2 were computed and compared for all operational modes (cruising, manoeuvring, hoteling) and ship categories. Log-transformed models generally exhibited superior performance on skewed data, particularly in Cruise Ship datasets with large emission ranges. However, in scenarios where emissions were more evenly distributed, raw data models outperformed. Notably, the non-logarithmic B-MARS variant delivered the lowest RMSE and MAE in multiple contexts, such as manoeuvring operations of Ro-Ro Ferries (MAE: 17,459 g), highlighting its accuracy in modelling balanced emission datasets.

Given its consistent performance across ship types and operational conditions, the B-MARS model without log transformation was selected as the predictive algorithm for Module 2. To further assess its accuracy, extended validation was conducted using unseen AIS and technical datasets from diverse periods of 2021, 2022, and 2023, encompassing an additional 15,930,840 reference points. The predictive outputs were compared against actual emissions calculated for Ro-Ro Ferries and Cruise Ships, selected as representative case studies due to their contribution of over 90% of the total recorded emissions. As illustrated in Figure 19, each scatter plot (panels a for Ro-Ro Ferries, b for Cruise Ships) shows predicted emission values (blue dots) alongside actual emissions (red dashed line) for all three operational modes. The alignment of predicted values with the reference trendlines demonstrates the model's ability to perform accurately beyond its training set. The strongest agreement was found in the cruising and hoteling modes, with only minor deviations observed in manoeuvring operations.

Overall, the B-MARS model trained on historical data successfully captured underlying patterns in ship behaviour and operational emissions, confirming its suitability for future forecasting scenarios and emissions trend analysis.



(a) (b)

Figure 19. Comparison of ship emissions based on real data and values predicted by non-log B-MARS module for Ro-Ro Ferries (a) and Cruise Ships (b) in C – Cruising, M – Manoeuvring, and H – Hoteling modes, from top to

bottom, as shown in Paper 3.

6.3. Module 3 – Ship Emissions Metric, Scaling, Classification, and Ranking Module

Although the second module generated accurate predictions of ship-sourced air pollutants, even under previously unseen operational scenarios, its outputs remained inherently tied to the specific temporal and spatial context of the baseline dataset, as defined by the emission estimations in Module 1. The findings from Papers 2 and 3 confirmed that emissions vary considerably depending on timeframes, vessel composition, and activity patterns, which limits the direct comparability of results across periods or ports. Moreover, the iterative process of producing, analysing, and validating these results is both computationally intensive and requires expert interpretation.

To overcome these challenges and facilitate efficient and more scalable evaluation of air pollution risks in ports, this research introduced a standardised system for metric-based analysis, integrated within the third module of the PrE-PARE DSS framework. Based on the analytical outputs produced in previous components, this module implements novel classification techniques, ship performance metrics, and scaling algorithms to provide a consistent, interpretable structure for ranking ship emissions and identifying optimisation opportunities. This approach directly responds to the needs outlined in the earlier studies, offering a more efficient pathway for ongoing emissions assessment, port-level risk classification, and targeted policy or operational interventions.

6.3.1. Standardised and Interpretable Assessment of Ship Emissions Efficiency and Impact through Novel Metrics and Scaling Frameworks

To establish a universally applicable and transparent framework for evaluating the emissions efficiency of individual vessels, this research introduced and implemented the VAPOR as a core metric within the third module of the PrE-PARE DSS system. Based on the emission outputs estimated in Module 1, VAPOR serves as a quantitative measure of the average hourly emissions per unit of working capacity for each ship, categorised by operational mode (cruising, manoeuvring, hoteling).

To derive standardised baseline values, the complete dataset composed of technical details and activities of all ships recorded during the 2019 as a baseline year was processed to calculate baseline VAPOR-b values (baseline) for each predefined ship category. These reference values represent emissions efficiency under expected conditions and enable subsequent benchmarking. In this context, working capacity was defined differently depending on the vessel type: for Cruise Ships, High Speed Crafts, Excursion Ship, Pleasure Craft, and Sailing Ships, passenger capacity was used; Ro-Ro Ferries included both passenger and vehicle capacity; Tugboats were evaluated using bollard pull; and Fishing Vessels were assessed based on cargo volume.

To establish a consistent reference framework, full working capacity was used as a fixed input parameter, irrespective of real-time utilisation, allowing for static comparison across ship types and visits. For port calls, where vessels typically load and unload passengers or cargo in both directions, the defined capacities were doubled to reflect total potential throughput. This adjustment did not apply to tugs or Fishing Vessels, as their work functions follow different operational logic.

The resulting VAPOR-b values for APSs, including SO_x, NO_x, PM_{10}, $PM_{2.5}$, NMVOC, and CO, are visualised in Figure 20 and highlight substantial variability across vessel classes and operational modes. Notably, Pleasure Craft demonstrated the highest emissions per unit of capacity during cruising, exceeding 760 g/h, a consequence of their small capacity paired with high engine demands. Contrarily, Ro-Ro Ferries, despite being among the largest total contributors to annual emissions exhibited the lowest specific rates due to their high capacity and relatively efficient operation. Sailing Ships also recorded high values (640 g/h), reflecting the conservative assumption of continuous engine operation, and representing a worst-case scenario within this research.

By standardising emission outputs against fixed working capacities and across discrete operational modes, the VAPOR framework provides a scalable foundation for the comparative analysis of emission efficiency. This lays the groundwork for the development of advanced classification, optimisation, and ranking methodologies in subsequent stages of the third module.

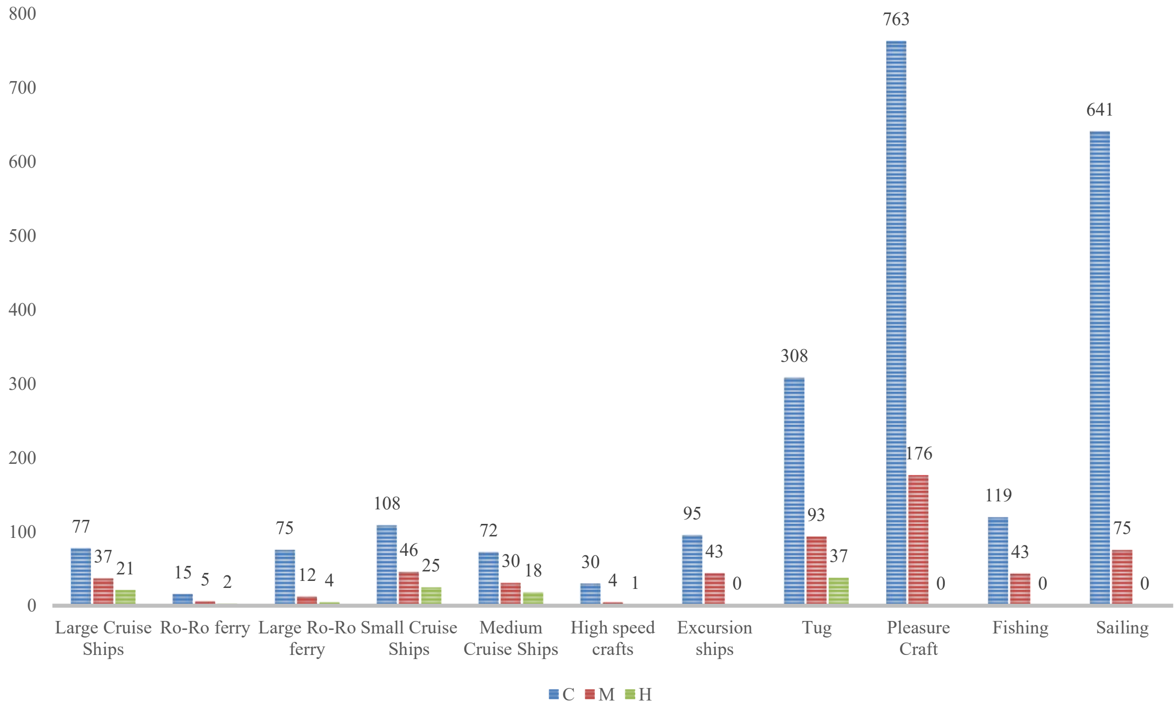
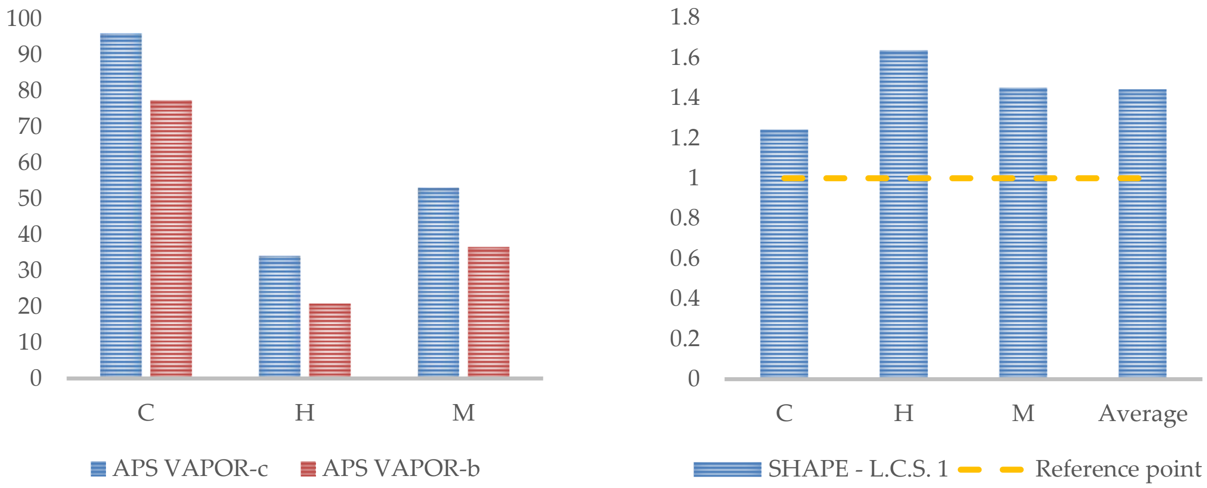


Figure 20. Overview of hourly rate of APS production in g per work capacity (APS VAPOR-b) in each mode (C – Cruising, M – Manoeuvring and H - Hoteling) across all ship types calling at Port of Split in baseline year 2019.

Following the establishment of VAPOR-b for each ship category and operational mode, a comparative scaling process was implemented. This involved calculating actual VAPOR (VAPOR-c) values for vessels calling at the Port of Split on 2 July 2019, ensuring consistency in the application of work capacity definitions between both baseline and actual cases. The comparison of VAPOR-c to VAPOR-b enabled the derivation of the SHAPE metric, a dimensionless indicator reflecting each vessel's emission efficiency relative to its expected performance. The SHAPE metric provides a clear interpretation: values above 1 signify lower emission efficiency, indicating a higher emission output per unit of work capacity, while values below 1 suggest that a vessel performed more efficiently than the average for its class. This process allows for a straightforward and objective benchmarking of individual ship performance.

To demonstrate the applicability of this metric, one large Cruise Ship (L.C.S. 1), identified as a major contributor to emissions on the analysed day, was used as a representative example. The left-hand panel of Figure 21 displays the actual (calculated) hourly emissions (VAPOR-c) compared with the corresponding reference values (VAPOR-b) in cruising, hoteling, and manoeuvring modes. For instance, during the hoteling phase, L.C.S. 1 on hourly basis emitted approximately 13 grams of air pollutants per unit of working capacity more than similar ships in its category. The right-hand panel presents the calculated SHAPE values, with each bar representing performance in a specific operational mode, and the dashed yellow line marking the standard reference point (SHAPE = 1). It is evident that in all three modes, L.C.S. 1 operated less efficiently than its peer average.



(a) **(b)**

Figure 21. (a) Comparison between recorded VAPOR-c and reference VAPOR-b values across different operational modes (C – Cruising, M – Manoeuvring and H – Hoteling); (b) Normalised SHAPE values for Large Cruise Ship 1. As depicted in Paper 3, the bars represent the calculated SHAPE for each mode, while the yellow dashed line marks the reference efficiency (SHAPE = 1), indicating that Large Cruise ship 1 performed less efficiently across all modes.

This example illustrates the practical value of the SHAPE metric. When used in conjunction with the VAPOR framework, it delivers a robust, transparent means of quantifying ship-level air pollution performance. Because the methodology relies solely on operational and emission data that are typically accessible, the calculation is both scalable and reproducible. Its intuitive visualisation, particularly through the use of normalised benchmarks, allows users, including non-experts, to interpret performance quickly and accurately. As a result, this dual-metric system not only supports more precise emissions monitoring but also offers a universal foundation for performance tracking at both local and international levels, aligning emission assessment with practical decision-making in port and shipping governance.

To supplement the technically focused emission metrics with a format that is more accessible to a broader port community, the SEIL was applied for the selected day of analysis. This user-friendly indicator compares the total emissions produced by each vessel during a single port call against those of a standardised reference, termed the “generic ship”. The reference value is calculated by dividing the total emissions by the total number of voyages recorded on that day, creating a consistent benchmark for comparative assessment.

As shown in Figure 22, SEIL offers a straightforward visual ranking of individual vessels, presenting emissions per voyage in relation to the average. Ships with a SEIL value above one are identified as higher-than-average emitters, drawing attention to those with a greater environmental burden. This clear format supports transparency and can serve as a communication tool for port authorities, stakeholders, and the public when evaluating and discussing ship-based air pollution.

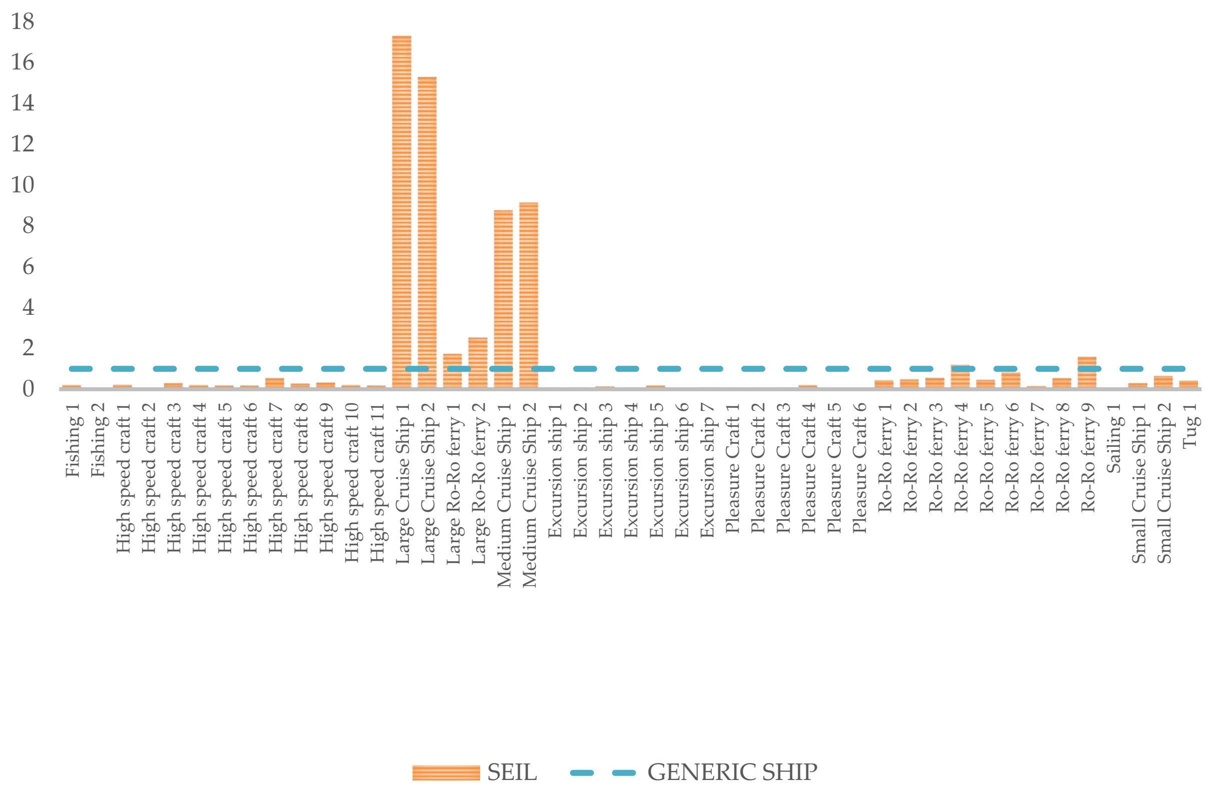


Figure 22. SEIL values for vessels that visited the port on 2 July 2019. The SEIL indicator represents the amount of emissions produced per port visit in comparison with a standardised baseline, referred to as the "generic ship" (illustrated by the dashed line with a value of 1). Significantly, Large Cruise Ship 1 recorded emission levels exceeding the average by more than a factor of 17. In contrast, the majority of vessels, including Ro-Ro Ferries and High Speed Craft, remained at or below this benchmark. This figure highlights the considerable variability in emission impact among individual vessels.

The SEIL results underscore the notable emissions disparities among vessel types. Most significantly, Large Cruise Ship 1 released over 17 times the pollutants of the generic ship during its port visit, illustrating its substantial environmental footprint. Although Ro-Ro Ferries collectively represent the second largest source of emissions on analysed day, and first on annual basis, the emissions from a typical Ro-Ro Ferry would require roughly 23 separate port calls to match the impact of a single visit by Large Cruise Ship 1. These findings emphasise the need for tailored emission mitigation strategies that reflect the operational characteristics and environmental influence of different vessel types.

6.3.2. Classification of Air Pollution Risk and Ranking of Ships by Emissions Intensity, Optimisation Potential, and Overall Performance

To enable effective assessment and regulation of emissions in port environments, a structured top-down classification system was developed. This system evaluates the overall risk of air pollution, emission intensity by ship type, and individual vessel performance-based on data generated through the first module.

As the initial step, the PERIL classification algorithm was applied to daily emission totals from 2019 as a reference year. Based on statistical distribution, this method categorises each day into one of five levels (Very Low, Low, Moderate, High, and Very High), by using the mean and standard deviation of the annual emission values as reference points. Figure 23 presents this categorisation, demonstrating that only a limited number of days fell into the highest risk categories, with Very High and High classifications accounting for just 13 and 50 days respectively. These days primarily occurred between April and November, confirming a seasonal pattern.

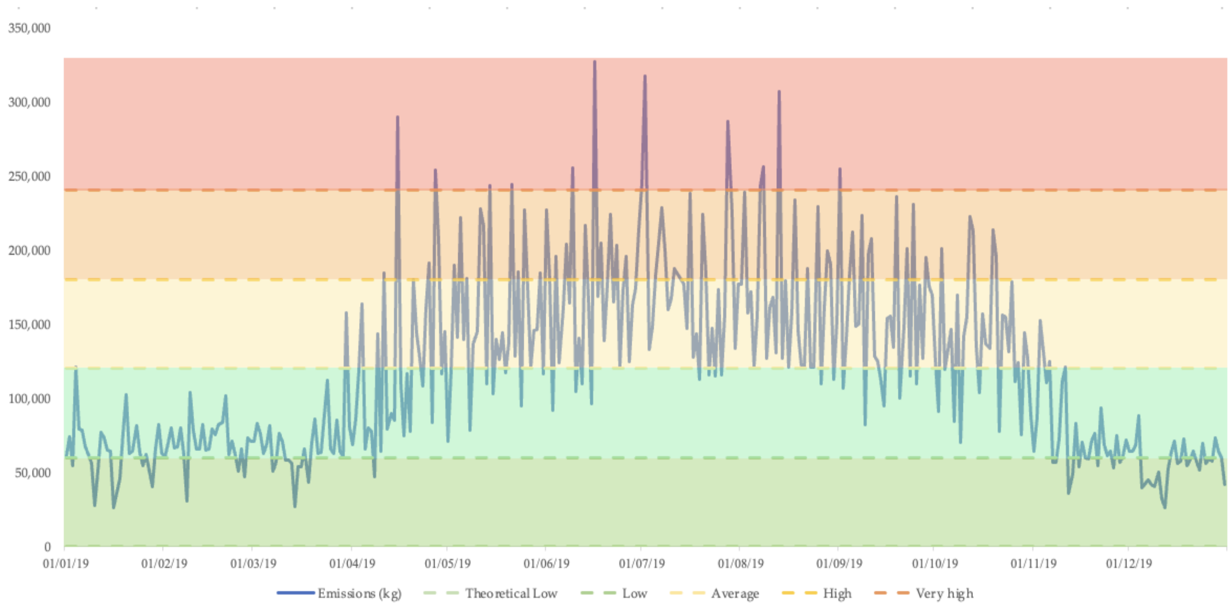


Figure 23. The PERIL classification algorithm applied on daily ship emissions quantified by the Module 1 for the baseline 2019 in are relevant to Port of Split, derived from Paper 3.

The day with the highest recorded emissions, 2 July 2019, was selected for detailed analysis, as it reached a total of 317,214 kilograms, exceeding the annual average by more than 2.6 standard deviations, thereby placing it within the Very High-risk category according to the PERIL classification.

In the second phase of analysis, the Ship Type Emission Intensity (ST-EI) method was used to assess which vessel types were most responsible for this output. As Figure 24 shows, Large Cruise Ships exhibited the highest pollutant intensity per voyage, prompting additional scrutiny of individual ships within this category.

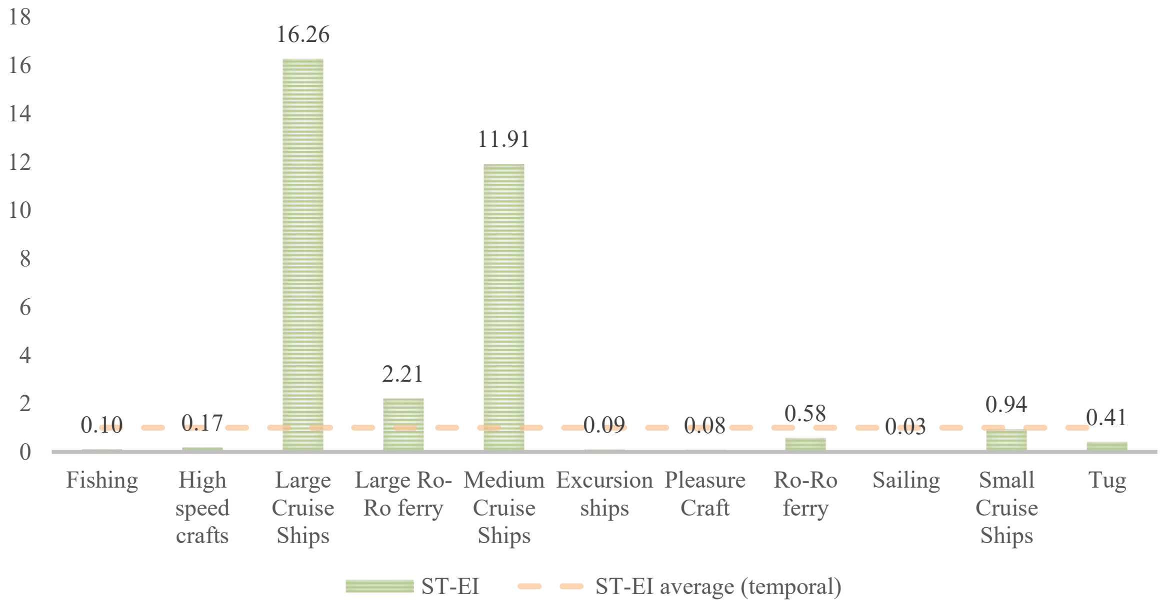


Figure 24. The Ship Type Emission Intensity (ST-EI) method for measuring the degree of air pollutants released in all ship types compared to temporal total ships emissions per all voyages, applied for APSs on 2 July 2019, and Present originally in Paper 3.

The third and final step involved calculating the EOP for specific vessels. This was achieved by comparing the actual emissions per unit of work capacity over the full voyage (S-EI actual) with each ship's own historical baseline (S-EI baseline). Unlike the VAPOR metric, which standardises emissions on an hourly basis, the S-EI metric captures emissions for an entire port visit, taking into account variations in operational time and pattern. It therefore allows intra-vessel assessment rather than comparison across different ships.

Figure 25 illustrates this analysis for two Large Cruise Ships. The results show that Ship 2 operated more efficiently across all phases, while Ship 1 produced 20 % more emissions during hoteling and 5 % more during manoeuvring compared to its historical performance. These findings demonstrate where targeted improvements could be made.

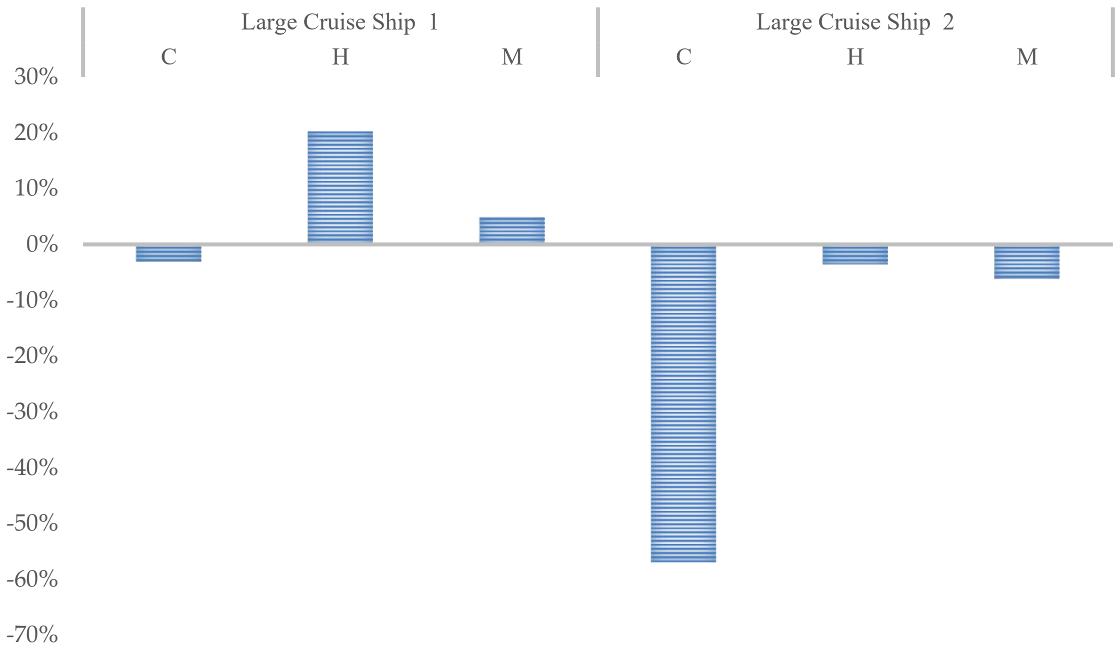


Figure 25. EOP results for air pollutant substances (APS) from Large Cruise Ship 1 and 2, expressed as percentages in different modes (C – Cruising, M – Manoeuvring and H – Hoteling), as presented in Paper 3. Large Cruise Ship 2 exhibited superior operational efficiency across all phases of the voyage, whereas Large Cruise Ship 1 displayed significant potential for emission reduction, particularly during hoteling and manoeuvring, where its outputs surpassed standard baseline levels.

To rank ships fairly, the EOP scores were combined with the previously established SHAPE metric to generate a SEPI. This composite score accounts for both relative emissions efficiency and optimisation potential. Table 4 presents the top ten ships ranked by ST-EI and SEPI. This multilayered classification system supports informed emissions management by identifying both the most impactful vessel types and the individual ships with the greatest potential for improvement.

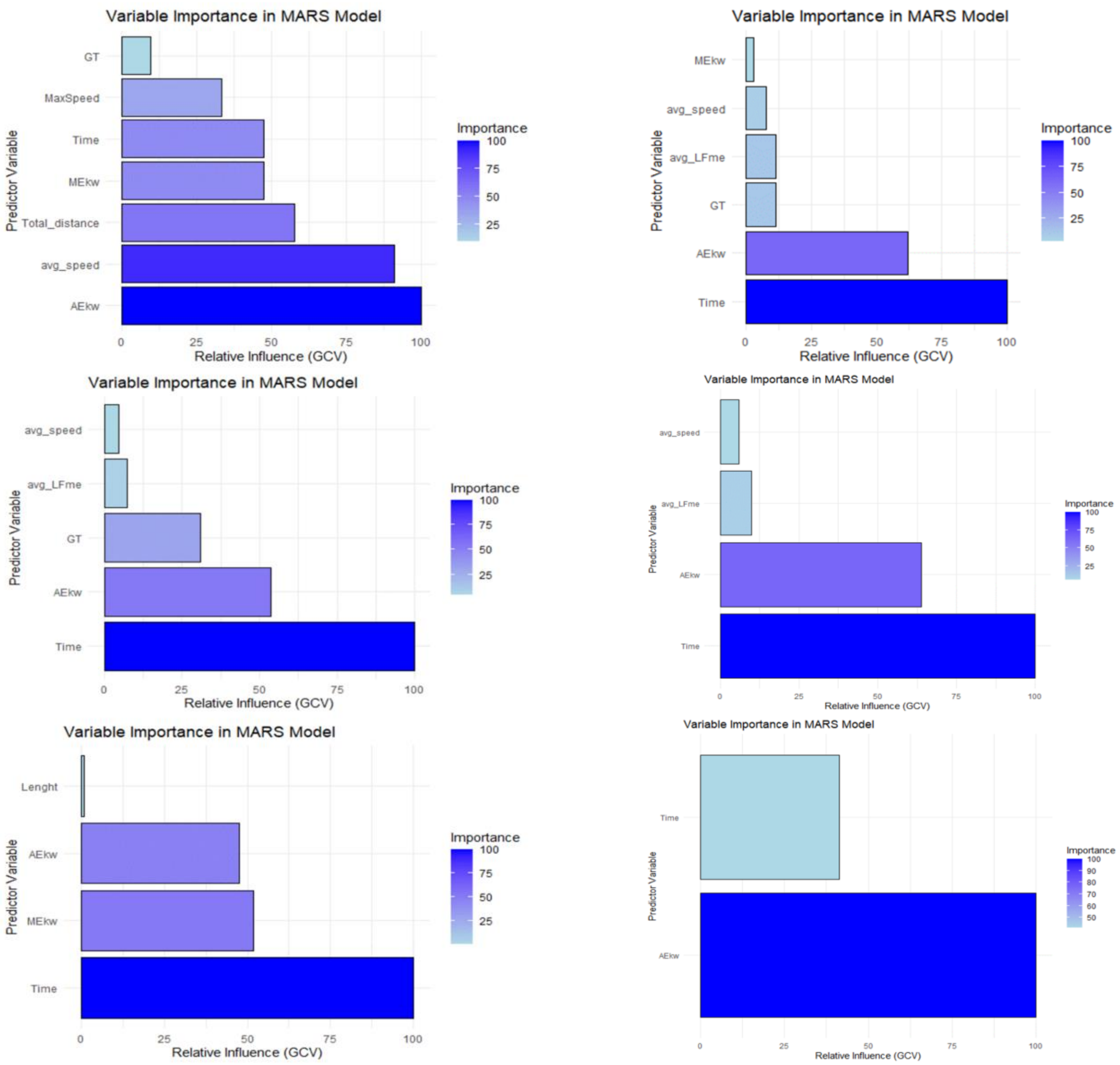
Table 4. Ranking of the top ten ships in the Port of Split on 2 July 2019, based first on the ST-EI, and SEPI indicators for the entire voyage, including the SHAPE and EOP values for each operating mode (C – Cruising, M – Manoeuvring and H – Hoteling).

Ranking	Name	ST-EI	Mode	SHAPE	EOP	SEPI voyage
1	Large Cruise Ship 1	16.26	C	1.24	0.97	1.56
			H	1.64	1.20	
			M	1.45	1.05	
2	Medium Cruise Ship 1	11.91	C	0.96	0.70	1.16
			H	1.17	0.95	
			M	1.04	1.62	
3	Ro-Ro Ferry 9	0.58	C	1.21	1.11	2.37
			H	1.20	3.37	
			M	0.99	1.75	

4	Ro-Ro Ferry 4	0.58	C H M	1.49 1.61 1.49	0.90 0.67 2.23	1.92
5	Ro-Ro Ferry 4	0.58	C H M	1.76 1.61 1.31	1.06 0.11 1.92	1.52
6	Ro-Ro Ferry 6	0.58	C H M	0.99 0.76 0.64	1.14 2.10 1.44	1.22
7	Tug 1	0.41	C M	0.99 2.16	1.11 0.47	1.05
8	High Speed Craft 1	0.17	C M	0.93 0.85	1.09 2.35	1.50
9	High Speed Craft 7	0.17	C H M	1.81 1.18 0.00	1.56 1.07 0.86	1.37
10	High Speed Craft 8	0.17	C H M	1.02 1.07 1.05	0.18 1.59 1.93	1.30

6.4. Module 4 – Optimisation Modelling and Application of Emission Mitigation Measures

To begin the emissions optimisation process within the PrE-PARE DSS framework, the B-MARS machine learning module was first utilised to identify the key predictors contributing to emission production by different ship types and operational modes for all ships in database. Since on 2 July 2019., six of the ten top-ranking ships based on SEPI scores were either Cruise Ships or Ro-Ro ferries, the emission-influencing factors for mentioned groups were analysed and visualised in Figure 26 for cruising, manoeuvring, and hoteling modes from top to bottom. These visualisations illustrate how different technical and operational parameters affect emissions from various ship types and voyage phases.



(a) **(b)**

Figure 26. Comparison of emission-influencing factors generated by the B-MARS machine leaning module based on technical and operational data for Ro-Ro Ferries (a) and Cruise Ships (b) in C – Cruising, M – Manoeuvring and H – Hoteling modes placed from top to bottom.

For both ship types and all three modes, activity duration (Time) and AE power consistently emerged as main or one of the most important emission-influencing factors. This is largely due to their variability among individual vessels within each group and their continuous influence on emissions, unlike main ME power which fluctuates with changes in vessel speed and voyage distance. Therefore, the auxiliary power, along with the duration of operation, were identified as crucial parameters in exhaust gas production for Cruise Ships in all modes, particularly during hoteling. For Ro-Ro Ferries, additional variables, such as ME power, vessel speed, and GT also proved to be the significant contributors to exhaust production, especially during cruising and manoeuvring. It can be noted that the power of the ME appeared as a relevant aspect for Ro-Ro Ferries even during hoteling, although mentioned system is not active while at berth. This can be attributed to variations among individual vessels within the same category and the interdependence between ME and AE design parameters, where a higher ME capacity often coincides with a more powerful AE system.

Although the identified features clearly contribute to ship-based emissions, several of them, such as installed engine power or vessel dimensions, represent fixed technical characteristics and cannot be directly influenced, particularly from the port perspective. These attributes help define a ship's emission profile but do not actively dictate the rate of exhaust output in the way operational parameters do.

Consequently, only activity duration and engine load can be directly influenced by applying targeted operational, regulatory or technological measures suggested by the model to finally mitigate emissions. These two emission-influencing factors serve as control variables connected to a range of available measures (e.g. berth scheduling, tariffs, or speed regulation), which the model uses to recommend appropriate adjustments. By focusing on these modifiable aspects, the optimisation module, when combined with quantified and evaluated emission-related data, enables effective and scalable pollution reduction at both ship and port levels.

Therefore, the results generated by the machine learning module were used in a first-tier optimisation process, where performance-based optimisation was applied, prioritising ships with the highest SEPI scores and EOP values for each mode within a specific voyage on stated day. However, the Port of Split, used as a case study, lacks infrastructure for shore power and port-specific emission regulations, so only a limited range of corrective actions could be considered. For Cruise Ships like Large Cruise Ship 1, the model proposed speed reduction during pilotage and improving coordination during manoeuvring and mooring operations to limit engine loads and time. While alternative fuels, application of abatement technologies, reduced energy consumption of secondary consumers, or usage of shore power could further reduce emissions, they were not viable at the time of analysis due to local constraints. Thus, in the hoteling phase, available mitigation measures were limited to shortening berth duration or rescheduling calls. Similarly, for ships such as Ro-Ro Ferry 9, the model suggested turnaround optimisation and scheduling, resulting in reduced time and engine loads during cruising, manoeuvring, and hoteling. Collectively, these actions led to a total emissions reduction of nearly 28%.

Despite this significant drop, the PERIL was only reclassified from Very High to High, prompting the intensity-based optimisation as a second-tier optimisation phase. In this stage, corrective measures were first directed toward ships within groups with the highest ST-EI metrics. Inside these groups, the logic then prioritised ships having the highest SEPI scores, focusing on voyage segments (modes) with dominant emission shares and targeting either the ME or AE depending on their relative contribution to overall air pollution in specific activity. To support this process, quantified emissions data derived from the Module 1 and evaluated by the Module 3 where integrated inside optimisation module extending the B-MARS analysis of emission-influencing factors. For instance, the distribution of total emissions in operational modes for Large Cruise Ship 1 on 2nd July 2019 was 23% for cruising, 11% for manoeuvring, and 66% for hoteling. The propulsion system of this ship accounted for 64% of emissions during cruising, while the auxiliary system was responsible for 89% and 100% of emissions during manoeuvring and hoteling, respectively. Although Large Ro-Ro Ferry 2 on the same date exhibited comparable ME/AE emission shares to Large Cruise Ship 1, the proportions between modes differed significantly with 74% of emissions occurring during cruising, 9% while manoeuvring, and 18% in hoteling. Based on these distributions, engine-mode combinations were targeted for further optimisation, using measures that correspond with ME or AE operations. Following the application of interventions based on operational performance and emission intensity, total emissions on the analysed day were reduced by 55%, leading to a PERIL reclassification from Very High to Moderate.

This outcome confirms the importance of combining both optimisation strategies to achieve effective air pollution mitigation during peak emission periods. In conclusion, the optimisation module completes the PrE-PARE DSS cycle by establishing a feedback mechanism where metric system is used as an indicator for data-driven interventions until the system stabilises under an acceptable PERIL level. By integrating predictive analytics with performance indicators and rule-based logic, the module proposes relevant and feasible measures for ship emissions control in port areas.

CHAPTER 4

7. Discussion

7.1. Progressive Development and Integration of a Modular Decision Support Framework for Ship Emissions Management

The research presented in this doctoral thesis introduces a comprehensive and modular decision support system, PrE-PARE DSS, designed to facilitate the analysis, prediction, evaluation, and mitigation of ship-sourced air pollution in port environments. Through the development and sequential integration of four analytical modules, the system was progressively expanded to address increasingly complex aspects of maritime emissions management.

Paper 1 laid the conceptual foundation for this work by applying a systematic review methodology to critically evaluate existing practices in ship emissions estimation. This analysis provided two essential outcomes. Firstly, it identified the most applicable and precise methodologies, such as the bottom-up energy-based approach, as the most suitable for localised port environments. Secondly, it highlighted the technical and operational datasets required to quantify emissions with spatial and temporal accuracy, including AIS records, ship characteristics, and engine parameters. Moreover, the review exposed significant gaps in traditional inventory based approaches, such as their limited temporal resolution, reliance on assumptions rather than actual movement data, and inadequate treatment of ship type variability. These limitations underscored the need for a more dynamic and data-rich system, informing the design requirements for the analytical framework introduced in subsequent papers.

Module 1, initially introduced in Paper 2 and later reused in Paper 3, serves as the foundational element of the PrE-PARE DSS. This component enables high-resolution quantification of emissions at the level of individual port calls using processed AIS data and technical specifications of ships. Its ability to produce structured, voyage-specific exhaust profiles underpins the subsequent analytical and predictive operations across the system.

Paper 3 introduced Modules 2 and 3, building on the datasets generated by Module 1. Module 2 employed machine learning, specifically a B-MARS model, to forecast emissions for unseen scenarios, thus extending the applicability of the system beyond observed data. Module 3 introduced a suite of innovative metric-based methodologies, such as VAPOR, SHAPE, SEIL, PERIL, ST-EI, EOP, and SEPI, that enabled the standardised interpretation, classification, and ranking of ship emissions performance. This addressed key limitations of traditional regulatory metrics by accounting for mode-specific behaviour, operational conditions, and non-CO_2 air pollutants. These novel approaches facilitated transparency, comparability, and stakeholder engagement in emissions evaluation.

Module 4, developed and presented in Paper 4 (currently under preparation), concludes the system by enabling targeted emissions reduction. Using results from the B-MARS predictive analysis, this module identifies key operational and technical predictors of emissions and applies a two-tiered optimisation framework. The first-tier addresses ships with the highest emissions performance scores, while the second focuses on the most impactful ship types and voyage segments. The integration of quantified, evaluated, and ranked emissions data within an optimisation logic enables tailored recommendations for control measures. Although infrastructural limitations constrained the feasible interventions in the case study of the Port of Split, substantial reductions in overall emissions (up to 55%) were demonstrated, showcasing the practical value of the approach.

Collectively, the four modules function as a harmonised system that provides detailed insights and actionable outputs across multiple levels, from ship-level operational behaviour to port-wide risk assessments. The modular architecture ensures the adaptability of the system to diverse port environments and regulatory frameworks. It also supports ongoing development, such as the incorporation of additional emissions factors or integration with external monitoring systems.

By progressively building the PrE-PARE DSS and validating each of its modules through real-world application and peer-reviewed dissemination, this thesis contributes a flexible, scalable, and practical framework for maritime air pollution management. The work aligns with the evolving environmental imperatives in shipping and provides a structured foundation for evidence-based, data-driven interventions in port sustainability practices.

The cumulative results of this research confirmed the initial hypothesis by demonstrating that machine learning techniques applied to ship activity data, when combined with a targeted optimisation algorithm, enable effective prediction and control of ship emissions in port areas. The accompanying development of a novel, scalable metric system further strengthened this approach, offering transparent, comparable, and operationally based evaluation of emissions performance. This integration represents a substantial advancement in harmonising predictive analytics with practical emission management at both local and broader regulatory scales.

7.2. Main research contributions

The overall aim of this doctoral research was to develop an adaptable, data-driven DSS capable of quantifying, predicting, evaluating, and optimising ship-related emissions in port environments. To achieve this, the research adopted a modular development strategy, progressively integrating methodological insights from existing literature and combining them with novel approaches and indicators introduced during the study. The resulting framework, the PrE-PARE DSS, was constructed through a phased, multi-paper research design that addressed five core research questions. These questions were formulated to sequentially identify current limitations, construct enhanced modelling methods, define new evaluation metrics, leverage machine learning for predictive accuracy, and demonstrate the practical implications of the system within real port contexts.

Each research question is directly aligned with a corresponding module of the PrE-PARE system and its development over the course of this thesis. The contributions are based on applied case studies and supported by both theoretical analysis and empirical validation. The five research questions and the corresponding methodological responses are summarised below:

- What are the methodological limitations and data inconsistencies in current ship emission inventories used in port areas, and how do these limitations hinder comparability and decision-making?

Paper 1 addressed this question by applying a systematic review methodology, critically assessing the prevailing ship emissions inventory frameworks. It identified key shortcomings, including the absence of methodological standardisation, spatial and temporal limitations confined to individual case studies, and variability of data quality. These limitations were shown to undermine the comparability of emissions data of different ports and timeframes, confining decision-making to a general standpoint. Paper 2 empirically validated these findings through the implementation of Module 1, which introduced a bottom-up, energy-based emissions quantification approach applied to each port visit. This analysis of outputs produced confirmed the inability of conventional methods to reflect operational and spatial variability at the individual ship and overall port levels.

- How can analytical modelling approaches be used to enhance the accuracy and interpretability of port-level shipping emission estimates?

This question was further addressed in Paper 2 through the development of Module 1, a data-driven emissions estimation module. By integrating AIS-derived movement trajectories with technical specifications of vessels, Module 1 enabled accurate and high-resolution emissions profiling per ship and per port call. The resulting model provided a transparent and reproducible framework that improved the interpretability of emissions in diverse port contexts by generating detailed technical, operational, spatial and temporal annalistic, thereby addressing critical issues identified in the first research question.

- What indicators or metrics can be formulated to standardise the evaluation of emission efficiency and intensities across different ships and port areas?

Paper 3 introduced and validated several novel metrics under Module 3 that allow for standardised, comparative, and interpretable emission assessment across vessel types and timeframes. These include:

VAPOR: Measures emissions in grammes per hour per unit of working capacity, enabling consistent evaluation of emission efficiency across different ship types and modes.

SHAPE: A scaling metric that normalises a ship's emission efficiency relative to baseline averages, allowing for cross-comparison between vessels with similar functional roles and dimensions.

SEIL: An intuitive, voyage-based ranking metric that expresses a ship's total emissions relative to the average vessel, aiding stakeholder and public understanding.

PERIL: A temporal classification tool using statistical thresholds to categorise port emissions into five risk levels (Very Low to Very High).

SEPI: Integrates emission intensity and efficiency to rank ships based on overall environmental performance.

EOP: Identifies deviation from baseline values (intra-ship performance) to highlight vessels with the greatest potential for improvement.

Together, these metrics establish a coherent and scalable framework for monitoring, classifying, and managing ship emissions, suitable for port operators, regulators, and researchers alike.

- How can machine learning methods improve predictive modelling of ship emissions in port operations?

In Paper 4, Module 2 was introduced, employing the B-MARS algorithm as a predictive engine for emission estimation. The model was trained on 2019 data and tested on new datasets from 2021 to 2023. It demonstrated robust generalisation capabilities across different operational scenarios and vessel configurations. Importantly, the model also offered interpretability through feature importance rankings, identifying time in mode and auxiliary engine power as the dominant predictors across ship types. This capability not only enhances emission forecasting but also supports targeted emission control by identifying modifiable parameters.

- What are the practical implications of the developed PrE-PARE DSS for port management, shipping industry, environmental monitoring agencies, maritime policy stakeholders, and the wider public?

This final research question was addressed in both Paper 3 and Paper 4, particularly through the implementation of Module 4. This module completed the decision support loop by translating model outputs into actionable emission reduction strategies. Through performance-based and intensity-based optimisation procedures, supported by indicators such as SEPI and ST-EI, targeted measures were proposed for specific vessels and activities. In the Port of Split case study, the interventions enabled a possibility for a 55% reduction in daily emissions and the downgrading of the port's PERIL classification from Very High to Moderate. This confirmed the practical utility of the system for real-world applications, including emission-based berth scheduling, environmental tariff formulation, or regulatory planning. Moreover, the metrics used are interpretable and accessible, ensuring that results can be communicated effectively to both expert and public audiences.

Although VAPOR was applied within the port area in this study, its calculation is not spatially limited. The model can be extended to evaluate emissions along the entire voyage, enabling continuous assessment from port to port across regional, sea, and oceanic passages. This flexibility enhances the relevance of the PrE-PARE DSS for broader applications, such as regional policy formulation, regional air pollution assessments, and international monitoring of emission performance of specific vessels or fleets.

8. Conclusion

This doctoral research introduced and developed the PrE-PARE DSS, a comprehensive, modular, and data-driven framework designed to quantify, predict, evaluate, and optimise ship-sourced air pollution in port environments. The system was conceived from a universal methodological foundation combining standardised emission estimation techniques with advanced statistical and machine learning tools applied to extensive emission-related datasets. Data processing and modelling were primarily conducted through RStudio, supported by Python scripting for preprocessing tasks and Excel for data visualisation and graphical interpretation.

The modular structure of the system ensured methodological flexibility, enabling the incorporation of novel metrics, updated datasets, and analytical enhancements without altering the core logic of the framework. Although designed to be universally applicable, the PrE-PARE DSS was implemented and validated through a detailed case study of the Port of Split. This application demonstrated the full operational capability of the system under real-world constraints, using it to generate detailed emission inventories, assess performance metrics, and implement predictive and optimisation scenarios.

On the example of a high-traffic day, 2 July 2019, the system successfully quantified emissions and disaggregated their technical, temporal, and operational characteristics. It accurately predicted emissions for various ship types and operational modes, even under unseen environmental conditions. Furthermore, it enabled the evaluation of ship-level emission efficiency, categorised the port-wide risk of air pollution, and proposed targeted mitigation strategies that ultimately achieved a 55% reduction in total daily emissions. These outcomes confirm the system's practical value for environmental management, operational planning, and regulatory support in seaport settings.

Nonetheless, several limitations and areas for further development have been identified, forming the basis for future work. First, while the emission estimation module (Module 1) demonstrated robustness, the overall accuracy of results depends on the quality and completeness of AIS data, as well as on appropriate assignment of EFs and LFs. Shortcomings in these parameters may introduce variability, particularly for ship types with inconsistent reporting patterns or atypical engine configurations.

Second, there is significant potential in combining diverse sources of emissions data, such as onboard measurements, fixed sensors, and satellite observations, to enhance data resolution and cross-validate modelled outputs. Third, environmental and behavioural parameters, including meteorological conditions and human decision-making, are currently not integrated into the system and could offer additional value for forecasting and risk analysis if appropriately modelled.

Expanding the application of the system to different port environments, ship categories, and regulatory contexts would further demonstrate its scalability. This includes adaptation for specialised fleets (e.g., LNG tankers, container vessels), as well as incorporating port-specific corrective measures such as shore power or emissions trading schemes.

In terms of methodological advancement, further refinement of the core metrics, particularly VAPOR and SHAPE, could support the development of dynamic, performance-based air pollution tariffs. These could incentivise cleaner operations and reinforce accountability among shipping actors. Additionally, stronger collaboration between the maritime industry, port authorities, and academic institutions will be essential for improving data transparency, standardisation, and adoption of such systems.

Future developments may also involve the integration of alternative fuels (e.g. LNG, hydrogen, methanol) into emissions modelling, accounting for their unique profiles and operational characteristics. Finally, while this thesis focused on air pollution, the PrE-PARE DSS framework could be adapted to other forms of ship-induced environmental impacts, such as underwater noise, carbon footprints, or water pollution, thus paving the way for a broader, cross-impact environmental monitoring system for maritime transport.

In summary, the PrE-PARE DSS offers an adaptable, scalable, and practical foundation for data-driven environmental management in ports. Its ability to combine quantification, prediction, evaluation, and optimisation within a single coherent structure represents a significant contribution to both maritime environmental science and applied decision support methodologies.

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Article 3

A Comprehensive Model for Quantifying, Predicting, and Evaluating Ship Emissions in Port Areas Using Novel Metrics and Machine Learning Methods

Bojić, Filip.; Gudelj, Anita.; Bošnjak, Rino

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Systematic Review

Port-Related Shipping Gas Emissions—A Systematic Review of Research

Filip Bojić *, Anita Gudelj and Rino Bošnjak

Faculty of Maritime Studies, University of Split, 21 000 Split, Croatia; anita@pfst.hr (A.G.); rino.bosnjak@pfst.hr (R.B.)
* Correspondence: fbojic@pfst.hr

Abstract: The global increase in shipping activity has contributed to the degradation of air quality, which particularly affects traffic-dense port areas. Due to the environmental and public health impacts of air quality in port cities, a number of inventories using varying methodologies have been conducted over the past two decades to manage gas emissions in specific areas. The objective of this work is to determine one relevant methodology for estimating ship emissions in ports through a systematic review of the relevant literature. In this research, PRISMA guidelines were followed through a multi-layer bottom-up analysis approach to ensure the validity of the proposed methodology. The aforementioned methodology, as the end result of this research, is intended to provide an empirically structured basis for further development of a novel indexing model of ship gas emissions in port areas.

Keywords: shipping emissions; port sustainability; systematic review; methodology

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1. Introduction

Shipping is the most efficient transportation mode in terms of energy usage per tonne of cargo, covering more than 80% of global trade by volume [1–3]. Although maritime transportation is still the least environmentally damaging mode of transport, it is responsible for about 2.2%, 15% and 5 to 8% of global anthropogenic carbon dioxide (CO_2), nitrogen oxide (NO_x) and sulphur oxide (SO_x) levels, respectively [4,5]. In addition to the mentioned gases, ships emit large quantities of particulate matter (PM), volatile organic compounds (VOCs) and carbon monoxide (CO). Despite the fact that maritime emissions have worldwide impact, some studies have indicated that about 70% of emissions from ships occur within 400 km of the coast, since most ships spend most of the time either harbored or near a coast [6]. While CO_2 is recognised as the leading greenhouse gas responsible for global climate change, the presence of PM, VOCs, CO, NO_x and SO_x in urbanised port areas requires even more attention due to the negative effects of these pollutants on human health [5]. Pollutants emitted from ships can be responsible for respiratory diseases, cardiovascular disease, lung cancer and even premature death, so it is necessary to monitor them and mitigate their presence in port communities [7,8]. The severity of air quality degradation is all the more serious when taking into account the fact that 90% of European ports are spatially connected to cities [9].

Mitigation of vessel gas emissions on a global scale was addressed by the International Maritime Organisation (IMO) in 1997 when Annex 6 "Prevention of Air Pollution from Ships" of the MARPOL convention was introduced [10]. The main changes that MARPOL Annex 6 brought in were a global progressive reduction in SO_x, NO_x and PM emissions and the introduction of emission control areas (ECAs) [10]. Over the years, MARPOL Annex 6 has been revised and from January 2020, or January 2025, depending on the availability of low sulphur for ships' use, the global limit for sulphur content of ships' fuel is reduced from 3.5 mass by mass percent (% m/m) to 0.5% m/m, while in ECAs the content is pushed down to 0.1% m/m [10]. Requirements for NO_x emissions were defined using a three-tier methodology, where different levels (Tiers) of control apply, based on ship construction date [11]. The less strict Tier 1 applies to vessels constructed on or after 1 January 2000, Tier 2 to vessels constructed on or after 1 January 2011, while the most demanding Tier 3 regulates NO_x emissions from vessels built after January 2016 that operate in the North American and United States Caribbean Sea, the Baltic Sea or the North Sea ECAs.

The issue of air quality inside the European Union (EU) port sector was first recognised in 2004 by the European Sea Ports Organisation (ESPO), while in 2013 it became a top environmental priority and has remained so to this day [9]. Due to the influence of air quality on the environment and public health of port cities, a number of different inventory studies have been conducted throughout the last two decades in order to manage gas emissions in particular interregional, national or local areas. For inventory development, two different approaches that are most commonly applied are the top-down approach and the bottom-up approach.

A top-down approach can be described as a fuel-based (FB) method, where fuel sales statistics are used to estimate the total mass of the fleet fuel consumption (FC) inside a specific area of interest in a certain time period. That information is then combined with the emission factor (EF), which denotes the mass of emitted pollutants per metric tonne (t) of fuel consumed in order to finally obtain the total mass of emitted pollutants (E), which is represented in Equation (1) [12]:

$$E = FC \times EF \quad (1)$$

The main advantage of this fuel-based (FB) concept is that it is not data-excessive. This means that data that only generally describe a particular fleet and its FC and EF can be used. Thus, this approach is recommended for situations where only limited traffic data are available [12]. However, applying generic data that are associated with a level of uncertainty can produce outputs that differ from realistic emissions. The corresponding EFs are highly aggregated, with averaged values, and do not take into account the specific conditions that lead to instantaneous emission production in any given circumstance [13]. Moreover, it has been proven that there is a significant discrepancy between banker fuel sales statistics and the actual fuel used by global fleets, so it cannot accurately reflect emissions in response to specific shipping activities [13,14]. This is especially relevant for small interest areas such as ports, where fuel sales data have lower accuracy. Therefore, the top-down approach is most commonly used in large-scale inventories where it is more practical to gain insight into shipping emissions by acquiring less detailed data based on FC.

When detailed information about a ship's movement dynamics and its technical data (TD) are available, then the bottom-up approach is recommended. This method is characterised as activity-based and data-demanding, since it requires a higher level of input parameters for each movement activity (MA); however, it is able to produce near instantaneous emission estimation on a vessel-by-vessel basis at high resolution (in time and space) [12,13]. In a bottom-up approach, emission estimations are obtained for each movement type by combining engine energy output (EO) or FC with EF and time (T) values that correspond to specific activities (e.g., hoteling, manoeuvring and navigation) [15,16]. To figure out the total shipping emissions in a certain area and time period, all estimated quantities of each activity are combined and scaled up over all trips [12]. In the bottom-up approach, both energy-based (EB) and FB methods can be applied. These methods are shown in the EB Equations (2) and (3), along with the FB Equation (4) [12,16]. When gas quantification is conducted by relying on an EB approach, EO is determined by multiplying total engine power (P) by the actual percentage of engine work output, expressed as load factor (LF). In this case, EF is defined as the mass of pollutants emitted per an engine's energy output:

$$E = EO \times EF \times T \quad (2)$$

$$EO = P \times LF \quad (3)$$

$$E = FC \times LF \times EF \times T \quad (4)$$

Since the bottom-up approach is data-excessive, it is generally applied in small-scale ship emissions inventories in regional and port contexts, and to aggregate the required data the Automatic Identification System (AIS) is often used. AIS transmits near real-time dynamic information about vessel speed, course and position, which is crucial for anticipation of ship-based emissions. Therefore, high-resolution ship motion data from AIS could be a source of reliable relative ship operation profiles, such as travel time and average speed between waypoints at sea in short time intervals, and could be used to identify ship routes [12]. Although the installation of AIS is required by the International Maritime Organisation (IMO) on commercial ships with 300 gross tonnage (GT) and all passenger ships, relying solely on information from this device, a proportion of marine traffic remains invisible [17]. To improve data quality, more than one source of traffic information should be considered in gas emission inventory development. However, regardless of data quality, the method by which it is used is of equal importance.

That is why, in this paper, a multi-layered analysis approach is applied with the aim of finding the most applicable methodology for the estimation of gas emissions from ships in port areas. The methodology, as the end result of this research, should provide an empirically structured basis for the further development of novel ship-sourced gas emissions indexing models in port areas. To ensure the adequate standard of the whole review process, Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) guidelines were followed in this paper [18]. Regarding the search strategy method employed, a bottom-up systematic review of the literature that explored port-related shipping emissions was conducted by applying relevant keyword and reference thread analyses in the Web of Science Core Collection, Scopus and Google Scholar databases. Search and screening of the selected papers was carried out by the authors.

2. Review Methodology

At the very beginning of the review process of the literature in which shipping emissions in ports were explored, it was possible to notice that various methodologies and data were applied, but with frequent similarities and mutual reference connections. Furthermore, it was recognised that the approaches and datasets used were mainly obtained from other studies. Therefore, in order to find a valid port-related ship emissions estimation methodology, a systematic review of the relevant literature needed to be carried out. That is why PRISMA guidelines were followed in this paper according to the proposed bottom-up multi-layered analysis approach presented in Figure 1.

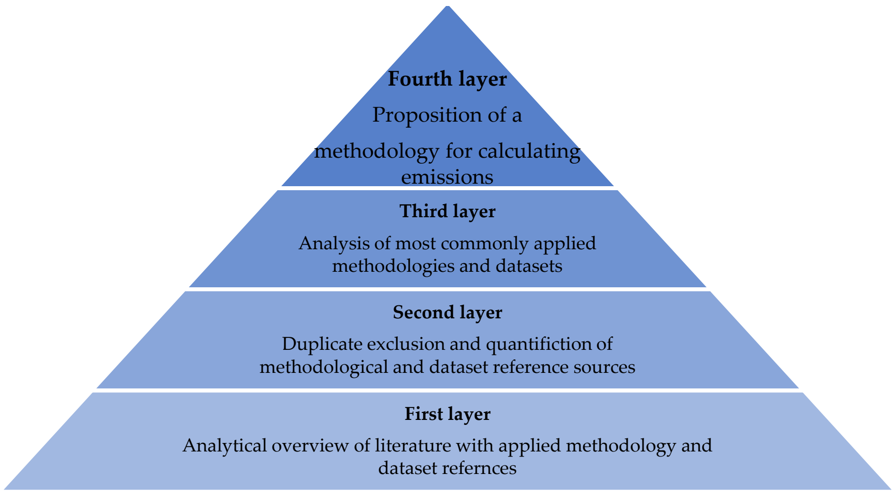

Figure 1. Bottom-up multi-layered analysis approach.

The review process began with keyword thread search of literature in the Web of Science Core Collection, Scopus and Google Scholar databases, using combinations of terms that included: port, ship, emissions, inventory, gas, pollution, quantification, method. After record screening, selected reports went through the analysis process, wherein references to the methods and datasets obtained from different sources were collected. These reference strings were used in the second review, expanding the search to websites of relevant organizations whose studies were cited. By applying both keyword and reference literature identification approaches, metrologies and data used in selected papers could finally be connected with the original sources, so that after completing the second screening it was finally possible to produce a full overview of the selected literature with the original sources of methods and datasets applied in them, thus finishing the first layer of the overall analysis. The complete review and analysis process is displayed in Figure 2 and a detailed explanation is provided below.

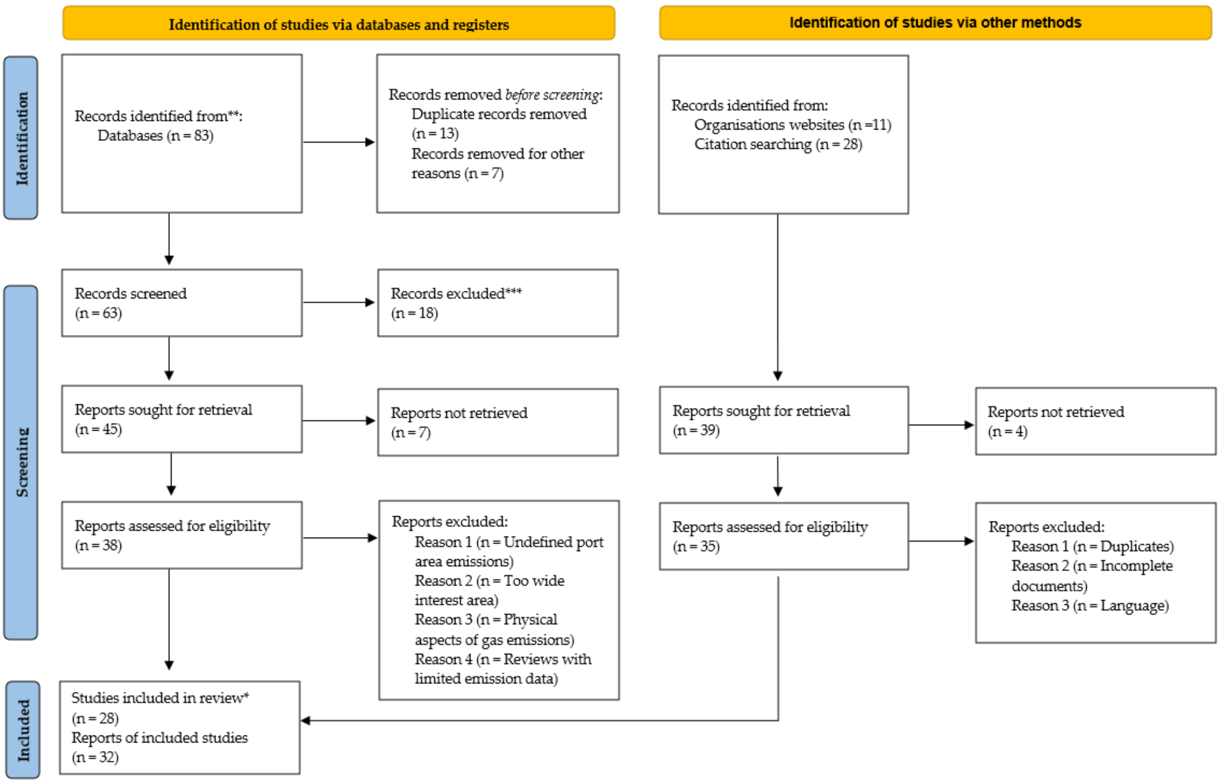

Figure 2. PRISMA 2020 analysis flow diagram for new systematic reviews which included searches of databases, registers and other sources [19] * According to the PRISMA glossary of terms, a study is defined as a larger scientific document that might have multiple reports, while a report is a document that supplies information about a particular study, such as a journal article, a conference abstract, a preprint, etc. [18]. That is why, in this research, the term "study" stands for large emission inventories that were mostly used as reference sources for methodologies and data. Accordingly, "report" is defined as a scientific paper of the sort reviewed in this research. ** Records that were identified were from the Web of Science Core Collection, Scopus and Google Scholar databases. *** Since no automation tool was used, all exclusions of literature were carried out by the authors of this paper.

The overview of the selected papers and their references were examined in the second layer, with the aim of determining the most influential methods and datasets through the quantification of their original sources. To ensure the relevance of reference quantification, the mutual citing connections between all sources used in the selected papers were first analysed with the aim of duplicate exclusion. This resulted in defining multiple sources that used the same methods and/or key data as an individual source. By performing mutual-referencing analysis, the exact number of different methodologies and key datasets cited were determined. Thus, the most influential sources could be defined and thoroughly examined.

A review of the most prominent studies was performed in the third layer of the process through an analysis based on the methodologies and datasets used in the selected literature. The analysis aimed to define the advantages and similarities of the most frequently applied approaches and datasets from the examined studies. This validation process enabled the determination of all vital components necessary for quantifying gas emissions from ships in ports.

Finally, validated components determined through the multi-layer bottom-up process were analysed and combined inside the methodology best fitted for calculating ship emissions in different port areas. The methodology proposed through the review process applied in this paper should ensure relevancy as the basis for the development of a novel ship-based gas emissions indexing model.

3. Discussion and Results

3.1. Analytical Overview of the Literature—First Layer

By conducting a systematic review of the literature according to PRISMA 2020 guidelines, 32 original papers that explored shipping emissions in 80 ports between 2008 and 2021 were selected for further analysis. With the aim of providing a transparent overview of the literature, Table 1 lists the abbreviations of the aforementioned studies and papers, while their reference numbers are listed at the end of the paper. The analytical overview of records was conducted by examining, comparing and linking applied methods and databases with studies and papers, which were the original refence sources, as summarised in Table 2.

Table 1. Abbreviations of cited studies and papers with their reference numbers.

Abbreviation	Reference Number	Abbreviation	Reference Number	Abbreviation	Reference Number
CAPSS/PAQman©	[20]	CARB 06	[21]	CARB 07	[22]
FEMA 09	[23]	EEA 09	[24]	EEA 13	[25]
EEA 16	[26]	EEA 19	[16]	EEM 10	[27]
ENTEC 02	[28]	ENTEC 05	[29]	ENTEC 07	[30]
ENTEC 10	[31]	IMO GHG 09	[32]	IMO GHG 14	[33]
SMED 04	[34]	IVL 05	[35]	L R 95	[36]
MAN	[37]	MEET 98	[38]	NEI 10	[39]
POLA 04	[40]	POLA 08	[41]	POLA 09	[42]
POLA 12	[43]	POLA 13	[44]	POLB 10	[45]
SEA	[13]	STEAM	[46]	US EPA 06	[47]
US EPA 09	[48]	PIRAEUS 09	[49]	SAMSUN 10-15	[50]

The analytical overview process allowed for the following conclusions to be drawn. Primarily, it was found that the authors of all papers relied on bottom-up methodologies, since they explored port-related emissions with good data coverage. An additional top-down approach was applied only for two records in order to make an output value comparison. Therefore, the EB method was predominant since it was used in 26 papers. By contrast, the FB approach was applied for only three publications, and for the same number of papers a combination of both methods was used. Datasets applied for calculating emissions were obtained both locally and from studies. Locally sourced datasets that were derived from Local Port Authorities (LPAs), Local Port Communities (LPCs), National Maritime Organisations (NMOs), AIS, Vessel Traffic Services (VTSs), traffic density data (TDD) or from studies offered information about marine traffic through TD on the ships and their MA. LF and EF data, as more complex components in the gas emissions determination process that depends on specific information about vessels and their activity, were either taken from studies as predefined default values or were estimated on a methodological basis from the same sources.

Table 2. Analytical overview of the literature that explores port-related ship emission sources.

Record Data				Methodological Base and Reference			Data Method and/or Default Reference Abbreviation		
No.	Paper	Port	Year	Method Base	Approach	Method Reference Abbreviation	MA and TD of Trafficgram	EF	LF
1	[51]	Mumbai	2008	EB	Bottom-up	MEET 98	LPA	US EPA 06/MEET 98	US EPA 06/POLA 04
2	[49]	Piraeus	2009	EB	Bottom-up	ENTEC 07/US EPA 06	LPA	ENTEC 02/ENTEC 07	PIRAEUS 09
3	[52]	Ambarlı	2009	FB	Bottom-up	MEET 98	LPA	MEET 98	MEET 98
4	[53]	Busan	2010	EB	Bottom-up	CARB 06	LPA	ENTEC 02/SMED 04	ENTEC 02/CARB 06
5	[54]	10 terminals—Turkey	2010	EB	Bottom-up	ENTEC 05	LPA/EEA 06	ENTEC 05	ENTEC 05
6	[55]	Barcelona	2011	EB	Bottom-up	US EPA 09	LPA/LPC	US EPA 09	US EPA 09
7	[56]	Kaohsiung	2012	EB	Bottom-up	ENTEC 07/US EPA 06	LPA	ENTEC 05/ENTEC 07	POLA 08
8	[57]	Hong Kong	2012	EB	Bottom-up	US EPA 06	AIS/LPA	US EPA 06/ENTEC 02/L R 95	US EPA 06
9	[58]	Shanghai	2013	EB	Bottom-up	ENTEC 02/SMED 04/POLB 10/IMO GHG 09	AIS/LPA	POLB 10/ENTEC 02/CARB 07/SMED 04	POLB 10
10	[59]	Izmir	2013	EB	Bottom-up	ENTEC 05	LPA	ENTEC 05	ENTEC 05
11	[60]	Incheon	2013	FB	Bottom-up	US EPA 06	LPA	POLA 08	POLA 08
12	[61]	Bergen	2013	FB	Bottom-up	US EPA 06/EEM 10	LPA	NEI 10	FEMA 09
13	[62]	Hong Kong	2013	EB	Bottom-up	US EPA 09	AIS/LPA/L MIU	US EPA 09/POLA 09	US EPA 09/POLA 09
14	[63]	14 ports—Spain	2014	EB	Bottom-up	EEA 09	LPA/ENTEC 05	ENTEC 05	ENTEC 02
15	[64]	Busan	2014	EB	Bottom-up	CARB 06/ENTEC 02	L MIU	ENTEC 02/ENTEC 05/ENTEC 07/SMED 04	ENTEC 02/CARB 06
16	[65]	3 ports—Taiwan	2014	EB	Bottom-up	ENTEC 05	NMO	US EPA 09/ENTEC 02	POLA 04/US EPA 06/US EPA 06
17	[66]	Las Palmas	2015	EB	Bottom-up	STEAM	AIS/LPA	STEAM	STEAM
18	[67]	Dubrovnik and Kotor	2015	EB	Bottom-up	US EPA 06/US EPA 09/ENTEC 07	LPA	US EPA 09	PIRAEUS 09
19	[68]	34 ports—Australia	2015	FB/EB	Top-down/bottom-up	ENTEC 02/SMED 04/POLA 12	AIS/LPA	ENTEC 02/SMED 04/IVL 05/POLA 12	US EPA 09
20	[69]	Tianjin	2016	EB	Bottom-up	ENTEC 02/SMED 04/POLB 10/POLA 12/POLA 13	AIS/LPA	SMED 04/US EPA 09/ENTEC 02	POLB 10
21	[70]	18 ports—Greece	2016	EB	Bottom-up	ENTEC 07	AIS/LPA	ENTEC 07	PIRAEUS 09
22	[5]	4 ports—Portugal	2017	EB	Bottom-up	EEA 16	L MIU	EEA 16/ENTEC 02/US EPA 09/SMED 04	ENTEC 02
23	[71]	Zadar	2018	EB	Bottom-up	EEM 10	LPA/ENTEC 02	ENTEC 10	ENTEC 02/US EPA 06
24	[50]	Samsun	2018	EB	Bottom-up	ENTEC 05	LPA	ENTEC 05	SAMSUN 10–15
25	[72]	Incheon	2019	FB/EB	Top-down/bottom-up	CAPSS/PAQman©	AIS/LPA	EEA 13/US EPA 09/ENTEC 02	US EPA 09
26	[73]	Split	2020	EB	Bottom-up	EEA 19	LPA/LPC/ENTEC 02	ENTEC 10	ENTEC 02
27	[74]	Split	2020	EB	Bottom-up	EEA 19	LPA/ENTEC 02	US EPA 09/EEM 10	US EPA 09
28	[75]	Šibenik	2020	EB	Bottom-up	ENTEC 10	LPA	ENTEC 10	ENTEC 02/US EPA 09
29	[76]	Incheon	2020	EB	Bottom-up	US EPA 09/EEA 19	VTS	ENTEC 02/SMED 04/US EPA 09	US EPA 09
30	[12]	Incheon	2021	EB	Bottom-up	US EPA 09/EEA 19	VTS	ENTEC 02/SMED 04/US EPA 09	US EPA 09
31	[77]	Kotor	2021	EB	Bottom-up	EEA 16	LPA	US EPA 09/EEM 10	US EPA 06/POLA 04
32	[13]	Trieste	2021	FB/EB	Top-down/bottom-up	SEA	TDD	IMO GHG 14	MAN

The data on the amount and type of emissions in all examined papers were analysed but were not comparable even for the same ports. This was due to several factors. First, the different papers used different methods and datasets for the emission calculations, so comparing the gas volume values would not describe the relationship between the measurements in a relevant way. Even if the same method was applied in the same interest area, all factors and datasets used for the calculations had to be identical to obtain comparable emission results. The most obvious examples of the mentioned discrepancies in factors are variations in gas types, ship types or shipping distances. However, in order to provide a valid systematic verification of the calculated emission data, regardless of the method and datasets used, it was necessary to establish a standardisation system for the main ship sources. Since no scalable solution was found in the selected work that would provide a basis for comparative data analysis, only the emission prediction methods and datasets were examined.

Finally, it was discovered that most methodologies and/or data segments used in the mentioned papers, were outsourced from the 5 papers and 28 large-scale gas emissions studies developed by, or for, national and interregional organizations responsible for air pollution monitoring and management. However, to specify which sources where predominantly used, and thereby expose the most convenient databases and methods, duplicate exclusion and quantification methods had to be performed in the next step.

3.2. Duplicate Exclusion and Quantification of Sources—Second Layer

The aim of this phase was to determine the most relevant methods and datasets for ship emissions estimation in ports through the quantification of sources used in the overviewed literature. During the overview, however, it was discovered that some reference records dating from different years had been declared as different sources, despite having the same methodological and data background. That is why, preliminarily to quantification, a reference exclusion based on method and dataset comparison was applied. In this procedure, all sources that were developed by or for the same organisations and explored similar interest areas, were considered for a cross-reference check of methodology and dataset aspects that corresponded with the overview in the first step. In the analysis processes, it was noticed that selected sources did employ the same methodologies for calculating emissions and determining data, though data values varied somewhat. That is why the methodological exclusion and quantification of reference sources is presented in Table 3, while the data were subjected to further analysis in order to find similarities relevant to exclusion based on datasets.

Table 3. Exclusion and application quantity of references based on methodology.

No. of Reports	Report	Report Type	No. of Reports after Exclusion	Application Quantity
1	CAPSS/PAQman©	Study	1	1
2	EEA 09	Study	2	9
3	EEA 16	Study		
4	EEA 19	Study		
5	EEM 10	Study		
6	ENTEC 02	Study	3	13
7	ENTEC 05	Study		
8	ENTEC 07	Study		
9	ENTEC 10	Study		
10	IMO GHG 09	Study	4	1
11	SMED 04	Study	5	3
12	MEET 98	Study	6	2
13	POLA 12	Study	7	4
14	POLA 13	Study		
15	POLB 10	Study		
16	SEA	Paper	8	1
17	STEAM	Paper	9	1
18	CARB 06	Study	10	12
19	US EPA 06	Study		
20	US EPA 09	Study		

In the analysis process, it was found that the noted data discrepancies between the reports that had the same research background was primarily relevant for MA and TD about marine traffic, which consequently affected LF and EF values. The main reason for the mentioned value diversity was the changes in fleet characteristics that happened over the time when the research was conducted. As a result of these changes, reports that had the same research background but different data values were considered as the same source, since the latest version was the most relevant for referencing. Therefore, Table 4 presents an overview of the reports whose data were most often applied in selected papers.

Table 4. Exclusion and application quantity of references based on data.

No. of Reports	Report	Report Type	No. of Reports after Exclusion	Application Quantity for EFs	Application Quantity for LFs
1	PIRAEUS 09	Paper	1	/	3
2	SAMSUN 10–15	Paper	2	/	1
3	CARB 06	Study	3	1	2
4	CARB 07	Study			
5	FEMA 09	Paper	4	/	1
6	EEA 13	Study	5	2	/
7	EEA 16	Study			
8	EEM 10	Study	6	2	/
9	ENTEC 02	Study	7	21	9
10	ENTEC 05	Study			
11	ENTEC 07	Study			
12	ENTEC 10	Study			
13	IMO GHG 14	Study	8	1	/
14	SMED 04	Study	9	8	/
15	IVL 05	Study			
16	L R 95	Study	10	1	/
17	MAN	Study	11	/	1
18	MEET 98	Study	12	2	1
19	NEI 10	Study	13	1	/
20	POLA 04	Study	14	4	7
21	POLA 08	Study			
22	POLA 09	Study			
23	POLA 12	Study			
24	POLB 10	Study			
25	STEAM	Paper	15	1	1
26	US EPA 06	Study	16	13	13
27	US EPA 09	Study			

After the exclusion of reports based on methodological and dataset duplication, the quantity of diverse reports decreased significantly. The number of reports used as method references was reduced from 20 to 10, while 16 different sources of datasets were acknowledged from the original 27 sources. In addition, all selected reports were recognised as studies, with the exception of three papers. Finally, quantification of the studies and papers used as references in the reviewed literature provided insight into the most commonly used methods and datasets. So, by combining the citation frequency from each report, the most relevant papers and studies are exposed and presented in Figure 3.

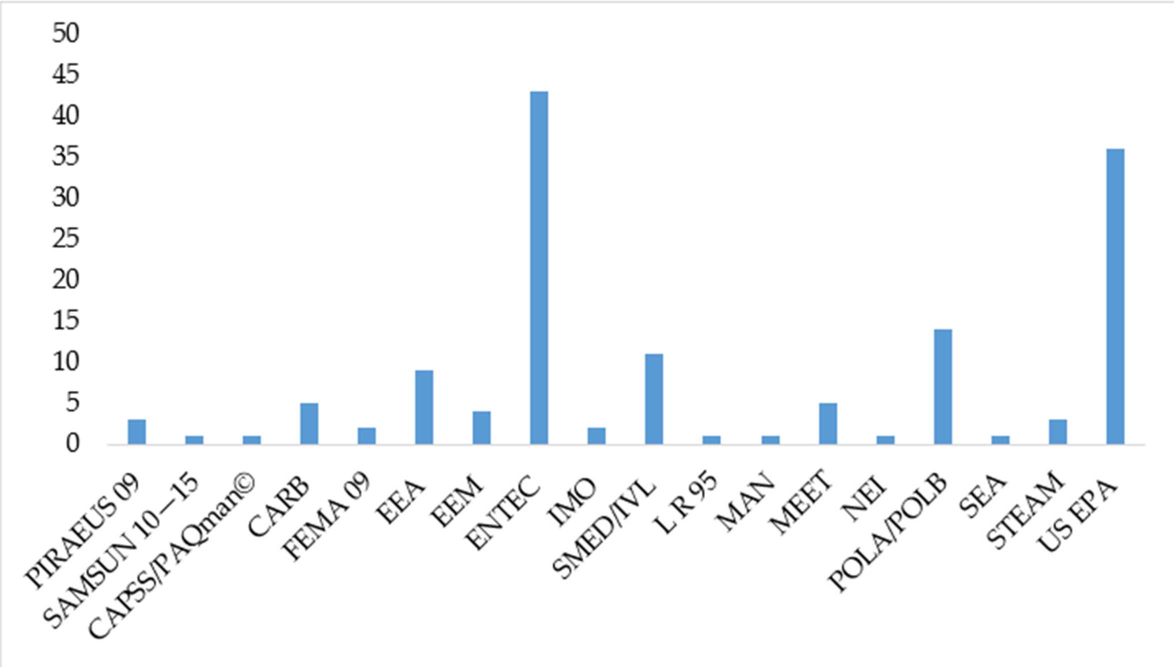

Figure 3. Citation quantity overview of methodologies and datasets originated from the papers and studies that explored ship emissions estimation.

3.3. Analysis of the Most Commonly Applied Methodologies and Datasets—Third Layer

By quantifying the reports used as methodological and data references in papers dealing with the estimation of ship emissions in ports, the seven most relevant studies stood out. The objective of this step was to examine the methods and data developed in these studies in order to determine the methodological and informational segments relevant to emission estimation. An overview and analysis of the equations, along with their methodological background and key data for determining emissions quantity, are presented throughout this examination process. However, since the methodologies and datasets may have changed over the years, the latest available and most actual editions of the commonly referenced studies were analysed.

3.3.1. ENTEC and NAEI Research

The primary objective of the ENTEC 10 research established by the Department for Environment, Food and Rural Affairs (Defra) was to develop a detailed ship emissions dataset that could be used to inform United Kingdom (UK) policies targeting shipping emissions [31]. Although this inventory was based on information about ship movements from 2007, it is a continuation of the ENTEC 02, ENTEC 05 and ENTEC 07 studies. The approach is consistent with the methodology for quantifying ship emissions in the EEA 09 and relies on information that largely dictates the emissions from a vessel: installed engine power, type of fuel consumed, vessel speed and distance travelled (or time spent travelling at sea), time spent in port and installed emission-abatement technology [31]. Although the methodology follows the EEA 09 guidelines, equations, types of vessels and EFs are different, so this research was analysed separately. Activity data on vessel movement and port entries was provided by the Lloyd's Marine Intelligence Unit (L MIU) which used AIS data for movements that were not recorded in the port arrivals statics. In addition, the aforementioned information was compared with the Department for Transport's (DfT) data in order to corroborate them. Static data that largely dictate emission volumes, such as vessel characteristics (type and service speeds) and main engine (ME) and auxiliary engine (AE) characteristics (type, speed and fuel type) were gathered from the L MIU database. Although this study has a UK focus, the generic values of key elements for quantifying emissions can be applied in different research areas since L MIU compiles one of the largest datasets containing vessel information. Although this research treats of three different movement activities, the equation for at-sea activity is separated from the equation for port emissions that is related to hoteling and manoeuvring activities. Equation (5), presented below, is applicable for determining port emissions [31].

$$E = T \times [(ME \times LF_{ME})) \times EF + (AE \times LF_{AE})) \times EF \tag{5}$$

where:

E: Emissions per vessel—in grams (g);
T: Average time spent at berth/manoeuvring per calling—in hours (h);
ME: Installed main engine power—in kilowatts (kW);
LF_{ME}: Average load factor of main engine at berth/manoeuvring—as a percentage of ME power (%);
AE: Installed auxiliary engine power—in kilowatts (kW);
LF_{AE}: Average load factor of main engine at berth/manoeuvring—as a percentage of ME power (%);
EF: Emission factors assigned to each vessel for at berth/manoeuvring depending on each fuel type and engine speed—in grams per kilowatt hour (g/kWh).

ENTEC 10 was the last research provided by Entec ltd. that explored shipping emissions for Defra, relevant to the UK waters [31]. That is why it should be emphasised that in the latest UK National Atmospheric Emissions Inventory (NAEI) conducted for Defra, EEA methodology was followed with differences in applied data [78,79].

3.3.2. US EPA Research

The purpose of US EPA 20 was to provide guidance for the development of a mobile source port-related air pollution emissions inventory within a designated area in a given time period. This document supersedes the previous April 2009 document US EPA 09 [80]. For the ocean-going vessel (OGV) sector, a bottom-up EB emission estimation methodology was presented, according to which both AIS and traffic statistics data could be applied using Equation (6). According to this document, the information necessary for emission calculations includes engine characteristics (that describe engine power, type, age, speed and category), ship speed, position and course. From the mentioned data, EF and LF can be obtained. In this publication, five different movement activities have been recognised (Transit, Manoeuvring, Restricted Speed Zone, Hotelling, Anchorage) and defined by LF. To obtain the value of LF, the propeller law is used. In the end, when actual activity is recognised, the predefined low load adjustment factors (LLAFs) can be applied [80].

$$E = P \times A \times EF \times LLAF \tag{6}$$

where:

E: Emissions per vessel by mode—in grams (g);
P: Engine operating power—in kilowatts (kW);
A: Engine operating activity—in hours (h);
EF: Emission factors of different pollutants in regard to engine group, engine type, fuel type, keel laid—in grams per kilowatt hour (g/kWh);
LLAF: Low load adjustment factor, a unitless factor that reflects increasing propulsion emissions during low load operations—always 1 for auxiliary engines and boilers.

3.3.3. POLA and POLB Research

The Port of Los Angeles' (Port or POLA) annual activity-based emissions inventories serve as the primary tool for tracking the Port's efforts to reduce air emissions from maritime industry-related sources. This study was prepared in coordination with the Port of Long Beach (POLB) and the following air regulatory agencies: the U.S. Environmental Protection

Agency, Region 9 (US EPA), California Air Resources Board (CARB) and the South Coast Air Quality Management District (South Coast AQMD) [81]. The methodology for estimating emissions was taken from the San Pedro Bay Ports Emissions Inventory Methodology Report, in which the EB approach was applied to every movement activity of OGVs within the harbour district for 40 nautical miles (NMs) [81,82]. The aforementioned methodological background is summarised in Equation (7). The traffic data for the emission estimation is provided through AIS and various statistical reports. The Energy component is determined by combining LF with the time spent in a particular activity mode [82]. Emission sources for all vessel categories include ME (propulsion), AE (generators) and auxiliary boilers (ABs). LF defaults are provided for AE and ABs for all movements (Transit, Manoeuvring, At Berth, Shift, At Anchorage), while ME load is estimated through propeller law [81,82]. In addition, average values of vessel characteristics relevant to emission estimation are introduced. The mentioned data correspond to the OGV traffic in the port area.

$$E_i = Energy_i \times EF \times FCF \times CF \tag{7}$$

where:

E_i: Emissions by mode—in grams (g);
$Energy_i$: Energy demand by mode as the energy output of the engine(s) or boiler(s) over the period of time—in grams per kilowatt hour (g/kWh);
EF: Emission factor depends on engine type, IMO tier and fuel used—in grams per kilowatt hour (g/kWh);
FCF: Fuel correction factors are used to adjust from a base fuel associated with the EF and the fuel being used—dimensionless;
CF: Control factor(s) for emission reduction technologies—dimensionless.

3.3.4. SMED—IVL Research

The methods for calculating emissions in Swedish emissions reporting have been developed in two reports (SMED 04 a, b), in which emission factors have been developed that can be used to calculate emissions together with statistics on fuel sales for domestic and international transport [83]. However, in recent years, the Swedish Environmental Research Institute (IVL) has developed a novel emission calculation model for ships in ports. With this model, it is possible to calculate the emissions of carbon dioxide, nitrogen oxides, particulate matter and sulphur dioxide, as well as the fuel consumption of ships during port calls [84]. Taking into account the evolution of engine and fuel characteristics from 2004, SMED 20 introduced effective emission factors that can be used for emissions reporting [83]. According to this new method, LFs are estimated by the propeller law, and by applying AIS data along with statistical information from ports it is possible to calculate ship emissions with greater accuracy. The aforementioned IVL calculation model for emissions from ships in port areas is constructed around Equation (8) [83,84]:

$$E = EF \times t \times P \tag{8}$$

where:

E: Resulting emissions—in grams (g);
EF: Emission factors that can depend on, e.g., engine age, type of engine, fuel used and exhaust gas aftertreatment—in grams per kilowatt hour (g/kWh);
t: Time in an operational mode—in hours (h);
P: Power needed in an operational mode—in kilowatts (kW).

The power requirements are most often calculated as the product of installed engine power and an engine load factor—an assumed value. Many generic values are used, and by comparing results with alternative datasets for input on ships' speeds, power requirements, etc., inaccuracies can be removed and rectified [84].

3.3.5. EEA Research

General guidance for the control of ship emissions in the EU has been provided by the European Environment Agency (EEA) through the EEE 20 Guidebook, Section 1. A.3.d. [85]. The key function of the EEA 20 Guidebook is to offer estimation methods and emission factors for developing inventories at various levels of sophistication that are transparent, consistent, complete and comparable [85]. Guidelines of different complexities for calculating ship-sourced gas emissions are incorporated in its three-tier system. The less data-demanding Tier 1 and Tier 2 approaches use fuel sales as the primary activity indicator and assume average vessel emission characteristics to calculate emissions estimates. The Tier 3 methodology is based on ship movement information for individual ships and requires detailed ship motion activity data, as well as technical information about ships [16]. The practical aspect of the Tier 1 and Tier 2 approaches is that they require less detailed data and are better suited for quantifying gas emissions at the national level, while the Tier 3 activity-based level can provide detailed site-specific results. For this reason, the Tier 3 methodology, applicable to port areas, is conceptualised in FB Equation (9) and EB Equation (10) [16].

$$E_{Trip,i,j,m} = \sum\nolimits_{p} (FC_{j,m,p} \times EF_{i,j,m,p}) \tag{9}$$

$$E_{Trip,i,j,m} = \sum\nolimits_{p} [T_{p} \sum\nolimits_{e}(P_{e} \times LF_{e} \times EF_{i,j,m,p}) \tag{10}$$

where:

E_{Trip}: Emission over a complete trip—in metric tonnes (t);
FC: Fuel consumption—in metric tonnes (t);
EF: Emission factors of different pollutants in regard to engine category, engine type, fuel type, activity mode—in kilograms per ton of fuel (g/t) or grams per kilowatt hour (g/kWh);
i: Pollutant;
m: Fuel type;
j: Engine type;
p: The different phase of trip (activity);
LF: Average load factor of engine at berth/manoeuvring—as a percentage of engine power (%);
P: Engine nominal power—in kilowatts (kW);
T: Average time spent in phase of trip (activity)—in hours (h);
e: Engine category.

3.4. Comparative Analysis of Key Components and Proposition of Relevant Methodology for Estimation of Ship Emissions in Ports—Fourth Layer

After reviewing the selected studies, it was concluded that the general methodologies for estimating ship emissions in ports are based on a combination of data about ship engines, fuel consumed and movements, along with their effects on engine performance and EFs based on energy consumption. Depending on their complexity, all of the aforementioned factors contain several key components that, by interacting with each other, largely determine the amount of gas emissions from the ship. The key components, that is, the data that define them, can be considered static and dynamic. The static data on particulars of the ships and their engines describe components for emission calculations, such as engine power (EP), engine function, engine type and fuel type. It can therefore be said that TD can be described as static while MA can be considered dynamic data. Ship MA is categorised by the operational mode of the ship's propulsion system and defined by dynamic information on the percentage of ME and AE working load expressed as LF. Since different activities do not have the same impacts on emissions, it is equally important to consider the time spent in each operational mode. Finally, as the central and most complex segment of the emissions quantification process, EF depends on both static data about engine function, engine type and fuel type and dynamic information about the characteristics of the ship's activities. Throughout the analysis of the studies, it was also found that mainly a combination of maritime traffic statistics from local or national maritime organisations and AIS information was used in data collection. Given this, traffic information can be compared and validated, resulting in more accurate emissions values estimates.

By combining all the analysed key data and methodological factors used in selected studies, a proposition of a relevant methodology for the estimation of ship emissions in ports can be introduced. To begin with emissions estimation, data acquisition should be carried out by combining multiple sources of marine traffic information. With the widespread use of AIS, better coverage of both static and dynamic information about ships and their movements is available. Therefore, a bottom-up EB approach is proposed. However, in order to validate AIS information and to get an overview of vessels that are not required to have an AIS onboard, statistical information representing the TD of the traffic inside the interest area should be applied. As can be seen in Figure 4, all key factors in emissions estimation are classified by colour and linked inside a methodology and data diagram for port-related calculation of emissions on a ship-by-ship basis. Within the diagram, grey colouring marks the static TD on the ship and its engines; blue indicates the combination of static and dynamic data for estimating LF through the propeller law and thereby determining a ship's MA; the colour yellow represents more complex datasets defined by TD and classified through methodological aspects relevant to traffic inside the research interest area; finally, orange indicates the key elements for calculating ship emissions as an output value, which is marked in red. The interactions of all key segments outlined in this research are presented in Equation (11) for estimating ship emissions in ports.

$$E = (P_{ME} \times LF \times EF_{ME} + P_{AE} \times LF \times EF_{AE}) \times T \times CF \quad (11)$$

where:

E: Emissions quantity by mode for each ship call—in grams (g);
$P_{ME/AE}$: Total power of main engines/auxiliary engines—in grams per kilowatt hour (g/kWh);
LF: Load factor expressed as actual engine work output—as a percentage of engine power (%);
EF: Emission factors of different pollutants in regard to engine function, engine type, fuel type, installation year—in grams per kilowatt hour (g/kWh);
T: Time spent in a certain movement activity—in hours (h);
CF: Control factor for emission reduction technologies—constant.

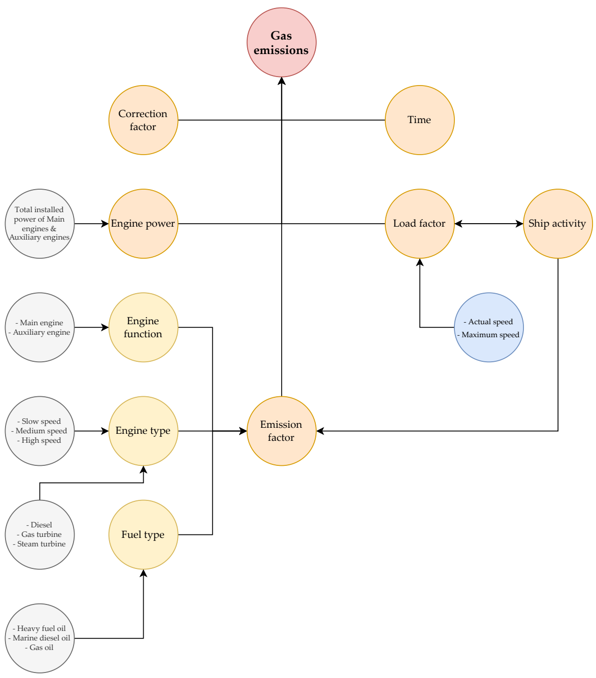

Figure 4. Proposal of methodological and data key factors for port-related calculation of emissions on a ship-by-ship basis.

4. Conclusions

The main goal of this review paper was to determine the most applicable methodology and datasets for quantification of port-related ship emissions through the presented bottom-up multi-layer analysis approach. The goal of the first layer was to provide an analytical overview of methodologies and datasets used in port-related ship emissions studies through a bottom-up PRISMA approach. After that, the methodological background of each selected scientific paper was thoroughly examined and connected to the original source of used methods. The methodological sources identified through the analysis were aggregated and quantified in the second layer to obtain the most commonly used methods in the relevant research. In the third layer, the methodologies and data of the most commonly used studies were examined and compared. By means of this, in the last layer, a proposal for the most applicable shipping emission quantification methodology for port areas was produced and explained through all key factors.

However, regardless of an approach used in examined studies, a scalable solution that would allow extensive insight into the main shipping sources of pollution was not introduced. The development of a unique standardisation system would not only enable better communication and integration with the wider port city community but could also serve as a basis for better predication and mitigation of ship-sourced emissions at a local and national level. Therefore, a method generated through the multi-layered analysis approach presented here will be used as the first step in future research into the development of a ship-sourced gas emission indexing model for port areas.

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Article 2

An Analytical Model for Estimating Ship-Related Emissions in Port Areas

Bojić, Filip.; Gudelj, Anita.; Bošnjak, Rino

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An Analytical Model for Estimating Ship-Related Emissions in Port Areas

Filip Bojić *, Anita Gudelj and Rino Bošnjak

Faculty of Maritime Studies, University of Split, 21000 Split, Croatia; anita@pfst.hr (A.G.); rinobo25@pfst.hr (R.B.)
* Correspondence: fbojic@pfst.hr

Abstract: Intensive shipping activity in port areas is considered one of the leading problems in the maritime sector, which has a negative effect on climate change and local air quality. The compilation of detailed inventories of combustion gases released by ships should therefore provide a more accurate overview of emission levels, which can serve as a basis for analysing impacts on the port community and lead to the establishment of better environmental measures. Thus, the aim of this study was to develop an adaptable and relevant analytical model capable of integrating a comprehensive methodology with large databases of ship movements and technical details to provide clear ship-related emission estimates in large port areas. Considering the lack of research in Croatia that includes the mentioned approach and the insufficient monitoring of air pollutants in ports, the model was used to produce an initial overall emissions inventory for the Port of Split, the busiest passenger port in Croatia. In the model, bottom-up logic with an energy-based method was applied to detailed technical and near-real-time shipping data from AIS, creating the first high-density spatial and temporal overview of shipping emissions in the City port basin. The results showed strong seasonal fluctuations and large discrepancies in the quantities emitted between different ship types and operating modes. The analysis therefore raised the question of the need for the future development and implementation of a scalable system that would provide a more transparent and efficient overview of the important characteristics of air pollution from ships and port areas.

Keywords: ship emissions; air pollution modelling; AIS; environment; Port of Split

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1. Introduction

Although shipping is widely recognised as the most sustainable mode of transport since large volumes of cargo can be carried in a single trip, extensive quantities of marine fuels are used for propulsion during transportation [1–4]. The internal processes of energy conversion and combustion in ship engines mainly produce air pollutant substances (APSs) such as sulphur oxides (SOx), nitrogen oxides (NOx), particulate matter (PM), carbon monoxide (CO), and volatile organic compounds (VOC), as well as carbon dioxide (CO_2), methane (CH4), and nitrous oxide (N2O), recognised as greenhouse gases (GHGs) [1,5–7]. While anthropogenic GHGs are responsible for global warming and the adverse effects of climate change, other air pollutants released from fuel combustion have serious impacts on human health in urban areas [1,7,8]. It was documented that exposure to the PM2, SOx, NOx, CO, and VOC is associated with respiratory illness, cardiovascular disorder, lung cancer, and premature mortality [8,9]. Given that 70 to 80% of world trade is seaborne, maritime transport contributes significantly to anthropogenic emissions [1,3].

Aiming to reduce ship-sourced air pollution, the International Maritime Organisation (IMO), in 1997, extended the MARPOL convention with Annex 6 "Prevention of Air Pollution from Ships". The main objective of the entry into force of MARPOL Annex 6 was to mitigate SOx, NOx, VOC, and PM emissions by establishing stringent fuel quality and emission control regulations applicable to ships and Emission Control Areas (ECAs) [10]. Under the revised MARPOL Annex 6, the global sulphur limit is reduced to 0.50% mass by mass percent (% m/m), effective from 1 January 2020, while the content in ECAs is reduced to 0.1% m/m [10]. Progressive reductions in NO_x emissions from marine diesel engines is regulated through a three-tier system. The less rigid Tier 1 applies to ships built on or after 1 January 2000, Tier 2 for ships built on or after 1 January 2011, while the most demanding Tier 3 regulates NOx emissions from ships built after January 2016, or 2021, and operating in ECAs [10]. It is expected that the measures for SOx and NOx should also reduce the quantity of PM and VOCs released into the atmosphere. Regarding the mitigation of GHGs, the IMO added a new Chapter 4 to MARPOL Annex 6, which provides two important measures. In the first one named the Energy Efficiency Design Index (EEDI), it is required for new ships to comply with minimum mandatory energy efficiency performance levels, increasing over time through different phases [11]. The Ship Energy Efficiency Management Plan (SEEMP) is an operational measure that establishes a mechanism to improve the energy efficiency of a ship in a cost-effective manner [11].

However, regardless of the numerous revisions to MARPOL Annex 6 and the continued application of more stringent emission control regulations, the IMO has recorded an increase in overall GHG air pollution from ships [12]. It was noted that, from 2012 to 2018, emissions of CO_2, NOx SOx, PM, CO, VOC, and CH4 increased by 5.6%, 1.2%, 5.5%, 3.5%, 10.2%, 7.6%, and 151%, respectively [12]. This rise of ship-related air pollutant volumes released into the atmosphere is mostly connected to the growth rates of fuel consumption due to increased shipping demand [12]. Although overall carbon intensity has improved by 20–30% over the same period, the study also stated that it will be difficult to achieve the IMO's GHG reduction goal of 50% by 2050 [12]. Therefore, countries should anticipate, prepare for, and adapt to climate change by fully understanding the risks, exposure, and vulnerabilities [13].

With the same tendency, but focusing on the regional aspect, the European Sea Ports Organisation (ESPO) has recognised the problems of air quality, climate change, and energy efficiency in the port sector of the European Union (EU) as three of the most important environmental priorities [14]. Ports account for a small share of global maritime traffic emissions, but their function as major transport hubs leads to intensive shipping activity and thus to a corresponding emission of air pollutants. Port-related emissions from ships engines have strong spatial and temporal significance that directly affects air quality in port communities. Considering that 90% of European ports are spatially connected to cities, the magnitude of air quality degradation is even more serious [14,15].

Although all EU countries are required to monitor their emissions under the EU Climate Monitoring Mechanism, and the European Environment Agency (EEA) compiles national inventories in accordance with the Intergovernmental Panel on Climate Change (IPCC) guidelines, emissions from maritime transport, particularly in port areas, are still vague in some regions [16–18]. An example of unclear monitoring of air pollution from shipping can be observed in Croatia. In the latest Croatian GHG inventory, general fuel consumption (Tier 1 method) was applied to estimate emissions from navigation, but without spatial, temporal, or technical details [19]. The Croatian part of the Adriatic coast is 1777 km long and has six ports of international economic importance open to public traffic, where most of the 359,223 arrivals of various types of ships were recorded in pre-pandemic 2019 [20,21]. Thus, it is necessary to obtain a better insight into air pollution from the maritime sector, especially in port areas with large communities [4,22–24]. Moreover, emission inventories should quantify not only GHG but also other pollutants that may compromise the health of the port-city population.

That is why the importance of high-resolution shipping emission inventories for port areas is recognised by both the port and scientific communities [14,15,23–27]. The results of a detailed air pollution study should reveal more accurate emission levels that can be used as a basis for analysing impacts on the port community, leading to the establishment of better environmental measures. However, to calculate quantities of air pollutants with higher accuracy, a bottom-up energy-based method should be applied on large datasets that contain relevant shipping information. IMO Regulation V/19, which requires the installation of an Automatic Identification System (AIS) on merchant ships of 300 GT (GT) and all passenger ships, has made near real-time data on ships and their movements available [1]. Accordingly, an increase in bottom-up energy-based gas emission inventories for ports has been noted, suggesting that by combining high-resolution data with the appropriate methodology, it is possible to obtain coherent estimates of air pollution from ships in ports [15]. The systematic review showed that the bottom-up approach was used frequently in papers analysing ship-related emissions in 80 different ports, with the energy-based method being predominantly applied [15]. However, as bottom-up approach requires large databases, calculating emissions is a complex and time-consuming operation, especially when estimation is not systematically processed.

Therefore, the focus of this research was to develop an adaptable and relevant analytical model capable of integrating a comprehensive methodology with large amounts of shipping data to produce clear ship-related emission estimates in large port areas. Considering the lack of research in Croatia that includes the mentioned approach and the insufficient monitoring of air pollutants in ports, the model was used to develop an initial overall emissions inventory for the Port of Split, the busiest passenger port in Croatia. The inventory with high temporal-spatial resolution can be used as a basis for developing strategies to control emissions. In the model, the bottom-up approach and the energy-based method were applied to detailed technical and near-real-time shipping data from the AIS to calculate levels of air pollutants released by ships in the City port area. Throughout the three-step process, estimates of CO_2 and CH4 as GHGs and SOx, NOx, PM10, PM2.5, NMVOC, and CO as APSs were determined on a ship-by-ship basis for the entire year of 2019. Exhaust gas volumes with relevant data on the production of air pollutants from marine engines are stored and can be handled by the model to generate various analytical results. The model was therefore able to produce a novel, high-density, activity-based ship emissions spatial distribution map, together with a detailed overview of technical, temporal, and operational aspects. In addition, a unique differentiation of ship types was developed to ensure proper and effective imputation of missing data while providing the background for a future extension of the model's predictive capabilities.

2. Materials and Methods

The methodology for estimating ship-sourced gas emissions in port areas applied in this research is based on a comparative analysis of relevant papers and studies within the PRIMSA approach and meets the requirements of the IPCC guidelines [15]. The mentioned paper stated that the bottom-up energy-based methodology is most reliable for estimating ship-sourced gas emissions in port areas since it requires a high level of input parameters [15,23]. Since this approach enables calculation on a ship-by-ship basis by combining energy output with emission factor (EF) and time, large databases that contain specific technical data on the ships and detailed information on movement activities need to be used. Static technical data on the details of the ships and their engines describe components for the emission calculations, such as main/auxiliary engine power ($P_{ME/AE}$), engine function, engine type, and fuel type [15]. Dynamic data on ship MA is categorised by the operational mode of the ship's propulsion and generator systems and defined by the percentage of ME and AE working load expressed as LF [15]. Considering that the specific workload of the engines has a direct influence on the emission production, the time spent in cruising, manoeuvring, and hoteling activities must be taken into account. As the central and most complex segment of the emissions quantification process, EF depends on both static data on engine function, speed, engine type, and fuel type and dynamic information on the characteristics of the ship's activities [15]. Therefore, the bottom-up energy-based methodology expressed in Equation (1) that contains key factors proposed in the systematic review is implemented in the emission estimation model presented within Figure 1 [15].

$$E = (P_{ME} \times LF \times EF_{ME} + P_{AE} \times LF \times EF_{AE}) \times T \times CF \quad (1)$$

where the following definitions apply:

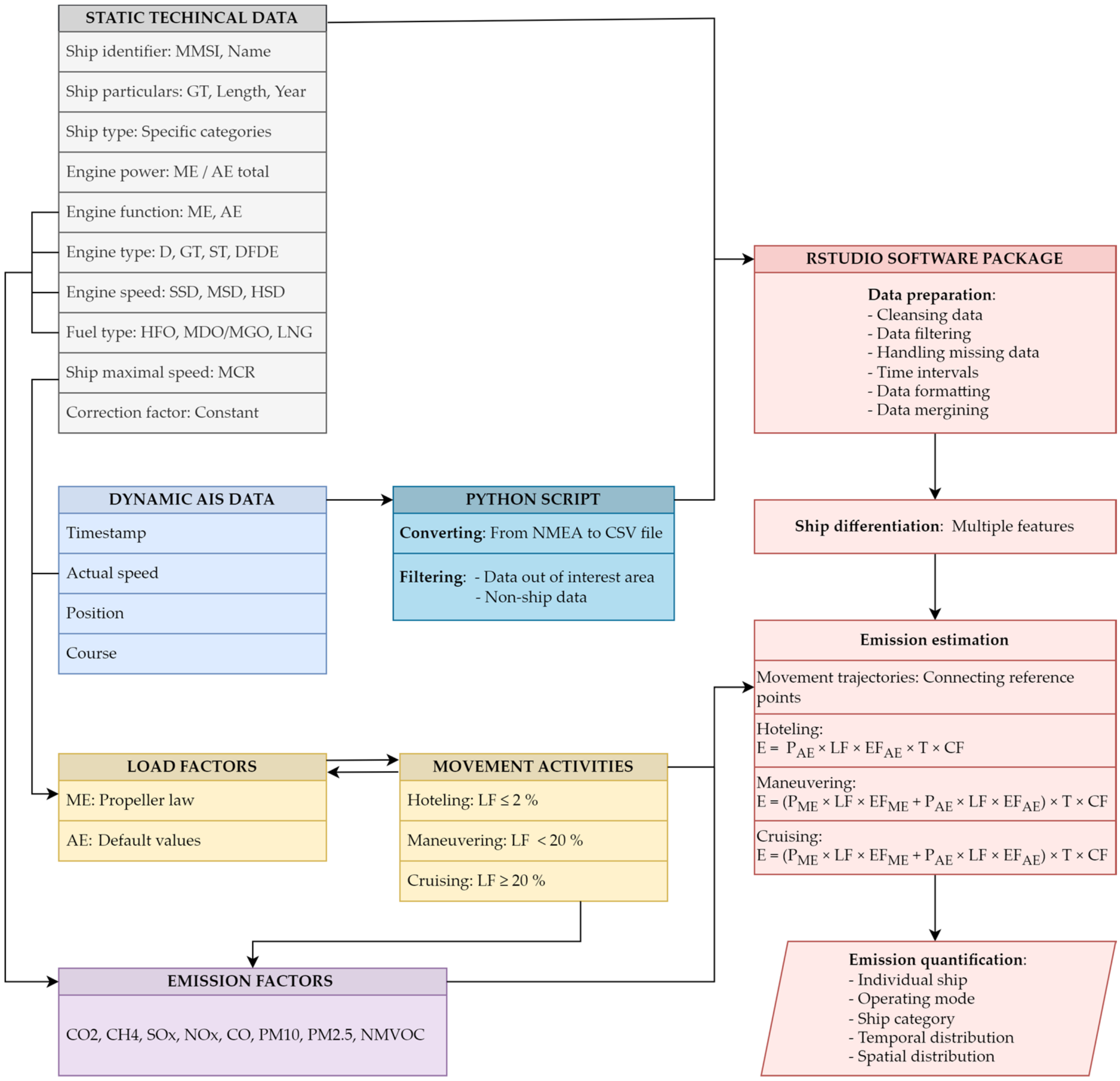


Figure 1. Flow diagram of the model for estimation of ship emissions in port areas.

E: E missions quantity by mode for each ship call—in grams (g);

$P_{ME/AE}$: total power of main engines/auxiliary engines—in grams per kilowatt hour (g/kWh);

LF: load factor expressed as actual engine work output—as a percentage of engine power (%);

$EF_{ME/AE}$: emission factors of different pollutants in regard to engine function, engine type, fuel type, and installation year—in grams per kilowatt hour (g/kWh);

T: time spent in a certain movement activity—in hours (h);

CF: correction factor for emission reduction technologies—constant.

The model for ship-related emissions estimation in ports has three complex and interconnected phases. In the initial preprocessing stage, data collection was carried out with recourse to several databases. The data from AIS had to be cleaned and converted from 'raw' format into a readable comma-separated values (CSV) file in order to be merged, filtered and structured together with the static technical data. Methods for ship type differentiation and emissions estimation were then applied on formatted technical and activity data as a part of the processing phase. Lastly, in the postprocessing phase, output data was stored and handled, aiming to create spatial and temporal visualisations of shipping emissions.

The dynamic AIS data was transferred through Python, while the handling and analysis were carried out using the RStudio 2023.09.1+494 software package. Within the grey box that contains technical features, MMSI stand for Maritime Mobile Service Identity, GT for gross tonnage, D for diesel engine, GTU for gas turbine, STU for steam turbine, DF for dual fuel, SS/MS/HS D for slow-/medium-/high-speed diesel engine, HFO for heavy fuel oil MDO/MGO for marine diesel/gas oil, LNG for liquified natural gas, and MCR for maximum continuous rating. MCR is defined as the manufacturer's tested engine power [28]. Usually, a ship operates at the nominal continuous rating, which is 85% of the 90% of MCR [26]. Inside the dark blue box, NMEA stands for National Marine Electronics Association sentence format.

Considering that the aspects of the main data processing components of the model are based on universal characteristics that have a significant effect on the production of air pollutants, it can be concluded that the model is not restricted to one case study and can be applied to different ports. Also, the flexibility of the model structure allows the inclusion of new insights and other aspects relevant to the port-based shipping emissions, expanding the quality and scope of the final output.

It is important to add that large quantities of technical data have enabled a specific differentiation of ship types based on the analysis of multiple characteristics. This feature allowed for more accurate and effective missing-data imputation and provided a basis for future expansion of the model's capabilities in emissions forecasting and scenario building.

2.1. Maritime Traffic, Spatial and Temporal Specifications

To determine the exact databases for the emission calculations, the temporal, spatial, and transportation characteristics of the research area must first be defined and analysed. As it was stated, the modelling of emissions was conducted by relying on historical data on shipping traffic in the Port of Split—City port basin in 2019.

The Port of Split is one of the busiest ports in the Mediterranean in terms of passenger and vehicle traffic, while cargo traffic remained within the bounds of local importance. For example, in 2019, the busiest year on record, 5,607,789 passengers and 829,594 vehicles were transported, but only 2,913,509 tonnes (mt) of cargo was transferred [29]. The distribution of maritime traffic is thus almost exclusively concentrated on various types of passenger ships, mainly Ro-Ro ferries, high-speed craft, cruise ships, and pleasure craft, which account for almost 90% of arrivals.

Spatially, the Port of Split is divided by the city of Split into two dislocated areas. One area, called North port, is situated on the northern side of the Split peninsula and consists of several basins, mainly for cargo ships. City port basin forms the second part of the port, which is intended for passenger ships and where, on average, about 90% of all maritime traffic is handled. The City port is located in the southern part of the Split peninsula, where it is spatially and infrastructurally integrated into the city centre, what can be seen in Figure 2. Due to the locational connection with the urban environment, high traffic density of City port and the fact that Split is the second most populated Croatian city, air degradation can represent a serious threat to public health. The city's connection with the Adriatic islands and the Apennine Peninsula via numerous shipping lines and its popularity as a cruise and tourist destination with a growth trend further emphasises the need for monitoring and control of pollutants from maritime traffic. Thus, this study focuses on the area of the City port with the aim of estimating and analysing ship-induced air pollution. The research area with the relevant coordinates is shown in Figure 3. The dynamic AIS data was transferred through Python, while the handling and analysis were carried out using the RStudio software package (https://www.r-studio.com/data-recovery-software/).

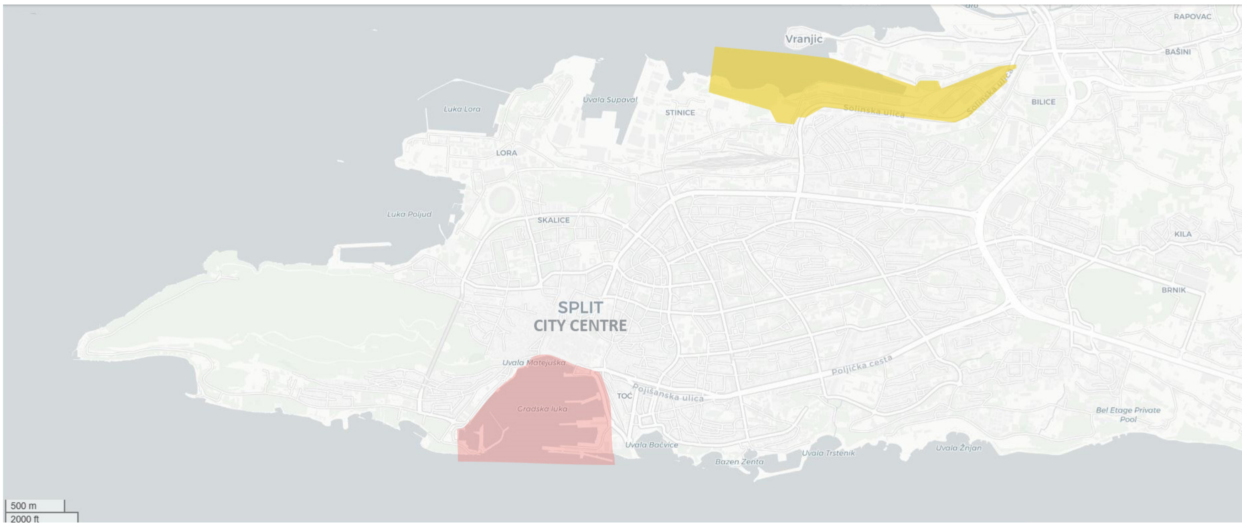


Figure 2. Overview of Port of Split basins and Split city centre.

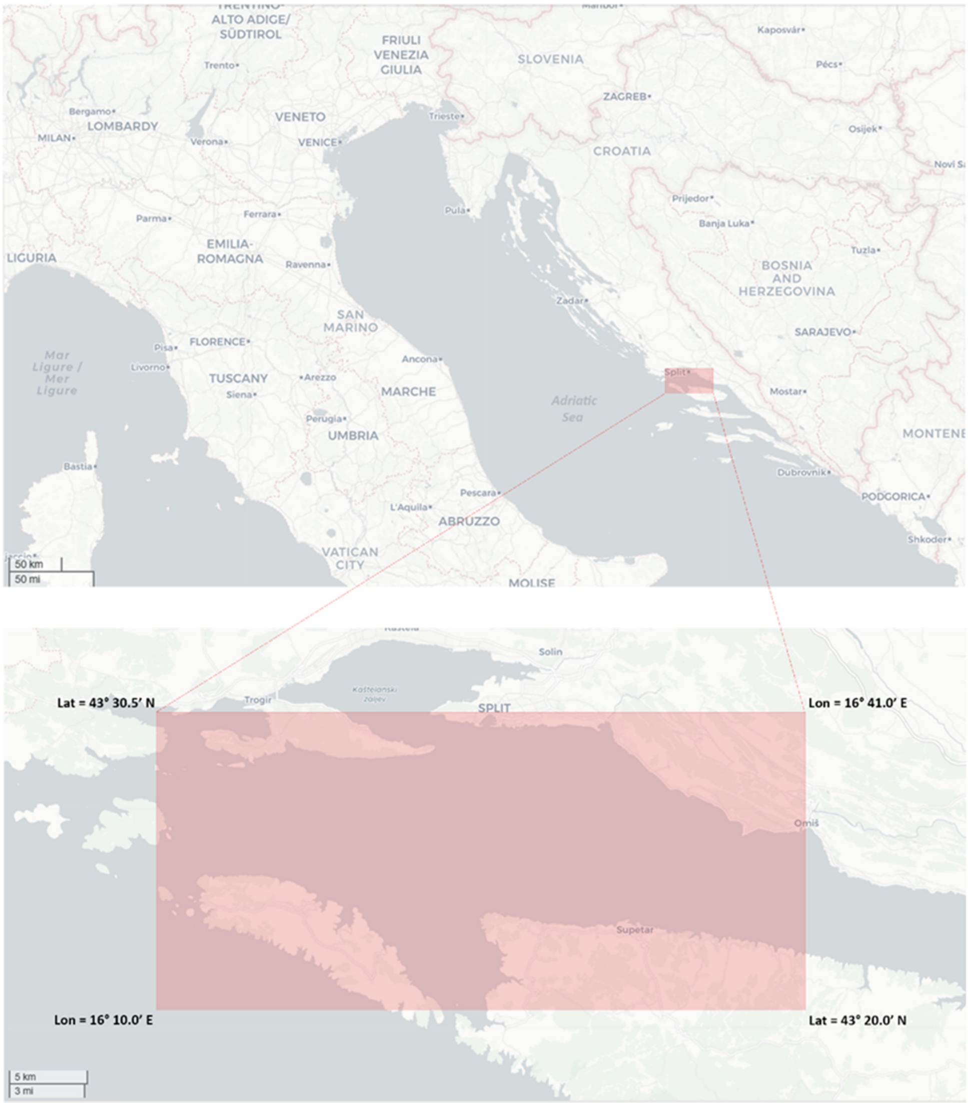


Figure 3. Research area in relation to the region with respective geographic coordinates.

Part of the area of the North port is marked in yellow, while the City port basin is in red. The grey area in between represents the urbanised parts and the locational connection of the City port with the town centre. Note: the map was generated with the RStudio software package and then modified.

2.2. Defining Input Databases—Technical Data and Activity Data

Based on the name, type, and MMSI number as identifiers, a database of technical information about ships and their engines was created by collecting attributes from the Croatian Registry of Shipping (CRS), the Croatian Integrated Maritime Information System (CIMIS), and web data (WD) from relevant shipping companies. Gathered data refers to GT, length, breadth, year, MA power, AE power, engine type, engine speed, fuel type, maximal speed at MCR, and relevant emission mitigation technology. Considering that several data sources were used, it was possible to corroborate mentioned information, and where data was redundant, the CRS database was prioritised.

The primary function of AIS is to ensure higher level of navigational safety by sharing timely information on ship characteristics and their movement between other vessels and the shore [30]. However, both static and dynamic data transmitted by AIS provide a detailed overview of ship movements and their characteristics, which is more often applied in emission estimation process [15,23]. Therefore, the AIS database that contains relevant shipping data applied in this research was provided by the Faculty of Maritime Studies in Split. Generally, the static data broadcasted through AIS refers to MMIS number, IMO number, ship type, length, name, and call sign [31,32]. Dynamic data on ship movement reveals the position of the ship, the timestamp, the course over ground (COG), and the speed over ground (SOG) [30,32]. As the AIS dataset does not contain all features required for the estimation of emissions, such as engine details or LF, only dynamic data was used, while static information represented by the above identifiers was included in the data merging process.

2.3. AIS Dataset Conversion and Filtering

A prerequisite for the integration of technical information with activity details is the conversion of the AIS data. AIS operates in the very high frequency (VHF) mobile maritime band or uses satellite communication for broadcasting messages in NMEA sentence format [33]. NMEA files are in 'raw' encoded form and as such are not readable by statistical data processing software. Therefore, a specific Python script was developed and integrated inside the model to convert the 'raw' data from AIS into a readable CSV format. Considering that the use of AIS is not limited to ships nowadays and that the AIS station used in this research covers a larger area than necessary, both spatial and non-ship filters were included in the script. As a final result of the AIS data preparation, timestamps with current speed, position, and course were extracted together with the corresponding identifiers for each transmitted point of each vessel that passed through the selected area in 2019. Since AIS generally generates and shares data every few seconds, 71,638,920 entries were obtained and taken into account for further preparation. Although processing a database of this size is very time-consuming and computationally intensive, it provided the basis for identifying emissions with high spatial and temporal density.

2.4. Data Preparation

In the last step of the preprocessing phase, the RStudio software package was used to develop code that enabled the cleansing, filtering, formatting, and merging of data. Cleansing was applied on AIS datasets, aiming to exclude duplicate and faulty data. In this process, entries missing identifiers and/or all particulars were screened out. Ships that passed through the interest area but did not arrive at the designated port basin were filtered out. The same principle was applied to the entries or the entire movement tracks with abnormal values for speed (more than 40 kt), position, and/or time. After eliminating inadmissible datasets, 49,540,895 entries were used for the research. Given that the technical and activity datasets were collected from several sources, their structure had to be formatted to establish a standardised form. Once a consistent display of the cleansed and filtered data was achieved, the specific technical details of each vessel were merged with all corresponding activity entries recorded in 2019 by linking the unique identifiers. Performing all the mentioned steps of the preprocessing phase within the model enabled emission estimation on a ship-by-ship basis, but also the implementation of the specific differentiation of ship types.

2.5. Ship Types Differentiation and General Characteristics

The two main functions of differentiating ship types based on the analysis of multiple characteristics are to ensure more accurate and effective imputation of missing data while also providing a basis for future expansion of the model's capabilities in emission forecasting and scenario building. Although AIS datasets already contain predefined information on ship type, their characteristics can vary considerably. This refers in particular to the ship's dimensions (GT, length), the MCR speed, engine details (power, type, speed), and also to the function of the ship. Thus, the ship type differentiation had to be performed in two steps.

Throughout the analysis of AIS datasets, it was found that most ship types were categorised in general terms (e.g., passenger, cargo, tanker, fishing) without additional information on the function of the ship (cruise ship, Ro-Ro, ferry, etc.). Therefore, as a first step, the ships were divided into specific groups according to their main function. However, large oscillations in technical and engine details were found in some categories. A good example is to compare two cruise ships, one of which had 2995 GT and an ME power of 2460 kW, while the other had 90,940 GT and an ME power of 50,000 kW. To create categories of ships with similar technical characteristics, certain types of ships were differentiated by applying the probability distribution to multiple characteristics that showed significant fluctuations. As a result of the second step, 11 specific ship types were identified based on the collected data:

- Large cruise ships;
- Medium cruise ships;
- Small cruise ships;
- Large Ro-Ro ferries;
- Ro-Ro ferries;
- High-speed craft;
- Excursion ships;
- Fishing;
- Tug;
- Pleasure craft;
- Sailing.

By subdividing categories of ships, it was possible to perform more specific and effective missing-data imputation. In this process, average values from corresponding group of ships were assigned to the features where data was missing. After operating the model, the imputed data displayed low level discrepancy, which allows for a more accurate estimation of emissions, even when all data is not available.

2.6. Emissions Estimation

In the last step of the processing phase, the model uses bottom-up logic where reference points are combined into specific movement trajectories to calculate the complete amount of air pollutants emitted during individual visits to the port basin for each ship included in the study. This way, the model is able to produce detailed estimates for each individual ship with high temporal and spatial density by applying the energy-based emission estimation method. However, throughout the port approach and departure operations, ships have to alter their speed, which leads to a change in the energy output of the engines, and consequently, to a trend in the production of air pollutants. Therefore, in order to estimate emissions based on energy demand, the operating modes with the time spent in them were determined for each trajectory.

2.6.1. Estimation of the LFs and Operating Modes

It is generally accepted that different rates of engines working load have direct impact on internal combustion processes that are responsible for releasing air pollutants into an atmosphere [12,34]. Some studies suggest that engines are the most efficient when operated at around 80% load and are not as efficient at lower loads. This applies in particular to LF of less than 20%, which are normally achieved when ships are preparing to berth or depart and are manoeuvring at low speed. Due to the mentioned low-load effect on engine efficiency, the model recognises three distinct modes of operation: cruising, manoeuvring, and hoteling. As the cruising mode is identified by engine loads above 20% and manoeuvring is defined with LF values that are lower, hoteling operation is considered when the ships have switched their ME off and only use the generators while at berth or at anchor. Since the load of the ME correlates with the speed, the collected AIS and technical data were used in the propeller law method expressed in Equation (2) to estimate LF and define the related operating modes for each trajectory, while the corresponding timestamps were used to calculate the operating time [12,34].

$$LF = (S_A/S_M)^3 \tag{2}$$

where the following definitions apply:

S_A: actual speed of the ship—in knots (kt);

S_M: speed of the ship at MCR—in knots (kt).

Although the workload of the ship's generators corresponds to the specific power requirements of the operating modes, it is not possible to anticipate it through the propeller law or similar methods, which is why the LFs of the AEs are generally vague [22–27]. In the absence of a specific study on AE workloads on ships navigating within the area of interest, static LF values from several large-scale studies and papers with similar traffic and spatial specifications were used [4,17,34].

2.6.2. Estimation of the EFs

As was stated, energy conversion in marine engines is a complex process with a number of variables that directly affect the production of air pollutants and may vary for different gases. Therefore, to calculate exact EFs for particular engines and the fuel they consume in specific operation modes, onboard measurements should be carried out, which requires specific research to be conducted on this topic. Since such studies are financially and logistically costly, the identification of the EFs is the vaguest area in the emission estimation process [12,15,22,23,25–27]. Therefore, in this study, collected technical data was combined with the estimated operating modes in comprehensive methods to determine the corresponding EF and connect them to the relevant reference points. The components used for identifying EFs are listed in Table 1, while the low-load adjustment values for all gases (except for NOx) included in the study were taken from the San Pedro Bay Ports Report and applied when the ships were operating in manoeuvring mode [34].

Table 1. Technical data and operating modes included in the model for EF identification.

EF Components					
Engine Function	**Engine Type**	**Engine Speed (rpm)**	**Fuel Type**	**Mode and LF**	
ME	D	SS D < 300	MDO/MGO	Cruising	$LF \geq 20\%$
AE	GTU	MS D 300–900	HFO	Manoeuvring	$LF < 20\%$
	STU	HS D > 900	LNG	Hoteling	$LF \leq 02\%$
	DF				

Emissions of CO_2 and SOx are directly proportional to fuel consumption. Thus, specific fuel consumption (SFC) load was calculated by applying the method from the third IMO GHG study and baseline values from the recent fourth IMO GHG study, as is shown in Equation (3) [12,35].

$$\text{SFC load} = \text{SFC baseline} \times (0.455 \times LF^2 - 0.71 \times LF + 1.28) \quad (3)$$

where the following definitions apply:

SFC load: SFC at a given engine load—grams of fuel consumed per kilowatt-hour (g/kWh);

SFC baseline: efficient SFC for a particular engine—engine load optimised at 80%.

After determining the SFC of engines under optimal and low-load conditions by applying LF values from 0 to 1, it was possible to determine CO_2 and SOx EF based on fuel usage. However, since the model developed in this study uses an energy-based logic, the methods presented in the fourth GHG study for calculating the EF for the mentioned gases had to be modified. For CO_2, a non-dimensional conversion factor (Cf) measured in g of CO_2 emitted per g of particular fuel consumed was taken from the MEPC.308(73)—2018 EEDI Guidelines [36]. As the Cf corresponds to the fuel used when determining SFC, Equation (4) was established to transfer the CO_2 EF from a fuel- to energy-based measure.

$$CO_2 \text{ EFe} = \text{SFC} \times \text{EFf} \quad (4)$$

where the following definitions apply:

EFe: energy-based emission factor—grams of pollutant emitted per kilowatt-hour (g/kWh);

EFf: fuel-based emission factor equal to Cf—grams of pollutant emitted per g of fuel consumed (g pollutant/g fuel).

As an air pollutant, SOx emissions vary with the sulphur content of the fuel and accordingly to fuel consumption. Therefore, Equation (5) presented in the fourth GHG Study was combined with Equation (4) to convert EFf of SOx to Efe [12].

$$\text{SOx EFf} = 2 \times 0.97753 \times S \quad (5)$$

where the following definitions apply:

S: sulphur content of a particular fuel — grams of pollutant per g of fuel (g pollutant/g fuel)

Since the EU Sulphur Directive applies to the area included in this research, the limit value of 0.1% sulphur content was taken into account when calculating the SOx EF [37]. Emissions of PM are a function of fuel sulphur content, where it is assumed that 97.753% of the sulphur in the fuel is converted to SOx and the rest to sulphate/sulphite aerosol, classified as a part of PM [12]. That is why both S and SFC had to be determined and applied inside Equation (6) to estimate PM10 EFe. Assuming that 92% of PM10 is actually PM2.5, Equation (7) was used [12].

$$\text{PM10 EFe} = 0.23 + \text{SFC} \times 7 \times 0.02247 \times (S - 0.0024) \quad (6)$$

$$\text{PM2.5 EFe} = \text{PM10} \times 0.92 \quad (7)$$

Emissions of NOx, CH4, CO, and NMVOCs vary depending on engine load; therefore, only values for low-load adjustment were used as stated before, without conversion of EF applied for CO_2, SOx, and PM. A set of EFs values for CO and NMVOCs described in the third IMO GHG study are applied, while for CH4, new insights presented in the fourth GHG Study were implemented [12,35]. This applies particularity to LNG fuel used by different marine engines [12]. The values of EFs for NOx emitted by diesel engines are limited by a three-tier system defined in IMO MARPOL Annex VI Regulation 13 (IMO, 2013b), where the EF of each tier is subdivided in relation to engine speed and construction date [38]. Since the NOx control requirements apply to installed marine diesel engines with an output power of more than 130 kW, values from the regulation corresponding to the technical data of ships were used as the NOx EFs in this research.

3. Results

The model performed an estimation of ship-related emissions based on relevant technical details and 49,540,895 AIS reference points that were previously processed with the aim of defining individual movement trajectories with respective operating modes and EFs. By combining the presented bottom-up logic with a relevant energy-based method, the model was able to produce high-density estimates of air pollutants released by individual ships for every port visit in 2019. Emission estimates for each port visit with all relevant features of individual ships are stored and can be handled by the model to generate various analytical results.

According to the processed data from AIS, the number of ships calling at the Port of Split—City port basin in 2019 was 16,429. This number corroborated the port traffic statistics, since the movement trajectories, such as datasets that represent port visits, form the basis for calculating emissions. The quantity of calls identified was found to match maritime transportation data with 100%, 98%, 95%, 96%, and 94% for all types of cruise ships, both types of Ro-Ro ferries, high-speed craft, tugs, and fishing ships, respectively. However, the arrival figures for excursion ships, pleasure craft and sailing ships were reported differently in the various sources of shipping statistics data and could not be compared as the other ship types. There is, therefore, a possibility that the emissions released by the mentioned ship types are greater than estimated in this research. The explanations for the discrepancies mentioned are explained in the section Uncertainties, while the distribution of port calls per ship type determined from the AIS database used in this research is shown in Figure 4.

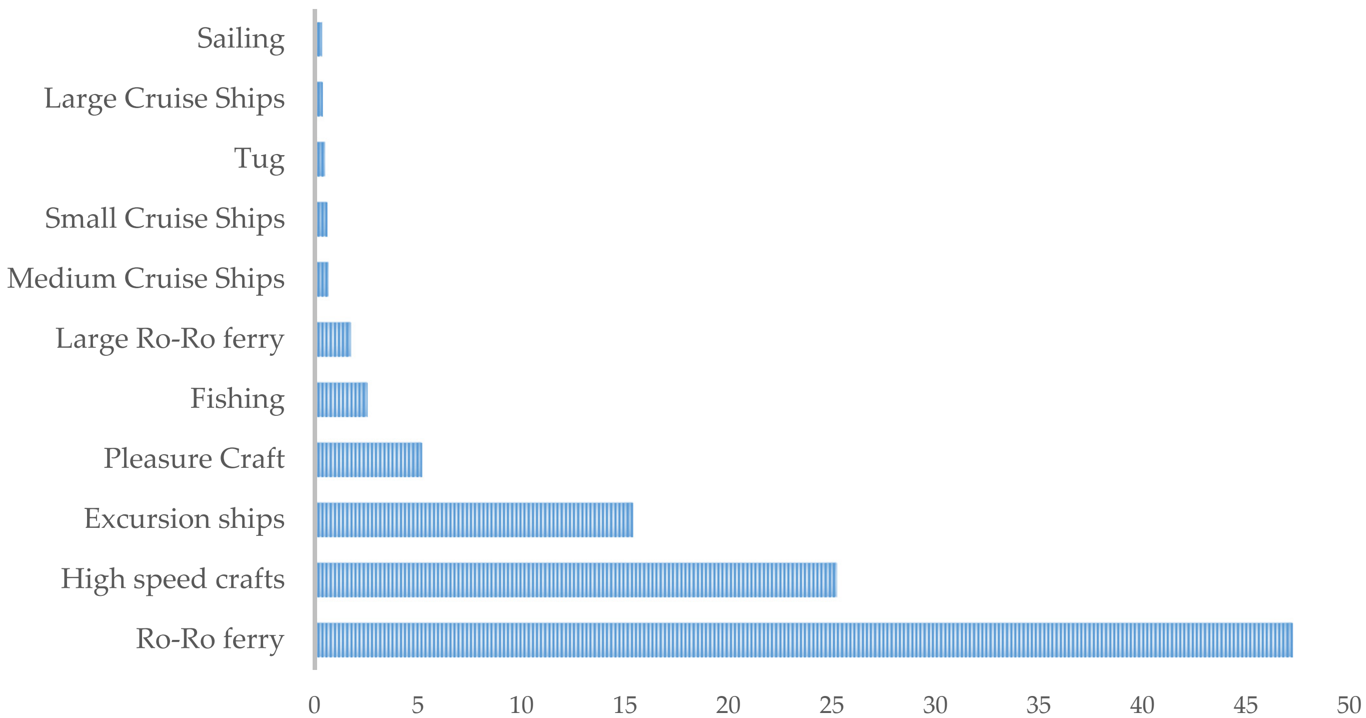


Figure 4. Share of visits to the Port of Split—City port basin in 2019 based on AIS data.

On all included ships, the most common engine type installed is a MS D engine (78%), followed by a HS D (22%) and a LS D (3%). GTU, STU, and DF are fitted on less than 1% of ships and therefore have no significant impact on emissions in the research area. With regard to the presented overview of engine details and the application of the EU Sulphur Directive, it is assumed that the entire fleet uses MDO/MGO with the limit value of 0.1% sulphur content during the entire port call.

3.1. Gas Emissions Quantification

The model was used to create an inventory of air pollutants generated by ships in the defined port area by summing the emissions from each movement trajectory for each ship, then for specific types of ships, and finally for the entire fleet. The annual emissions quantified with the model for the Port of Split—City port basin in 2019 are presented in Table 2 as totals for each ship type and released gas. In the comparison, the emissions per ship type match the distribution of port visits only for Ro-Ro ferries and high-speed craft, while a significant deviation can be observed for the other groups. The reason for this lies in the technical requirements of the propulsion and generator systems on board and the different energy demand of the individual ship types.

Table 2. Annual emissions quantified by the model for the Port of Split—City port basin in 2019 expressed in mt.

Ship Type	GHG		APS					
	CO_2	CH4	SOx	NOx	PM10	PM2.5	NMVOC	CO
Ro-Ro ferry	19,734.524	0.345	11.694	297.449	6.484	5.966	16.857	12.132
High-speed craft	5962.247	0.105	3.533	85.349	1.945	1.789	5.475	5.037
Large Ro-Ro ferry	4697.735	0.088	2.782	86.684	1.619	1.490	4.085	0.698
Large cruise ships	4276.095	0.080	2.532	77.546	1.471	1.354	3.617	0.772
Medium cruise ships	4160.025	0.077	2.464	75.264	1.427	1.313	3.509	0.821
Excursion ships	1431.938	0.033	0.849	26.338	0.526	0.484	1.870	0.836
Small cruise ships	1156.656	0.020	0.685	16.751	0.378	0.348	0.899	0.838
Pleasure craft	525.652	0.013	0.312	11.866	0.203	0.187	0.777	0.173
Fishing	351.700	0.007	0.208	4.610	0.117	0.108	0.350	0.331
Tug	135.243	0.003	0.080	1.770	0.049	0.045	0.167	0.141
Sailing	30.074	0.001	0.018	0.739	0.011	0.010	0.038	0.007
Totals	42462	1	25	684	14	13	38	22

The effects of the different groups of ships on air pollution in the port area are therefore shown in Figure 5. By examining presented overall impact of specific ship types, it can be noted that Ro-Ro ferries contributed an average of 47% of all estimated emissions, while the average share of gases released by high-speed craft is 15%. Large Ro-Ro ferries and large- and medium-sized cruise ships have a general share of 10%, while all other ship types combined are commonly below 10%, leading to the conclusion that their impact on air pollution is of limited importance.

However, the connotations of GHG and APS emissions should be considered separately, as the first group has a global impact on climate change, while the second group poses a direct threat to human health on local scale [39].

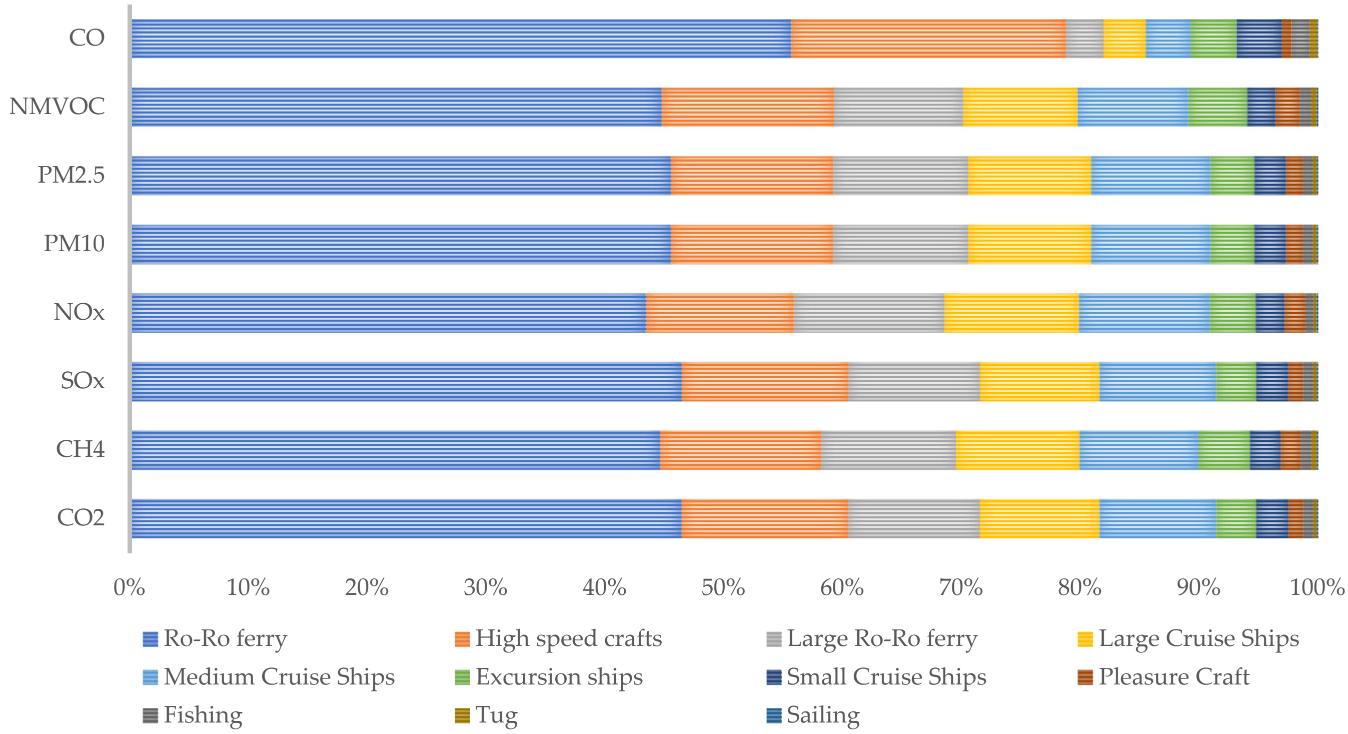


Figure 5. Proportions of emissions produced by different ship types.

3.1.1. Greenhouse Gases (GHGs)

The reason why CO_2 is the predominant GHG in the port area, with a share of more than 99.99%, is due to the almost exclusive use of MDO/MGO by the fleet, which is primarily powered by diesel engines. The amounts of CH4 released annually are therefore insignificant but could increase given the global trend towards the introduction of LNG-powered ships. As depicted in Figure 5, the GHG emissions of Ro-Ro ferries are roughly equivalent to those of High-speed craft, large Ro-Ro ferries, and medium and large cruise ships combined. To mitigate annual CO_2 emissions in the relevant area of the City port basin, the focus should therefore be on operational and technical measures aiming to increase the energy efficiency of ships which contribute most to GHG pollution.

3.1.2. Air Pollutant Substances (APSs)

At 86%, the amount of NOx emitted by ships accounts for the largest share of the total APS released. The cause for the larger NOx levels could be in the engine speed and the age of the fleet, which are particularly high in the most active ship types. Mentioned engine details are directly related to the tier system, which assumes larger EFs, resulting in the amount of emissions stated. The modernisation of liners and the introduction of exhaust gas reduction technologies such as selective catalytic reduction would be beneficial to mitigating overall NOx levels. Annual total of SOx is not severe since the 0.1% sulphur content was applied in the estimation process. However, the specified limit was based on an assumption that entire fleet used low-sulphur fuel for the entire period of arrival, berth, and departure. However, according to the EU Sulphur Directive, fuel changeover is mandatory only after arrival at berth, and since data on the content of the fuel used was limited, it is possible that SOx emissions are higher than estimated through the model [37]. The same conclusion can be drawn for PM 2.5 and PM 10 emissions, as it is assumed that sulphur not converted to SOx is released as PM [12]. As products of incomplete combustion of fuel, both CO and NMVOC are part of the total APS emissions. The estimated NMVOC values correlate with the predominant passenger ship types found in the research area, as this pollutant is generally produced primarily by evaporation from takers [40]. Higher CO emissions, especially for Ro-Ro ferries, can be explained by longer periods of low-load operation associated with the partial combustion process, which indicates the application of a higher EF in the estimation [12].

3.2. Operating Modes and Spatial Distribution

A general overview of the emissions produced in the different operating modes indicates that 59%, 8%, and 33% were released in cruising, manoeuvring, and hoteling activity, respectively. However, this fact varies considerably with the different types of ships, which is shown in Figure 6. On an annual basis, Ro-Ro ferries, high-speed craft, excursion ships, pleasure craft, and sailing ships emitted most of the pollutants during cruising activity. On the other hand, all types of cruise ships and large Ro-Ro ferries produced larger volumes of emissions during the hoteling phase, while for tugs, the manoeuvring mode was dominant.

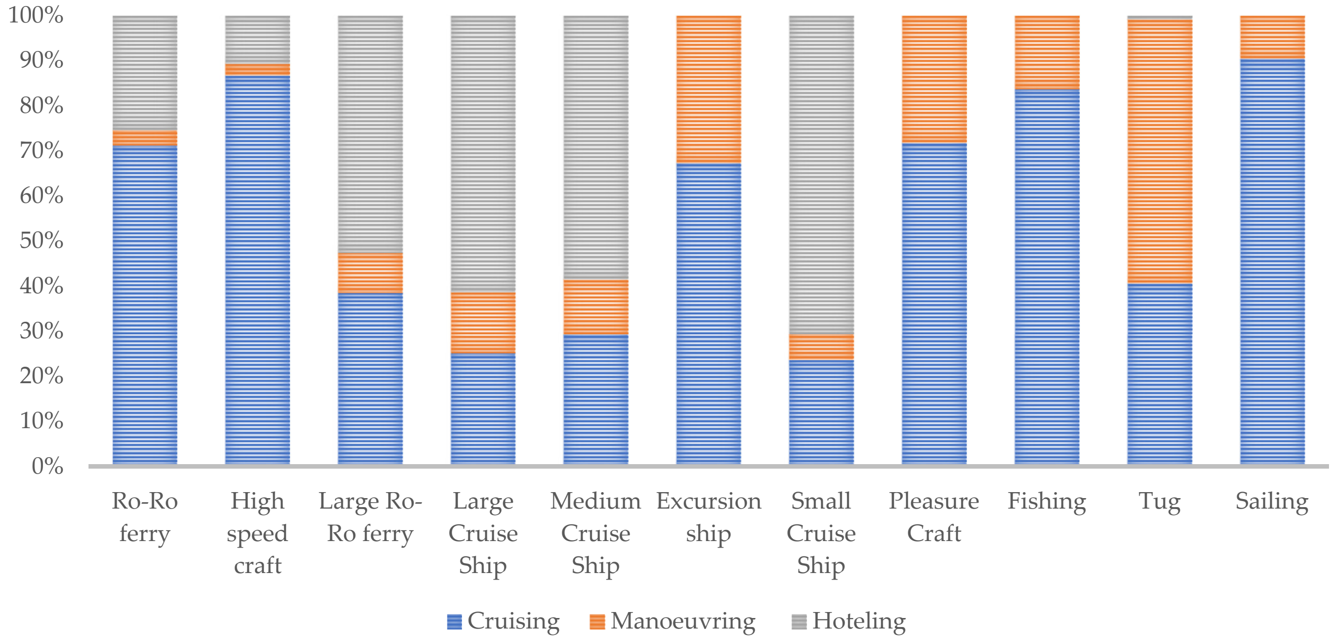


Figure 6. Distribution of quantified emissions released in different modes of operation by ship types on an annual basis.

This insight is particularly valuable for future mitigation planning based on characteristics associated with a particular operating mode. It is also important to note that APSs emitted near urban areas have a greater impact on local air quality. That is why the model was used to produce the unique high-density spatial distribution of emissions based on activities to provide an overview of the main air pollution dispersion points quantified on an annual basis for each type of ship, as is depicted in Figure 7. The figure shows that 59% of emissions released in cruising activity are within a radius of 13 NM, while 41% (manoeuvring and hoteling emissions combined) are mostly concentrated in an area with a maximum distance of 0.5 NM from the city centre.

The divergence found between the points of emission generation for different modes for Ro-Ro ferries and large cruise ships is shown in Figure 8 with a radius of 1 NM from the spot where most emissions are released. This map shows even more detailed information about the air pollutants released, as it displays the total values for each visit with a colour scale, where green stands for lower emissions and red for higher emissions, revealing the proximity of air pollution production points to the populated area. In addition to the aforementioned difference between emission production in various modes, the variance in the emission quantities released by two types of ships is also shown. For example, the legend in the top right corner of the map suggests that large cruise ships released anywhere from 35 to 45 mt of air pollutants in hoteling, while Ro-Ro ferries released 1.2 mt while operating in cruising mode.

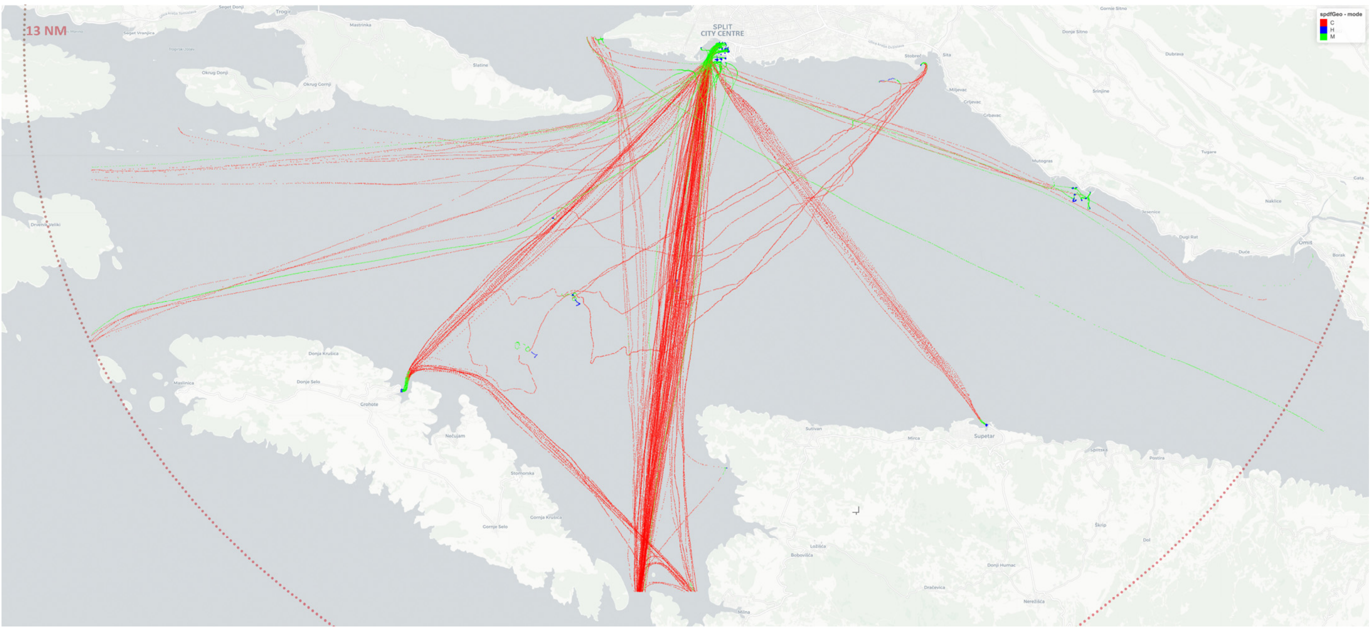
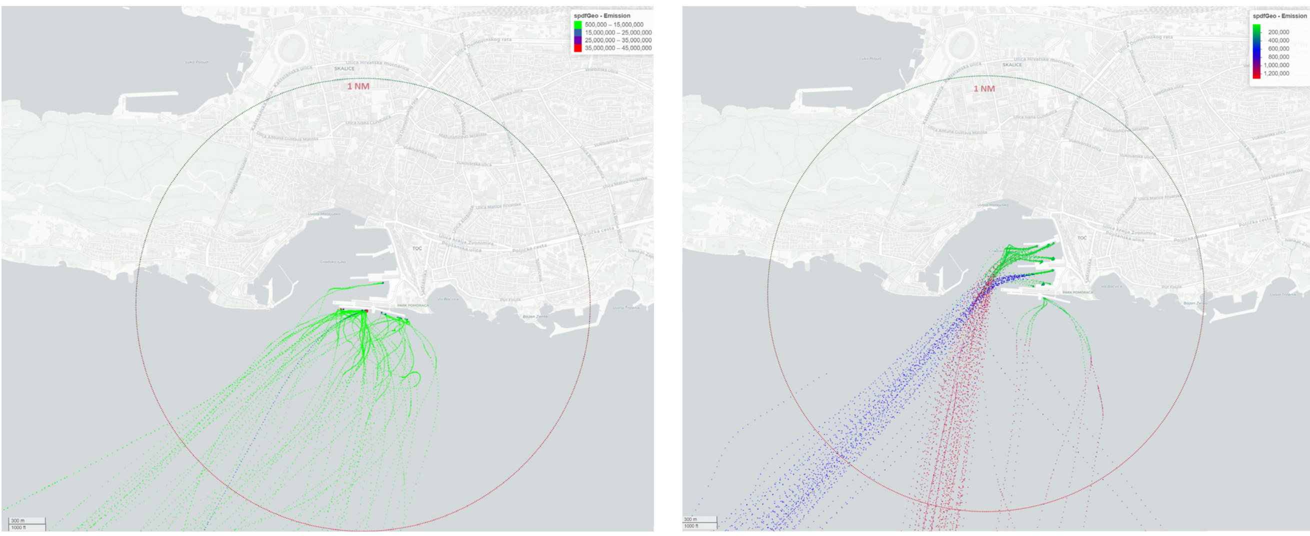


Figure 7. Activity-based ship emissions spatial distribution map. As can be seen from the activity-based ship emissions spatial distribution map, the distances between the emission dispersion points and the populated area are not great. All cruising dispersion points marked in red colour are located within a radius of 13 NM from the city centre, while most of them start at a distance of 11.5 NM and 9 NM. The proximity to the urban area applies in particular to the emissions released in the manoeuvring and hoteling phases, displayed in green and blue, respectively, as they are concentrated in an area with a maximum distance of 0.5 NM from the city centre.



(**a**) (**b**)

Figure 8. Activity-based ship spatial distribution map of emission sums (in g) per port call for a period of one month (October) with radius of 1 NM from the point where the largest levels of emissions are released: (**a**) large cruise ships, (**b**) Ro-Ro ferries.

3.3. Temporal Distribution—Seasonality

The increased demand for shipping services is strongly connected to the tourist season, as this industry is a major source of income for the local economy. Therefore, a higher volume of emissions was generated during the summer months, which correlates with seasonal traffic intensity. Since the different types of passenger vessels are predominant in the transportation mix, both GHG and APS production show almost the same trend, so their temporal distribution over the twelve-month period with annual average for 2019 is shown in Figure 9. It can be observed that there is a particular difference between months in which the average emissions were significantly exceeded and those in which they were approximately the same or lower. In this case, the months in which the recorded values are above average individually had emissions more than twice as high as months from the rest of the year. This difference is particularly significant for July, when emissions are generally three times higher than those estimated for January, February, March, November, or December, and almost double the annual average of 3605 t.

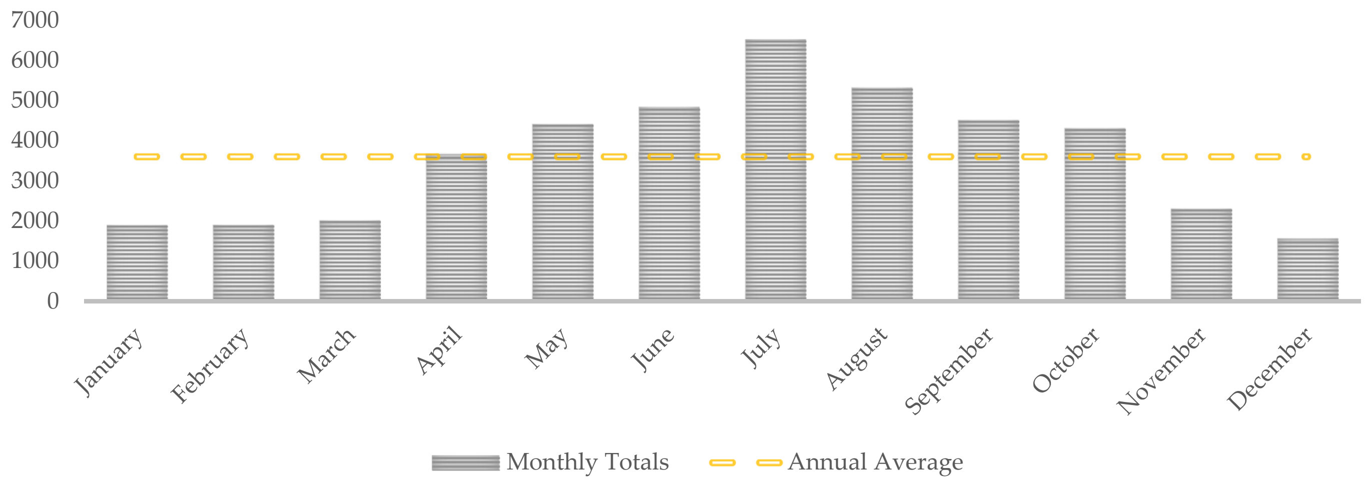


Figure 9. Temporal distribution of emission totals based on monthly fluctuations and the annual average for 2019 in mt.

Based on the analysis of intra-month variations, we propose considering two annual periods: a season when emissions are higher than the annual average and an off-season when emissions are low or close to average. Considering this, emissions are expected to increase with projected demand from tourism and shipping industry, resulting in higher concentrations of APSs in a shorter timespan, elevating the risk to the health of local population. Therefore, optimisation of emissions at peak periods should be considered, with the goal of achieving moderate values closer to the annual average.

3.4. Uncertainties

The uncertain aspects induced in this research that directly affect the level of estimated emissions are addressed in the relevant chapters. However, to provide a better overview of the unclear elements, they are examined in the following subsections.

3.4.1. AIS Data

Since the IMO Regulation V/19 states that not all ships are required to have AIS on board, a proportion of marine traffic remains invisible [1]. As this applies in particular to smaller ships that have only a minor impact on air pollution, it is assumed that the emission totals are not significantly higher. However, the technical and human errors that usually occur when the AIS is operated can lead to data loss during transmission/storage or to erroneous values which were filtered out of the database used for emission calculation. Thus, in this research, port calls estimated based on AIS data have been cross-checked with shipping statistics databases where applicable. It is therefore possible to assume emission levels based on the difference between port calls and add them to the calculated totals.

3.4.2. Unknown Technical Details

The imputation of missing data was based on linking ships with an incomplete data set to the corresponding ship type and calculating average values for attributes with unknown information. This procedure was applied to all ships whose technical data were incomplete. Since the databases used in this research contained, on average, less than 10% of unknown information on technical characteristics per ship type and a specific differentiation of ship types was made, the imputed data show little differentiation.

3.4.3. LFs

While the LFs of the MEs were calculated on the basis of the propeller law, the same method was not applicable for estimating the workload of generators. As there was no research or database that would provide values on LFs of AEs operated in interest area, static values from several large-scale studies and papers with similar traffic and space specifications were used for the workload values of the AEs.

3.4.4. Fuel Composition

Even when the fuel type used by ships in the navigating area is known, the composition of the fuel may vary for each supply of the same product. Therefore, fuel composition assumptions were made based on the regulations in force in the research area and the details of the engine.

3.4.5. EFs

As the most complex feature that is dependent on both technical and movement characteristic, EFs can be described as the component with the highest level of uncertainty. Since the specific research on EFs involving accurate data on the engine details, fuel composition, and its consumption or workload in specific mode was not conducted on the ships operating in the research area, the EFs values have been calculated on the basis of comprehensive methods applied to the collected data.

3.4.6. Weather Conditions

Sea and air temperature, wind, currents, and wave force and direction can significantly affect fuel consumption/engine load, leading to a change in EF values and consequently emissions released by the ship. As the vessels operating in the area included in this research do not navigate in extreme weather, the influence of the mentioned conditions is limited. Also, LF values for AEs are assumed based on temperature fluctuation between warmer and colder periods, which is specifically important for passenger ships [4]. However, in future work, and for different areas, the model should include meteorological data.

4. Discussion

The annual inventory of emissions released by ships in the relevant port area, produced by the model developed in this research, provided an overview of technical, temporal, spatial, and operational aspects. Presented results are based on calculations applying relevant methodologies to a large AIS database and detailed technical data, and thus can be used for establishing broad guidelines for emissions management in port.

However, mentioned insights have a general standpoint and as such do not include the aspect of equivalence between the emission-related characteristics of different ships or port areas. For example, Ro-Ro ferries were identified as the ships that emit the greatest amount of air pollutants overall, especially when operating in cruising mode. To achieve this, they had to account for almost 50% of the total port visits. On the other hand, large cruise ships released more than four times less emissions, most of them in the hoteling phase, but only for a fraction of the total arrivals. The difference in emission production and quantities also varies with the observed period and changes the proportion of air pollutants released between the ships. In order to introduce strategies for control of the emissions, all aspects must therefore be examined and considered, which can be a computational and time-consuming process as large databases and connections between different factors need to be analysed.

Furthermore, the volumes of calculated emissions are not comparable, even for the same ports, as the inventories often apply different methods and datasets for emission calculations [15]. A comparison of the gas volume would therefore not describe the relationship between the measurements in a meaningful way [15]. Even if the same method was used in the same area of interest, all factors and datasets used for the calculations must be consistent in order to obtain comparable emission results [15]. The most obvious examples of the discrepancies mentioned can be found in the values for gas types, ship types, EFs, LFs, or transit distances [15].

The lack of specified comparability between ships and ports is common in emissions inventories aggravates the process of an appropriate assessment of insights into the production and effects of air pollution from ships [15]. Therefore, the introduction of a scalable system based on the analysis of emissions-related data from inventories could provide a more transparent and efficient overview of the important characteristics of air pollution from ships and port areas. The application of the above system may serve as a coherent framework for the control of air quality in port communities.

Since the model presented in this research already integrates a large database of emission features with calculated results, it is possible to extend its capabilities by including a comparison logic in future work.

5. Conclusions

In this research the analytical model for estimation of ship-sourced emissions was developed and used to produce an inventory of combustion gases released in the area relevant to the Port of Split—City port basin for 2019. To estimate emissions of GHGs and APSs, technical details and ship movement data from AIS were integrated inside the model where bottom-up logic with an energy-based method was applied. Therefore, to obtain a high-density overview of emissions, the modelling was carried out using three main interconnected components.

First was the preprocessing segment, where the technical and AIS datasets were prepared by applying conversion, cleansing, filtering, formatting, and merging techniques to create the specific data arrangement of features relevant to the ship-based emission estimation.

In the second, the processing component, unique categories of ship types were defined based on different classifiers to ensure a more accurate and effective imputation of missing data, while also providing the background for a future extension of the model's predictive capabilities. Estimates were then made of the GHG and APS quantities released for all ships recorded in the AIS database for the year 2019 within the research area.

Finally, the results produced by the model show that 42462, 1, 25, 684, 14, 13, 38, and 22 mt of CO_2, CH4, SOx, NOx, PM10, PM2.5, NMVOC, and CO were emitted from ships in the relevant area of the Port of Split—City port basin, respectively. It was noted that most annual emissions are generated during the tourist season, as this period has the highest frequency of port calls. Because of the high arrival rate, Ro-Ro ferries were identified as the ship type that emitted the largest amount of air pollutants, while C activity was the dominant mode of operation for emission production overall.

Emission estimates with all datasets containing information on characteristics that are important for the production of air pollutants are stored and can be handled by the model to generate various analytical results. Therefore, the model was able to produce detailed inventory and reports with various statistical features that can be used by experts and decision-makers for managing emissions in port areas. Furthermore, as the structure of the model's components is flexible and an adaptable approach to database imputation is taken, it is possible to extend its potential by pursuing the following:

- Modelling emission estimates for different port areas by integrating location-specific AIS data and technical details of related ships.
- Applying new insights, mainly named in the chapter on uncertainties, to the production of combustion gases from marine engines with the aim of obtaining even more accurate calculations.
- Introducing a scalable system to provide a more transparent and efficient overview of the important characteristics of air pollution from ships and port areas.
- Extending predictive capabilities by relying on large shipping databases to create scenarios for the future development of air pollution from the fleet in a specific port area.

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A Comprehensive Model for Quantifying, Predicting, and Evaluating Ship Emissions in Port Areas Using Novel Metrics and Machine Learning Methods

Filip Bojić *, Anita Gudelj and Rino Bošnjak

University of Split, Faculty of Maritime Studies, 21000 Split, Croatia; anita@pfst.hr (A.G.); rinobo25@pfst.hr (R.B.)

* Correspondence: fbojic@pfst.hr

Abstract: Seaports, as major transportation hubs, generate significant air pollution due to intensive ship traffic, directly affecting local air quality. While emission inventories are commonly used to manage ship-based air pollution, they reflect only the emission-related aspect of a specified period and area, limiting the broader interpretability and comparability of the results. To overcome the mentioned challenges, this research presented the PrE-PARE model, which enabled the prediction, analysis, and risk evaluation of ship-sourced air pollution in port areas. The model is composed of three interconnected modules. The first was applied for quantifying emissions using detailed technical and movement datasets, which were combined into individual voyage trajectories to enable a high-resolution analysis of ship-based air pollutants. In the second module, the Multivariate Adaptive Regression Splines (MARS) machine learning method was adapted to predict emissions in varying operational scenarios. In the third module, novel metric methods were introduced, enabling a standardised efficiency comparison between ships. These methods are supported by a unique classification system to determine the emission risk in different periods, evaluate the intensity of various ship types and rank individual ships based on their operational efficiency and emission optimisation potential. By combining new methods with technical and operational shipping data, the model provided a transparent, comparable, and adaptable system for emissions monitoring. The results demonstrate that the PrE-PARE model has the potential to improve strategic planning and air quality management in ports while remaining flexible enough to be applied in different contexts and future scenarios.

Keywords: Sustainable shipping; Air pollution; Metric system, Machine learning, Risk assessment

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1. Introduction

To keep in line with the Paris Agreement, in 2023 the International Maritime Organisation (IMO) reinstated the Initial Strategy on the reduction of greenhouse gases (GHG) with a more ambitious Strategy aiming complete decarbonisation of ships by or around 2050 [1,2]. However, emissions released by ships are continuously rising. The 4th GHG Study showed the significant increase in GHG emissions from international shipping, which reached a share of 2.9 % of global anthropogenic GHG pollution [3]. Future projections for shipping's GHG emissions also do not support the process of full decarbonisation, as global maritime trade continues to grow, the sector is still heavily reliant on fossil fuels and regulatory standards lag far behind those that apply to other modes of transport [3,4]. Although the IMO has not yet adopted reduction requirements that would unequivocally cut down emissions, the implementation of global compulsory technical and operational measures coincide with the reduction in the carbon intensity of ships, which in 2018 is on average 20 to 30 % lower compared to the base year 2008 [3–5].

The first of these requirements to enter into force in 2013 were the Energy Efficiency Design Index (EEDI) and the Ship Energy Efficiency Management Plan (SEEMP) as part of the International Convention for the Prevention of Pollution from Ships (MARPOL) Annex 6, Chapter 4 [6,7]. SEEMP is a framework designed to support ship owners in improving the operational efficiency and carbon intensity of their fleet [7–9]. Divided into three parts, the recent guidelines include a plan to improve energy efficiency (through hull and propulsion maintenance, use of automated engine management, voyage planning, weather routeing, speed optimisation, etc.), a plan to record fuel oil consumption and methods for monitoring ship's carbon intensity [7–9]. The EEDI is a mandatory measure that sets minimum energy efficiency requirements for newly built ships of 400 GT or more for the international voyage [7,10]. The EEDI is determined by combining parameters from the fuel-based method for emission estimation, such as the power of the engines, their specific fuel consumption and the carbon content of the fuel consumed in relation to the ship's capacity and different correction factors corresponding to the specific type of ship and the energy-efficient technology installed [11]. The idea behind the EEDI was to encourage ship owners to apply efficient technical solutions to improve the fuel efficiency of a ship at the design stage [5,7]. The CO2 reduction level (grammes of CO2 per tonne-mile) for the first phase was set at 10% compared to a reference line calculated from the average efficiency of ships built between 2000 and 2010 and will be increased every 5 years [7]. In the meantime, MARPOL Chapter 4, including the SEEMP and the EEDI, has been extended and improved with additional requirements to try to achieve the objectives set out in the Strategy. Accordingly, in 2023 it became mandatory for relevant ships to calculate their achieved Energy Efficiency Existing Ship Index (EEXI) and to initiate data collection for reporting of annual operational Carbon Intensity Indicator (CII) and the associated CII rating [7,9,10]. The EEXI achieved by a ship indicates its energy efficiency compared to a baseline value. The obtained EEXI is then compared to a required value based on an applicable reduction factor expressed as a percentage relative to the EEDI [12,13]. This index must be calculated for in-service ships of 400 GT and above according to the different values for ship types and size classes, using a method based on the EEDI guidelines [7,13]. The calculated attained EEXI value for individual ship must be below the required EEXI to ensure that the ship fulfils a minimum standard for energy efficiency [7]. As one of the recent monitoring mechanisms included in the SEEMP, from 2024 the CII must be calculated for ships of 5,000 GT and above and reported together with the aggregated data for the previous year [14]. The CII measures the efficiency of a ship in transporting goods or passengers and is expressed as the mass of CO2 emissions emitted relative to capacity/size and distance travelled [15]. Based on their efficiency, ships are given an environmental rating from A as the best to E as the worst performance level [16]. The annual amount of CO2 released by ships is calculated by applying the fuel-based method, in which the total mass of fuel used is multiplied by the corresponding carbon content, while the transport work can be estimated by combining various factors depending on the type of ship and the available data [17]. Therefore, IMO proposed several indicators for determining transport performance such as Annual Efficiency Ratio (AER), cgDIST, Energy Efficiency Operational Indicator (EEOI) [3,9,17].

Although it is expected that the implementation of all the above measures will further improve the efficiency of the global fleet and reduce its carbon intensity, there are still major limitations in terms of both technical and monitoring requirements. While the 4th IMO GHG study has shown a decrease in the carbon intensity of international shipping on the AER, research conducted by CE Delft has indicated that this reduction is mainly influenced by high fuel prices and freight rates [18]. Costs and demand in the shipping market have a direct impact on orders for fuel-efficient hulls and the number of new-builds, but also on fuel-saving measures [18]. According to the study by the International Council on Clean Transportation (ICCT), the EEXI would only reduce CO2 emissions from the 2030 fleet by 0.7% to 1.3% compared to a baseline, as low-speed transport would continue to predominate [19]. The EEXI/EEDI will not directly reduce fuel consumption and CO_2 emissions if ships already operate slower than the speed limit proposed in the IMO requirements [19]. This means that the effectiveness of technical efficiency measures like the EEXI need to be evaluated against real-world conditions [19]. Mentioned conclusion implies not only the weakness of regulatory standards, but also of the approach based on vessel design and theoretical emission parameters rather than real operational data [20–22]. Also, even though the calculation method for the CII should include the annual amount of fuel consumed, the time spent at berth and/or anchorage is not considered, which can lead to inconsistencies in the final categorisation of the ships. This applies in particular to ship types that frequently operate within port areas, such as cruise ships, container ships, ro-ro ferries, etc. [23]. In addition, the Strategy on reduction of GHG emissions and all the current technical and monitoring mechanisms on which it is based focuses only on CO_2 and is not accounting other exhaust gases [1,9,10]. Due to their contribution to global warming, black carbon (BC), nitrous oxide (N_2O) and especially methane (CH_4), as a gas that has 84 times greater potential than CO_2 to trap heat in the atmosphere over a 20-year period, should also be included in the Strategy and all associated requirements [24,25] .

But more importantly, GHGs are only part of the problem. Throughout the internal processes of energy conversion and combustion, marine engines also discharge nitrogen oxides (NOx), carbon monoxide (CO), sulphur oxides (SOx), particulate matter (PM), and volatile organic compounds (VOC) recognised as one of the main air pollutant substances (APSs) [26,27]. The presence of mentioned pollutants in the atmosphere and their uptake by humans can cause mortality as well as diseases such as pneumonia, ischaemic heart disease, chronic obstructive pulmonary disease, lung cancer, and stroke [28,29]. Diverse health problems can occur with both short- and long-term exposure, especially to PM, CO, ozone (O_3), NOx and SOx [28,29]. Because of the direct interaction between the shipping sector and port cities, the local urban environment is directly exposed to negative effects of air pollution. The impact on the environment and the deterioration of air quality can be severe along coastal zones and especially near seaports, as these areas are usually characterised by heavy shipping traffic [30,31]. Given the fact that 90% of European ports are spatially connected to cities, the extent of the deterioration in air quality is even more serious [32,33]. To monitor emissions at national level, all countries in the European Union (EU) are required to provide GHG inventories to European Environment Agency (EEA) in accordance with the Intergovernmental Panel on Climate Change (IPCC) guidelines [33–36]. However, mentioned inventories are only supposed to include GHGs, and emissions from maritime transport, particularly in port areas, are still not required to be specified.

Considering the realistic need to obtain a better insight into air pollution from the maritime sector, establishing shipping emission inventories for seaports is recognised by both the port and scientific communities [30,33,37–41]. Port-related ship emission inventories are generally conducted by combining either a top-down or bottom-up approach with a fuel or energy-based method to determine the quantity of pollutants emitted in a given period [37]. But to calculate the amount of emissions with higher accuracy, a bottom-up energy-based method should be applied to large datasets that contain both technical and movement data of ships [37]. Basic technical details should include information on the type of vessel, dimensions, identifiers and engine specifications regarding type, power and speed. Movement data is generally gathered from the Automatic Identification System (AIS) and provides near real-time information on the vessel's position, actual speed and course with corresponding timestamps. As the mentioned approach is data-excessive, it can provide detailed overview into various aspects of ship-based emissions that can be used to establish guidelines for emissions management in particular ports.

However, mentioned insights have a temporal and location-specific standpoint and as such do not include the aspect of equivalence between the emission-related characteristics of different ships or port areas. A systematic review of the literature on port-related ship emission inventories has shown that the quantity and type of emissions in all analysed works were not comparable between or even for the same ports due to the inconsistency of data used [37]. Emission-related factors such as the types of pollutants included, diverse technical and movement data between ships or the area and time frame covered vary with each calculation and are specific to individual inventories [37]. Furthermore, estimated emission quantities alone do not provide sufficient data to unconditionally categorise air pollution intensity between ships or the impact on overall pollution over different time periods [33]. In other words, without a standardised scaling system and corresponding baseline values that would allow a comprehensive comparison of emission levels between ships and overall traffic in different time windows and locations, it is difficult to determine whether a ship, a group of ships or even an entire port area is efficient or rather an excessive polluter. To predict the risk of air pollution from ships and introduce strategies for its control, all aspects must be examined and considered, which can be a computational and time-consuming process as large databases and connections between different factors need to be analysed and compared [33]. The introduction of a scalable system based on the analysis of emissions-related data from inventories could provide a more transparent and efficient prediction and evaluation of air pollution intensity of ships and port areas.

That is why the aim of this research was to develop a unique metric, scaling, classification and ranking methods implemented inside a novel model for predicting and evaluating the air pollution risk and efficiency of different ship types and overall marine traffic in port areas. The port-related emissions prediction, analytics and risk evaluation (PrE-PARE) model presented in this research is therefore based on new emission evaluation approach and machine learning methods applied to actual ship technical and activity data with the goal of creating an adaptable, relevant, and transparent overall system for calculating ship-related emission and classifying the level of risk for port areas in standardised manner. In the first of three main modules, the collected shipping data was prepared and used within bottom-up and energy-based methodologies to estimate emissions with high temporal and spatial density. Upon the analysis of the results, a Multivariable Adaptive Regression Spline (MARS) approach was adopted in a second module and applied to the processed datasets to assess the influence of emission-related factors and predict the levels released in various scenarios. Finally, the implementation of the novel metric, scaling, classification and ranking algorithms enabled standardised categorisation of the air pollution efficiency and impact, and the temporal risk level evaluation of emitted emissions. By integrating high-resolution technical and operational data with novel metrics and machine learning methods, the proposed PrE-PARE system enables accurate scenario-based forecasting under varying traffic conditions, along with comprehensive, comparable, and scalable evaluation of ship performance and port-wide pollution risk. Although the logic of the PrE-PARE system differs from ambient air monitoring frameworks like the European Air Quality Index, the underlying ambition is similar, to establish a clear, interpretable, and quantifiable basis for evaluating pollution focused specifically on ship-based emissions in port areas [42,43]. By providing ship air pollution quantification, predictive capabilities, and novel evaluation metrics, the proposed framework pushes the boundaries of current practice in ship emissions assessment and aligns with broader interdisciplinary goals in maritime policy and urban air quality management. As this paper is part of a larger research project that continues the work presented in a systematic review and the article on an analytical model for estimating ship-related emissions in port areas, the Port of Split and the corresponding emissions-related data were used as a case study [33,37].

2. Materials and Methods

In contrast to the carbon efficiency and intensity indicators proposed so far, the PrE-PARE model is based on bottom-up approach and energy-based method that combines the energy output with the related emission factor (EF) and time, what provides more realistic results for the calculated emissions and the corresponding air pollution metrics of ships. As the approach described above enables the estimation of emissions for each voyage of a ship based on technical details and operational data derived from the AIS, the emission impact and efficiency in different operating phases, including idle times, could be determined. Cruising, manoeuvring, and hoteling are modes of operation that correspond to the relevant workload of a ship's engines and are often performed differently between ship types or individual vessels. These ship-specific operational patterns directly affect the production of emissions and related impact. Since the model incorporates detailed emissions-related data, it was possible to determine the operational and air pollution profile of individual ships in different segments of voyage. This feature is a key component for predicting future emissions in different scenarios and consistently determining the associated air pollution impact and efficiency through metric algorithms, not only for individual ships, but also for groups of ships with similar characteristics classified into ship types. The calculation of emissions was therefore carried out according to the bottom-up principle, i.e. for each segment of the voyage and then totalled for the ship, the associated ship types and the entire port area in the assigned period. However, the air pollution risk assessment was first carried out for complete shipping traffic by applying a classification system to determine whether the impact in the port area is very low, low, moderate, high or very high. If the system classifies the risk as high or very high, the emission intensity of the group of ships and the optimisation potential of the individual ships are determined by applying the feature scaling method to the calculated values to finally rank the ships by their emission performance.

To perform the entire process, the model consists of three complex and interconnected modules, depicted within Figure 1. In the primary module for quantifying and analysing emissions, the collected technical and movement data were initially prepared with the aim of defining the voyage trajectories of each port arrival, stay and departure for individual ships. These voyage datasets along with specific differentiation of ship types, enabled not only a high-density estimation of the air pollutants released by the individual ships together with various analytical results, but also provided a basis for the extension of the model's forecasting capabilities. Therefore, in the second component, machine learning algorithms were applied to the previously processed extensive technical and operational data to create a predictive module. Since the respective voyage trajectories of the individual ships represent complex data clusters that contain important factors influencing emission production, a Multivariable Adaptive Regression Spline (MARS) approach was adopted in this research to determine the effects of included factors and predict the emission quantities released in different scenarios. To evaluate the performance of the predictive module, ten runs of k-fold cross-validation were performed, with additional validation by comparing the predicted and actual results based on unseen data. The final component of the model is based on the data generated by the two previous modules and includes methods for assessing the emission intensity of ships, operational efficiency and the temporal risk of air pollution. This has been achieved through the integration of novel metrics, scaling and risk classification and ranking approaches, resulting in a transparent, comparable and efficient overview of ship-based air pollution impact in port areas. Since, the system does not only focus on carbon pollution but also includes the leading GHGs and APSs, it was able to calculate and evaluate risk of shipping emissions for CO_2 and CH_4 as GHGs and SO_x, NO_x, PM_{10}, $PM_{2.5}$, NMVOC, and CO as APSs for each ship, a group of ships and an entire port area.

Given the basic components of the model are derived from universal characteristics that significantly influence emissions production, the model is therefore not limited to a single case study but can be applied to different ports. In addition, the modular structure of the model facilitates the integration of new insights and other relevant aspects of port-related shipping emissions, thereby improving the quality and scope of the final output. It is important to emphasise that algorithms embedded in the PrE-PARE model and the data-handling were produced with the software package RStudio 2023.09.1+494.

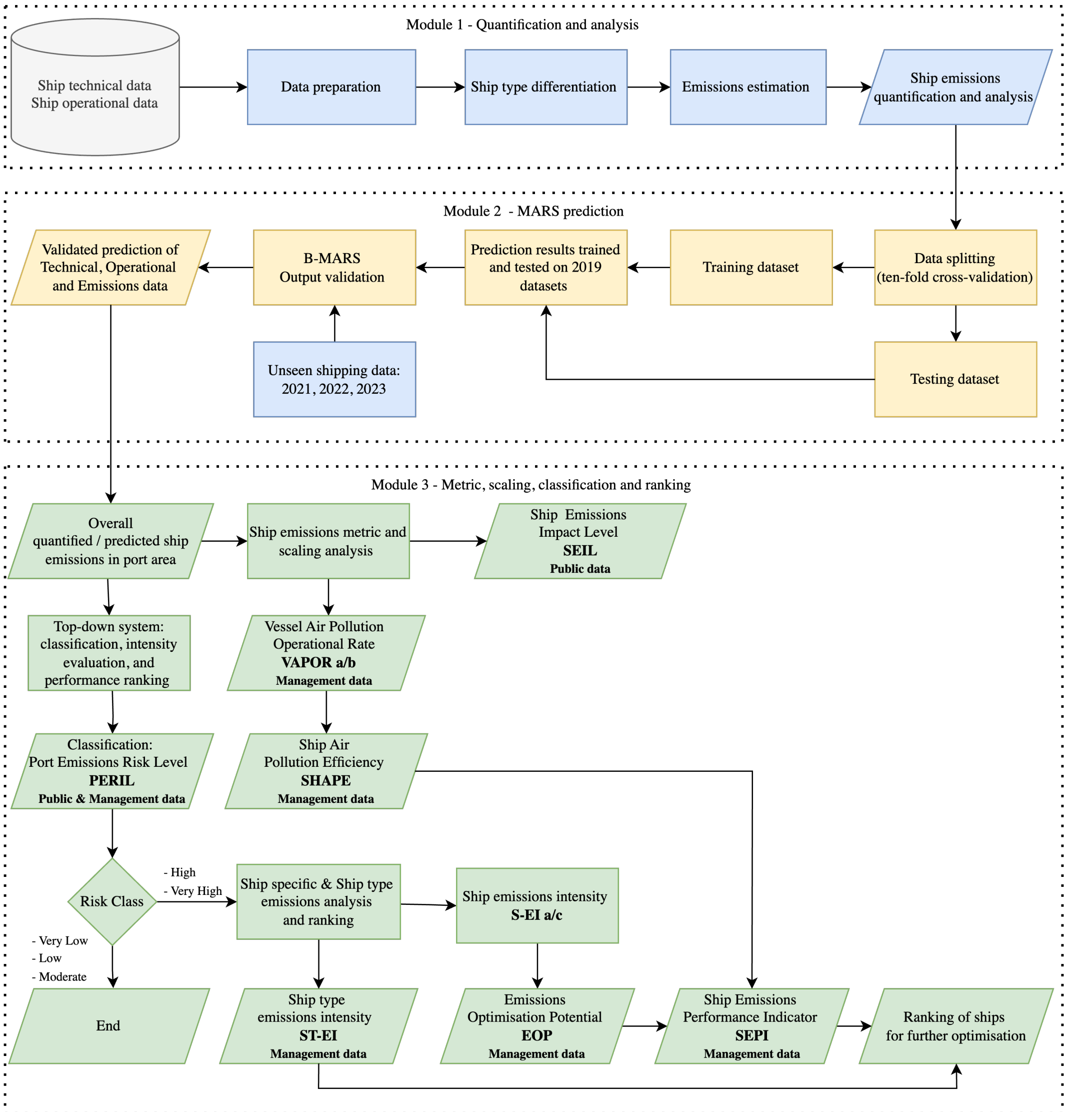


Figure 1. Flow diagram of the PrE-PARE model.

2.1. Emissions estimation and anlayisis module

As it was stated, this paper builds on earlier work by the authors, in particular a systematic review and an article on an analytical model for estimating ship-related emissions in port areas [33,37]. The model presented there served as the initial module, which was adapted and integrated with novel predictive and, risk evaluation and metrics modules to form the PrE-PARE system. While the full details of this component and its methodologies are discussed at length in the cited papers, a summary is provided in this chapter to ensure a comprehensive understanding of the system introduced in this study [33].

The estimation and analysis module was therefore able to produce an inventory of ship emissions for large port areas, providing a detailed overview of technical, temporal, spatial and operational aspects. To obtain the emission-related analytical results, the module integrates three main components [33]. In the initial phase, the technical and AIS datasets were pre-processed by applying conversion, cleansing, filtering, formatting and merging methods. These steps were essential to configure the collected data so that it was suitable for calculating emissions through the module. The technical data recorded relate to the gross tonnage (GT), length, breadth, year, main engine (MA) power, auxiliary engine (AE) power, engine type, engine speed, fuel type, sped at maximum continuous rating (MCR) and the relevant emission mitigation technology. The activity data derived from the AIS comprised 49,540,895 reference points, which were linked to the above-mentioned technical details of the corresponding ships via name, type and MMSI number as identifiers [33].

This was followed by the differentiation of ship types and the estimation of emissions during the processing phase. To create categories of ships with similar technical characteristics, data on the function of the ship and details on ship dimensions, speed and engines were considered. When certain ship types showed significant variations in some features (e.g. engine power), a probability distribution was applied to obtain more specific categories, eventually resulting in identifying 11 ship types:

- Large Cruise Ships
- Ro-Ro ferry
- Large Ro-Ro ferry
- Small Cruise Ships
- Medium Cruise Ships
- High speed crafts
- Excursion ships
- Tug
- Pleasure Craft
- Fishing
- Sailing

Differentiating vessel types based on multiple characteristics improved the accuracy and efficiency of imputing missing data while providing the groundwork for the predictive capabilities of the next module [33].

In the second step of the processing phase, the bottom-up approach was applied, where reference points that contain technical and operational data are combined into specific movement trajectories. Then the energy-based method, which meets the requirements of the IPCC guidelines and is expressed in Equation 1, was used to calculate the total amount of air pollutants emitted during individual port call for each ship [34]. Since altering speed during port approaches leads to change in energy output and consequently emission production, three operating modes (cruising, manoeuvring and hoteling) with the time spent in them were determined for each trajectory [44]. It was done so by estimating workload of propulsion engines known as load factor (LF) through propeller law method expressed in Equation (2) [44]. As the cruising mode is identified by engine loads above 20% and manoeuvring is defined with LF values that are lower, hoteling operation is considered when the ships have switched their ME off and only use the generators while at berth or at anchor [27]. Subsequently, calculations were performed to estimate the quantities of greenhouse gases and air pollutants emitted by all vessels documented in the AIS database for the year 2019 within the study region.

Lastly, the output data was stored and handled with the goal of producing spatial and temporal visualisations of shipping emissions as well as a detailed overview of various technical and operational aspects [37].

$$E = (P_{ME} \; x \; LF \; x \; EF_{ME} + P_{AE} \; x \; LF \; x \; EF_{AE}) \; x \; T \; x \; CF \qquad (1)$$

where the following definitions apply

E: Emissions quantity by mode for each ship call—in grams (g);
$P_{ME/AE}$: total power of main engines/auxiliary engines—kilowatts (kW);
LF: load factor expressed as actual engine work output—as a percentage of engine power (%);
$EF_{ME/AE}$: emission factors of different pollutants in regard to engine function, Engine type, fuel type, and installation year—in grams per kilowatt hour (g/kWh);
T: time spent in a certain movement activity—in hours (h);
CF: correction factor for emission reduction technologies—constant.

$$LF = (S_A/S_M)^3 \qquad (2)$$

where the following definitions apply:

S_A: actual speed of the ship—in knots (kt);
S_M: speed of the ship at MCR—in knots (kt)

2.2. Predictve module

Since the first module already performed preparation of detailed emissions-related data, it was possible to develop a predictive algorithm as the second component of the PrE-PARE model. However, as the production of different APSs and GHGs form marine engines is influenced by a variety of factors that interact with each other, the prediction of emissions cannot be determined by linear functions. The relationships between the predictor variables such as engine power, type and speed, fuel type, actual speed, energy output and time in the different operating modes and the released emissions are nonlinear. In addition, the values of the parameters and their interactions vary between the ship types and individual ships. To overcome the complexity of predicting ship-related emissions, the MARS method was adopted in this research.

2.2.1. Multivariate Adaptive Regression Splines (MARS)

The MARS is a nonparametric, piecewise regression technique applicable in the modelling and analysis of complex, nonlinear relationships between multiple dependent and independent variables [45]. To examine the interactions and capture nonlinearity, this method automatically creates piecewise polynomials that characterize the data [46]. These polynomials, referred as splines, are basis functions inside the MARS model, and prediction is made by summing the weighted output of all the basis functions in the model [47]. Simple BFs involve a single variable (x) and come in pairs of the form $(x − t) +$ and $(t − x) +$ where t is the knot, $(x − t) + = (x − t)$ if $x > t$, and 0 otherwise; and $(t − x) + = (t − x)$ if $x < t$, and 0 otherwise [47]. The modelling process has two main segments, the forward stage that has the same idea as forward stepwise regression and the backward stage or pruning where model is improved and validated [45–47]. The forward stage starts by including the constant mean of target variable (intercept). This allows for determining the breakpoints or knots for each predictor variable. Between each point, a fitting basis function is added. This process is being done iteratively until the threshold is reached [45–47]. Once the full set of features has been created, the algorithm sequentially removes individual features that do not contribute significantly to the model equation to avoid overfitting [46,47]. This "pruning" procedure assesses each predictor variable and estimates error rate aiming to eliminate basis functions with the least contribution [46,47]. This procedure is applied automatically through the Generalized Cross Validation (GCV) technique [45]. The GCV can be expressed as follows (3) [47]:

$$\mathrm{GCV(M)} = \frac{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}_M\,(x_i)^2)}{(1 - C(M)/n)^2} \tag{3}$$

where the denominator is a complexity function, and C(M) is defined as C(M)=(M+1) + dM of which C(M) is the number of parameters being fit and d represents a cost for each basis function optimization and is a smoothing parameter of the procedure [47]. Larger values for d will lead to fewer knots being placed and thereby smoother function estimates [45].

With the aim of obtaining more accurate results for the prediction of ship emissions, standard MARS and Boosting MARS (B-MARS) methods, with and without log normalisation, were applied in this research to historical data processed by a previous module. This approach resulted in four distinct predictive models. Their performance was assessed and compared to determine the accuracy and reliability. To ensure an unbiased selection of data and evaluate the models, k-fold cross-validation was used during the hyperparameter tuning process for MARS models where ten-fold approach was applied. The data used for testing and training, with validation results averaged over ten runs, includes technical details and operational data derived from the AIS of ships that called at the port in 2019.

2.2.2. Prediction performance validation metrics

To evaluate the performance of above MARS models, the Root mean squared error (RMSE), Mean Absolute Error (MAE) and Coefficient of determination (R^2), presented in Equations (4), (5) and (6) where applied in this research [46]. Above metrics asses the accuracy of the predictions by quantifying the errors between predicted and actual values [48]. The R2 score measures the proportion of variance in the dependent variable that the model explains [48]. Its value ranges from 0 to1, with a value closer to 1 indicating stronger relationship between variables and better predictive accuracy [49]. The RMSE calculates the square root of the mean of the squared differences between predicted and actual values [46]. As the errors are squared before averaging, the RMSE is more sensitive to larger errors and directly relates to Euclidean distance [46]. Lower value indicates better performance. MAE is used to measure the average absolute difference between predicted and observed values [45,48]. Unlike RMSE, this method treats all errors equally without squaring them, making it less sensitive to larger deviations [48]. A low MAE indicates higher prediction accuracy.

Although the above criteria are commonly used to evaluate the prediction of the models, additional validation was performed in this research by including unseen shipping data from 2021, 2022 and 2023. These datasets were first used to calculate ship emissions, and the results were then compared to those predicated by the module relying on historical data from 2019 aiming to gain a clear insight into its forecasting capabilities.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (X_i - Y_i)^2}{(\sum_{i=1}^{n} (\overline{Y} - Y_i)^2} \tag{4}$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} |X_i - Y_i| \tag{5}$$

$$\text{RMSE} = \sqrt{\frac{\sum_{i=1}^{n} (X_i - Y_i)^2}{n}} \tag{6}$$

where X_i is the predicted i^{th} value, and the Y_i element is the actual i^{th} value, while n stand for the number of samples [48,50].

2.3. Ship emissions metric, scaling, classification and ranking module

As outlined in the introduction, the IMO has implemented various measures to regulate and assess the carbon efficiency of ships, which have become basic tools in the global effort to reduce CO2 emissions from the shipping industry. However, significant methodological limitations have been identified in mentioned measures. These constraints are particularly evident in the narrow focus on CO2, that disregards other exhaust gases and can lead to the overall environmental impact of ship emissions being overlooked, especially in urbanised port areas. Also, the carbon intensity calculations exclude the hoteling phase, leading to inconsistent results that may not accurately reflect a ship's total emissions profile. Adding to these issues, the measures do not fully incorporate operational data of the ships, which means that valuable insights into more realistic performance and efficiency are missing. Lastly, current imposed air pollution limitations are generally considered insufficient to address the full scope of the industry's environmental impact, emphasising the need for more comprehensive and differentiated approaches to assessing and regulating the sector's environmental footprint.

Consequently, the final objective of this research was to determine the air pollution impact and efficiency of ships while also providing a risk evaluation of temporal emission levels for individual ships, groups of ships and the entire port area. This was achieved in the third module, where novel metric, scaling, classification and ranking methods were applied to the outputs of the first and second modules.

2.3.1. Novel metric and scaling systems for standardised measurement and transparent overview of the emission efficiency and impact of ships

To establish a systematic approach for assessing the efficiency and impact of air pollution from individual ships while ensuring standardised measurement, the operational output of maritime transport must first be defined and weighted. Given that the primary objective of the shipping industry is to provide safe and efficient transport, emissions should be evaluated in relation to this goal.

Therefore, Operational Efficiency (OE) should be defined as the ability of a ship to complete a voyage on schedule with minimal energy consumption per unit of time, as represented in Equation (7). In the context of port approach, a voyage includes arrival, stay, and departure, encompassing cruising, manoeuvring, and hoteling as three operational modes, ensuring a comprehensive assessment of the vessel's operational profile. By integrating the time required to reach the expected EO with a ship's capacity for the intended operation and by comparing it against the emissions generated during the voyage, it becomes possible to determine the Vessel Air Pollution Operational Rate (VAPOR) for each mode, as defined in Equation (8). Unlike the metric system proposed by the IMO, the VAPOR considers available operational data and emissions over the entire voyage by evaluating air pollution in each mode (cruising, manoeuvring, and hoteling) separately giving the average hourly rate of exhaust production per work capacity. This allows for a standardised and detailed metric of emissions efficiency within specific operational phases. To ensure relevance, clarity and comparability, the feature scaling technique is therefore applied. The calculated VAPOR (VAPOR c) for a specific ship is normalised against the baseline VAPOR (VAPOR b) of the corresponding ship type, revealing the Ship Air Pollution Efficiency (SHAPE), as depicted by Equation (9). The VAPOR b is calculated by relying on extensive emissions-related database for each predefined ship-type groups, which are classified in the first module. This enables SHAPE to indicate whether a ship is operating more or less efficiently compared to the expected performance of its category. It also provides an insight into the progress made in the emission efficiency of certain ships and groups over time.

In addition, a simplified and user-friendly metric system has been developed to make the contribution of specific ships to air pollution in ports more transparent to the general public. Therefore, the Ship Emissions Impact Level (SEIL) compares the emissions released by a certain ship during a voyage relative to the average emissions per voyage of a generic ship within a defined time window, as shown in Equation (10). This approach provides a clear and intuitive visualisation of a ship's air pollution impact during an entire port visit, making it easier for the wider port community to assess and compare emission levels using a standardised emissions impact scale.

$$\text{EO (kWh)} = \sum_{\text{C,M,H}} \text{Operational LF (kW) x Operational time (h)} \quad (7)$$

$$\text{VAPOR} = \frac{\text{Emissions (g)}}{\text{Work capacity} * \text{Operational time (h)}} \quad (8)$$

$$SHAPE = \frac{\text{VAPOR c}}{\text{VAPOR b}} \tag{9}$$

$$SEIL = \frac{\text{Ship emissions in voyage (kg)}}{\text{Generic ship emissions in voyage (kg)}} \tag{10}$$

2.3.2. Comprehensive top-down system for classifying air pollution risk in ports, evaluating emission intensity, and performance ranking of ships

While emission estimation follows bottom-up methodology, this system first evaluates the exhaust gases released in the entire port, then relevant contribution from ship types, and finally performance of specific vessels. Mentioned stepwise process allows for a structured assessment by first identifying the risk level of overall emissions in a relevant area, followed by determining the air pollution intensity for different ship types, and finally evaluating the ship-specific indicator of emission performance where the potential for emissions optimisation is calculated and combined with the SHAPE. The aim of this three-stage procedure is to ensure a fair and data-driven framework for the control of ship-sourced air pollution in ports by providing an overview from both a macro and micro perspective.

To achieve this, the Port Emissions Risk Level (PERIL) classification algorithm is developed aiming to determine the degree of severity of overall ship emissions in the entire port area for a specified period as a first of three steps. The algorithm categorises emissions into five levels (Very Low, Low, Moderate, High, and Very High) by comparing the calculated emission rates with threshold values derived from the annual average and the standard deviation. This approach uses the average as a central reference point, allowing a clear and standardised classification of emission intensity based on statistical distribution rather than setting arbitrary thresholds. Upon determining the limit values, the system can automatically classify quantified shipping emissions. If the total emissions exceed the high-risk threshold, further analysis is conducted in a second step where the contribution of each ship group to total emissions is analysed.

This includes the application of the Ship Type Emission Intensity (ST-EI) assessment, which determines the degree of air pollution of each ship group by comparing their average emissions per voyage with the average emissions per voyage across all ship types in a given period, as shown in Equation (11). This method is used to create a relevant emissions contribution scale aimed at prioritising certain ship types for possible emissions improvement.

As a part of a final step, the Emission Optimisation Potential (EOP) is calculated for each ship by comparing its actual emissions per work capacity in each mode of voyage defined as Ship Emission Intensity (S-EI) against a reference baseline, as depicted in Equation (12). The EOP is therefore used to determine the range of possible emission optimisation by displaying emission exceedances with values greater than 1 or improvement of operations in stated voyage with values lower then 1. The baseline values of individual ships represent the volume of emissions released typically per work capacity in each mode of voyage and are determined by relying on historic recodes from database provided in first module. If the database lacks the operational and air pollution profile of a ship (first port visit), the second module is used for predicting the emission quantities by relying on technical and movement data of similar ships in the corresponding category.

Although the EOP exposes the performance of individual ships in terms of air pollution in each segment of specified voyage, some vessels may already operate efficiently, leaving little room for further optimisation. Therefore, to ensure objective ranking of ships, the Ship Emissions Performance Indicator (SEPI) is applied where emissions efficiency determined through the SHAPE is combined with the EOP as measure of ship's operational performance in specific voyage, as displayed in Equation (13). By incorporating both factors, SEPI enables a fair emissions attribution and ranking, ensuring that the ships with the highest improvement potential are prioritised in the final step.

$$ST\text{-}EI = \frac{E_{st}\ x\ V_{tot}}{V_{st}\ x\ E_{tot}} \quad (11)$$

$$EOP = \frac{\mathrm{S-EI\ a}}{\mathrm{S-EI\ b}} \quad (12)$$

$$\mathrm{SEPI} = \mathrm{SHAPE}\ x\ \mathrm{EOP} \quad (13)$$

where the following definitions apply:

ST-EI: Ship Type Emission Intensity — normalised value (dimensionless);
Est: Total emissions for a specific ship type —in kilograms (kg);
Vst: Number of voyages for that ship type — dimensionless value
Etot: Total emissions for all ship types in the period —in kilograms (kg)
Vtot: Total voyages for all ship types in the period— dimensionless value
EOP: Emission Optimisation Potential — normalised value (dimensionless)
S-EI a/b: Ship Emission Intensity actual/baseline — as emissions mass in entire voyage per units of work capacity (kg/wcu)

2.3. Data

All the above methodologies integrated inside the PrE-PARE model were applied on technical and activity data of the ships that visited the Port of Split in 2019 as a case study. Mentioned datasets, along with corresponding EFs and LFs where preprocessed in the first module as briefly explained in section 2.1., creating extensive database of emission-related inputs used throughout all three components of the PrE-PARE model.

Technical details of relevant ships were sourced from the Croatian Register of Shipping (CRS), the Croatian Integrated Maritime Information System (CIMIS) and relevant shipping company websites. The attributes collected include ship dimensions, work capacity, year built, ME and AE power, type and speed, fuel type, max speed at MCR and emission reduction technologies along with identifiers such as name, type and MMSI number [33].

Since the AIS is used for sharing timely information on ship characteristics and their movement between other vessels and the shore to improve navigational safety, recorded data is also often applied for estimating emissions [30,38,51,52]. Therefore, the position of the ship, the course and speed over ground (COG, SOG) with corresponding timestamps along with name and MMSI number of specific ships as identifiers were applied in this research. For collecting mentioned datasets, the AIS station of the Faculty of Maritime Studies in Split was employed. However, as the AIS transmits messages in National Marine Electronics Association (NMEA) sentence format that is unrecognisable to RStudio software, a specific Python script was developed and integrated inside the first module to convert the ‘raw’ data from AIS into a readable CSV format [33]. In the earlier mentioned preprocessing stage, erroneous and non-ship entries where then removed to finally obtain 49,540,895 records of ships in 2019 used for emission estimation in the initial module but also for testing and training in the predictive module. Same procedure was applied to acquire additional 15,930,840 AIS reference points of ships visiting the same port in different periods of 2021, 2022 and 2023 that represented unseen data used for extended validation of outputs produced by second module.

These AIS reference points where then connected with technical data of particular ships via respective identifiers finally creating individual trajectories for each port visit.

This process enabled the identification of operating modes with corresponding temporal and spatial characteristics in each recorded voyage by estimating the energy output of ME through the propeller law method [44]. The LFs for AE were taken from relevant studies as constant values [31,35,44]. Since all emission-related technical and activity details were identified and connected into a single database, the EFs could be determined as the final and most complex dataset required for estimating and evaluating ship emissions by applying the relevant methodologies described in the 3rd and 4th IMO GHG Study and the San Pedro Bay Ports Report [3,44,53]. The types of EFs along with elements for identifying them are presented in Table 1 [33].

Table 1. Engine details, modes of operation and types of EFs incorporated in the model

Elements for determination and types of EFs							
Engine function	**Engine type**	**Engine speed (rpm)**	**Fuel type**	**Mode & LF**		**GHG EFs**	**APS EFs**
ME	D	SS D < 300	MDO/MGO	C	LF = > 20 %	CO_2	SO_x
AE	GTU	MS D 300 - 900	HFO	M	LF < 20 %	CH_4	NO_x
	STU	HS D > 900	LNG	H	LF = < 2 %		PM 10, 2.5
	DF						NMVOC
	D-E						CO

Within the Table 1. D stands for diesel engine, GTU for gas turbine, STU for steam turbine, DF for dual fuel engine, D-E for diesel-electric engine, SS/MS/HS D for slow-/medium-/high-speed diesel engine, HFO for heavy fuel oil MDO/MGO for marine diesel/gas oil, LNG for liquified natural gas [33].

3. Results

The integration of technical details with activity data within the PrE-PARE model enabled the determination of operating modes and EFs for each of the 65,471,735 AIS reference points. These complex emission-related datasets were then combined into individual voyage tracks for each ship that called at the port, creating a foundation for modelling, predicting and evaluating ship emissions in large port areas. Therefore, the model has recognised 48,256 voyages to the passenger basin of the Port of Split in 2019 and in different periods of 2021, 2022 and 2023. However, it is important to emphasize that 2019 was used as the base year in this research, so the datasets from this year were used for defining reference points, and records from other periods served for validation. The recorded number of visits closely matched port traffic data, showing an average deviation of only 3% across all ship types, except for pleasure crafts, excursion and sailing ships, which lacked consistent arrival figures in the different sources. This discrepancy is largely due to their irregular schedules, often resulting in underreported AIS data. In addition, the 3% deviation partly reflects the ability of AIS to capture even minor vessel movements, offering higher quality input for accurate emissions estimation compared to standard port statistics. The share of port calls between ship types is illustrated in Figure 2.

Of all the ships surveyed, the most frequently installed engine type is MS D (78%), followed by HS D (22%) and LS D (3%). Share of engine types other than D is below 1%, so their influence on overall emissions is limited. Given the engine specifications and the enforcement of the EU Sulphur Directive, it is assumed that the entire fleet operates on MDO/MGO with a maximum sulphur content of 0.1% for the duration of each voyage [33].

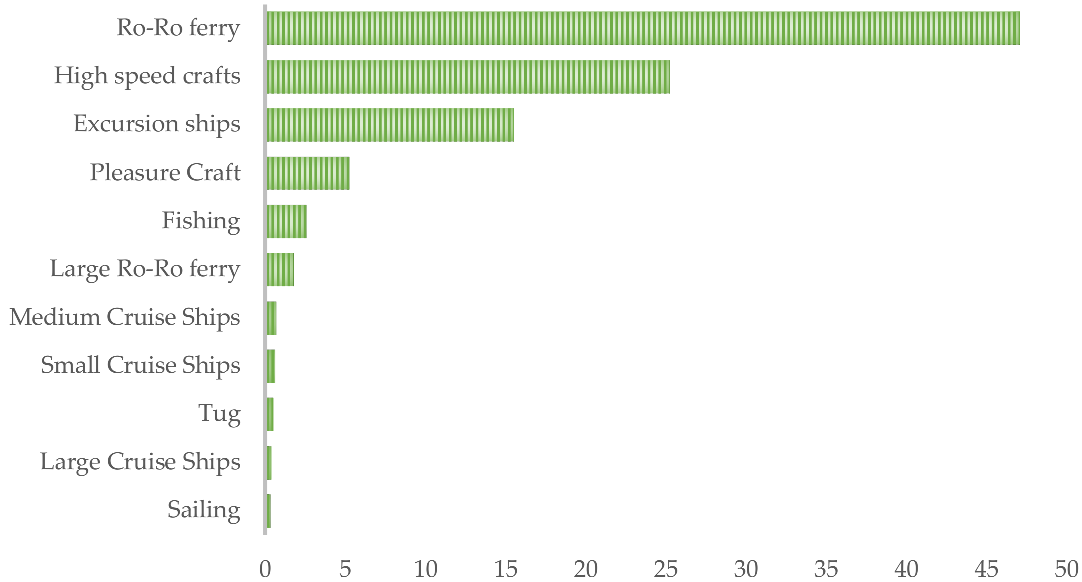


Figure 2. Proportion of voyages to Port of Split in periods covered by AIS data

3.1. First module – emissions estimation and analysis

As already mentioned, the first module was based on the analytical model presented in the earlier research created by the authors of this paper. Thus, an overview of various detailed technical, temporal, spatial and operational aspects of ship emissions were presented inside inventory of combustion gases released in the area relevant to the Port of Split—City port basin for 2019 [33]. Apart from an examination of monthly fluctuations relative to the year average, mentioned analysis was focused on different elements of annual emissions. This approach, standard for emission inventories, reveals only general insights, as emission levels and their distribution between ships changes with intervals considered. To enable a detailed analysis and a comprehensive evaluation of the risk and impact of emissions, the production of air pollution from marine engines should therefore be assessed over shorter timeframes. Given that a strong correlation was found between high emission levels and intensive seasonal traffic, a further and thorough examination of emissions at peak times should be considered.

That is why, the first module that combines energy-based method with bottom-up logic was used in this research to additionally analyse the fluctuation of daily emissions in the baseline year. The graph of daily emission totals in Figure 3, represented by the blue line, confirms the seasonal trend, but also shows considerable differences in day-to-day air pollutant levels released, not only between summer and winter periods, but also within the same months. The magnitude of the emission spikes becomes even more apparent when compared against the annual average of 120,164 kilograms (kg) marked by the yellow line, with emissions on some days being more than twice as high as the mean. Given the evident daily variability of ship emissions, further analysis of different aspects focussed on a particular day in July, as this month was identified as the most critical.

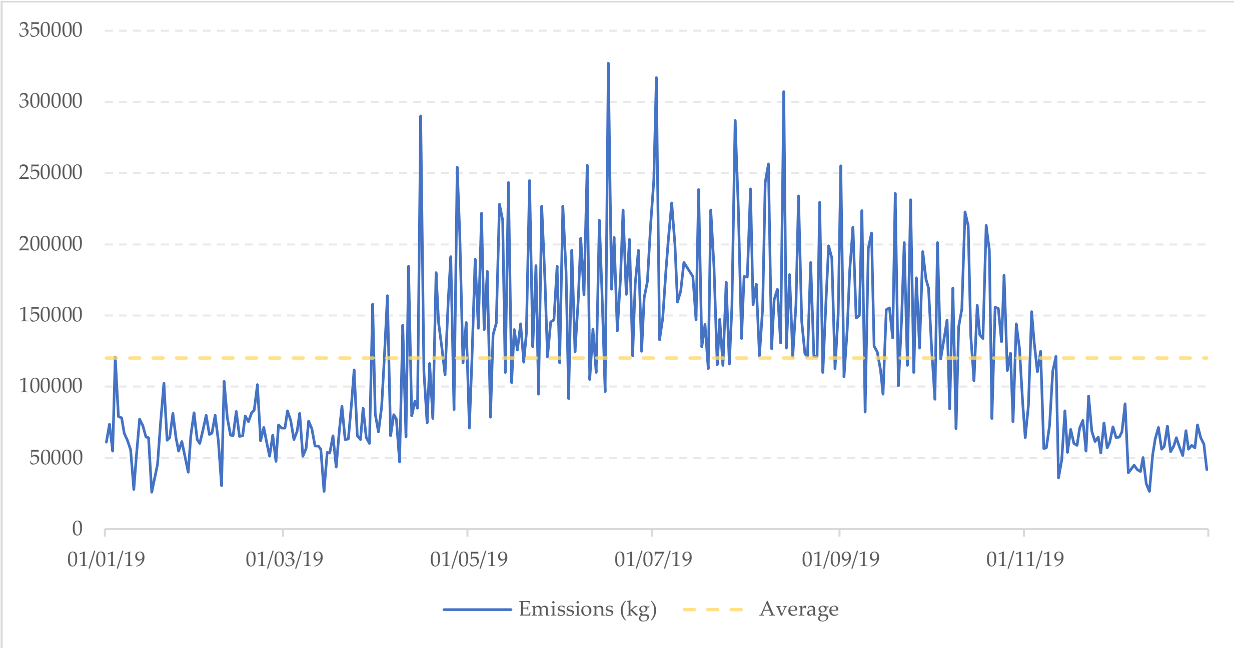


Figure 3. Distribution of daily emission totals and annual average expressed in kg, released by ships calling at the Port of Split passenger basin in 2019.

Table 2 therefore shows the emissions quantified by the estimation and analysis module for the Port of Split passenger basin on July 2nd, 2019, as the most emission-intensive day in the selected month. The table clearly shows that total ship emissions on the date indicated were more than 2.5 times higher than the average for the base year, illustrating the severity of risk that air pollution poses to the urban environment in the short timespan. It is also evident that Large Cruise Ships are responsible for about 37% of the emissions on that day, releasing almost twice as much as Ro-Ro ferries as second largest contributors to pollution, and only 5% less than all other groups combined. This result contrasts with the annual totals and confirms the differences in the distribution of emissions over time.

Table 2. Emission totals in kg for Port of Split passenger basin on July 2nd, 2019, quantified by the first module.

Ship type	GHG		AP						SHIP TYPE TOTALS
	CO2	CH4	SOx	NOx	PM10	PM2.5	NMVOC	CO	
Large Cruise Ships	116,161.249	2.133	68.801	2174.880	39.936	36.741	94.975	9.674	118,588.391
Ro-Ro ferry	63,221.461	1.102	37.466	885.589	20.553	18.908	54.663	48.716	64,288.459
Large Ro-Ro ferry	39,378.559	0.758	23.300	733.636	13.703	12.607	36.573	3.364	40,202.501
Small Cruise Ships	35,969.292	0.642	21.315	655.656	12.220	11.242	27.581	5.751	36,703.699
Medium Cruise Ships	31,222.711	0.591	18.481	582.766	10.817	9.951	26.038	2.642	31,873.997
High speed crafts	19,380.975	0.346	11.486	262.921	6.312	5.807	17.733	17.273	19,702.854
Excursion ships	21,46.156	0.051	1.272	35.847	0.783	0.720	2.849	1.456	2,189.134
Tug	14,60.308	0.028	0.865	18.785	0.480	0.442	1.324	1.413	1,483.644
Pleasure Craft	1,349.716	0.047	0.800	26.445	0.584	0.537	2.797	0.616	1,381.542
Fishing	691.295	0.021	0.410	9.374	0.272	0.250	1.081	0.765	703.468
Sailing	94.409	0.002	0.056	2.026	0.035	0.032	0.117	0.038	96.715
EMISSION TYPE TOTALS	311,076	6	184	5388	106	97	266	92	317,214

By comparing the calculated exhaust gas values of the individual ship types with the corresponding number of voyages in the same period, expressed as a percentage in Figure 4, the disparity between the emissions released and the number of port calls for some groups becomes clear. For instance, High speed crafts, which account for the largest share of voyages (37%), caused 6% of total emissions on a given day, while Large Cruise Ships produced 37% of total emissions from only 2% of visits. This example alone provides additional insight into the disproportionate contribution supporting the need for a thorough analysis of the conditions that cause greater production of on-board exhaust gases.

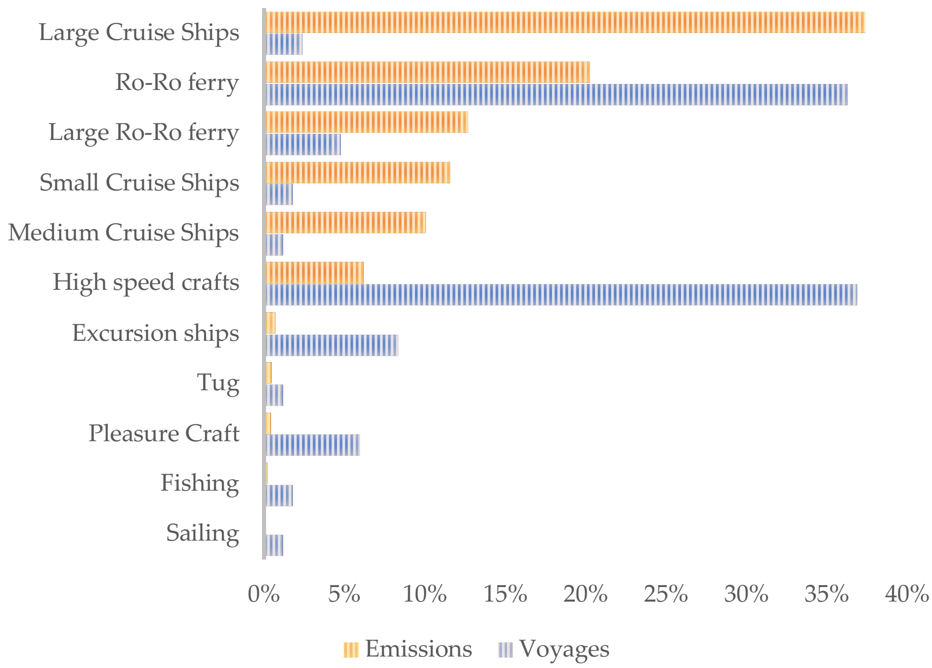


Figure 4. Share of emissions (orange) and voyages (blue) between ship types relevant in research area on July 2nd, 2019.

In this context, the first module was also used to examine the operational and spatial aspects of the emissions released on the selected day. Therefore, the distribution of emissions across operational modes was found to be 43%, 12% and 46% during cruising, manoeuvring and hoteling respectively. These values deviate notably from the annual averages, highlighting the temporal variations in emission patterns and confirming the difference in generation of air pollutants between ship types in the diverse operational modes, as illustrated in Figure 5. As can be seen, all types of Cruise ships released most of the emissions in the hoteling phase, Fishing and Pleasure crafts while manoeuvring and all others through cruising mode.

Since the identified activities and their corresponding emissions occur in distinct zones within the study area, a detailed map of the emission dispersion points was generated and presented in Figure 6 to illustrate the spatial distribution of air pollution. An analysis of the emission release locations, categorised by operating modes within individual voyages, revealed that almost all air pollutants were released within a 12 nautical miles (NM) radius around the city centre of Split. Notably, emissions from hoteling and manoeuvring operations, comprising 58% of the day's total, occurred only 0.5 NM from the urban area, highlighting their impact on the local atmosphere. This finding is especially relevant for APSs, which pose a direct threat to human health.

The development of a high-density map correlating emission dispersion points with operating modes provided a detailed overview of ship-based air pollution patterns in the port area. However, as shown in Figure 4, ships often operate differently, what directly affects emission output. Furthermore, composition and workflow of fleet involved changes with the timeframe examined, meaning that even reports based on large datasets only reflect conditions specific to examined period. In order to achieve a comprehensive evaluation of ship emissions, the machine learning techniques must therefore first be applied to provide relevant prediction of emissions in different scenarios on the basis of all the features analysed.

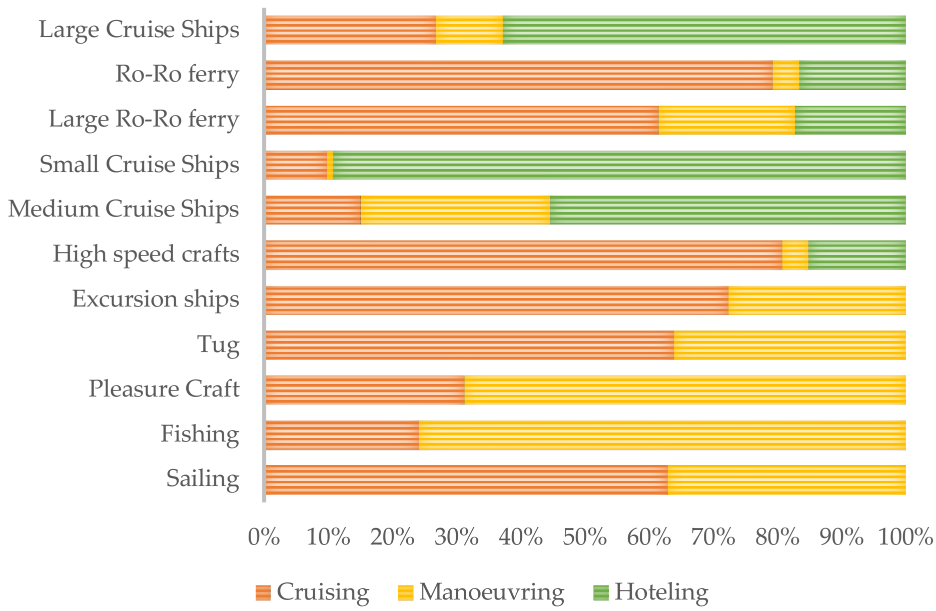


Figure 5. Distribution of emissions produced in operating modes for each ship type that visited the passenger basin of Port of Split on July 2nd, 2019.

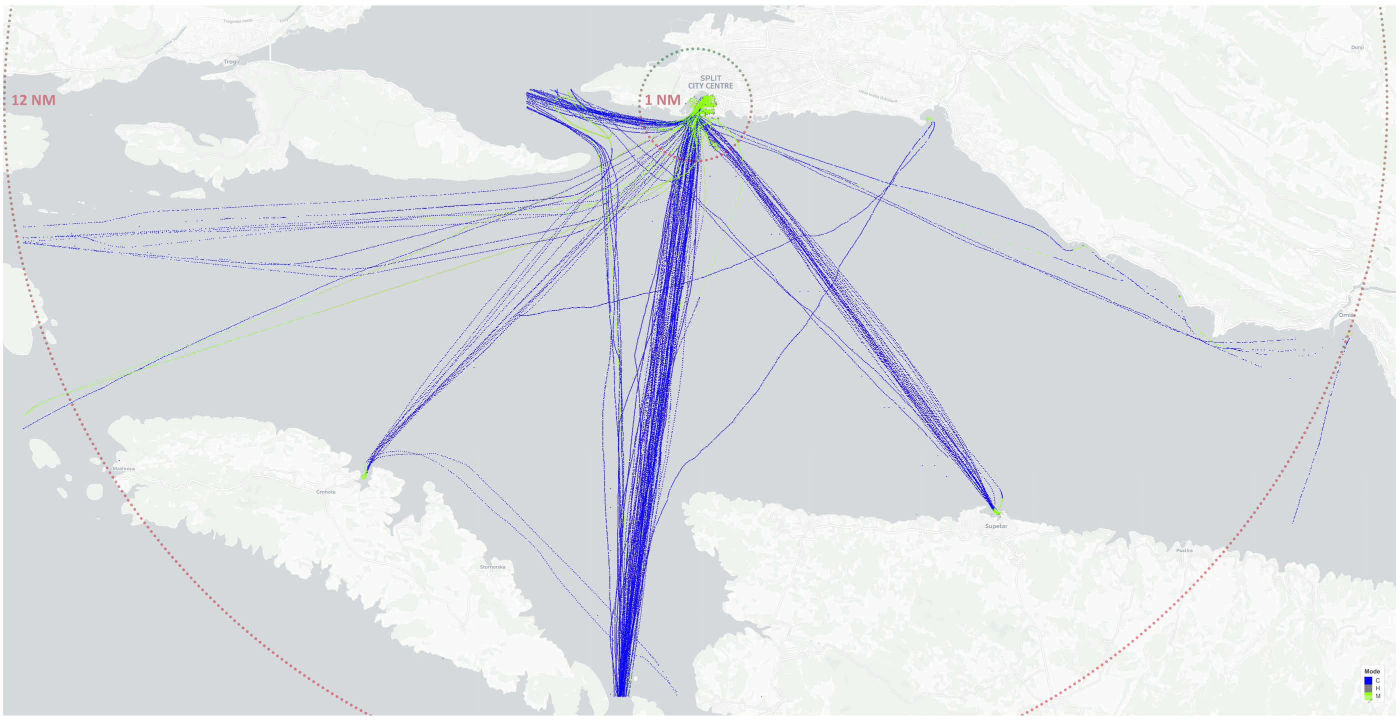


Figure 6. Spatial distribution map of ship emissions based on operating modes. The reference points shown represent the individual voyages of each ship that visited the passenger basin of the Port of Split on 2 July 2019 and contain a complete set of emission-related data. As can be seen, most of the cruising emissions, marked in blue, were released in the 11 NM parameter of urbanised area. The manoeuvring emissions shown in green extend over 12 NM but are almost entirely released within the port basin (0.5 NM from city centre). The air pollution from hoteling operations, marked in grey and identified as the largest contributor on set date, occurred just metres from populated areas, highlighting its direct impact on the local atmosphere.

3.2. Second module – emissions predction based on MARS approach

In the second module, different MARS methods were applied to extensive emission-related datasets preprocesses and structured in the previous component, aiming to achieve more accurate and reliable predictive outputs. Specifically, standard MARS and B-MARS, both with and without log normalisation, were used on technical and 49,540,895 AIS records of ships that visited the Port of Split during the base year 2019.

As previously described, in each MARS model a ten-fold cross-validation was implemented where data was partitioned into ten equal subsets. Each of ten iterations interchangeably included different 90% of the datasets into training fold and 10% in testing fold ensuring randomised and unbiased selection of inputs. To obtain clear and data-driven evaluation of outputs produced by each MARS model, RMSE, MAE and R^2 were calculated as key performance metrics and compared across all runs. Given the operational and technical differences between ships, each MARS variant was validated separately for distinct ship categories and operational phases. Table 3 presents the average key performance metrics for all categories of Cruise ships and Ro-Ro ferries, selected as representative case studies due to their contribution of over 90% of the total recorded emissions. These examples effectively illustrate the predictive capability of developed models across dominant ship types and operational scenarios.

The performance metrics of all four predictive models included RMSE, MAE and R^2 values for all categories of Cruise ships and Ro-Ro ferries in three operational modes. Models trained with log-normalised emissions were evaluated in both logarithmic units (Log-Scale MARS and Log-Scale B-MARS) and their anti-logarithmic equivalents (Original MARS and Original B-MARS), resulting in some metrics being expressed in grammes to provide interpretable, real-world error values. On the other hand, metric results for the models trained and evaluated entirely on raw emission values (MARS and B-MARS without log) where shown only in grammes since no normalisation was applied.

Table 3. Performance metric comparison of ship emissions predictive models

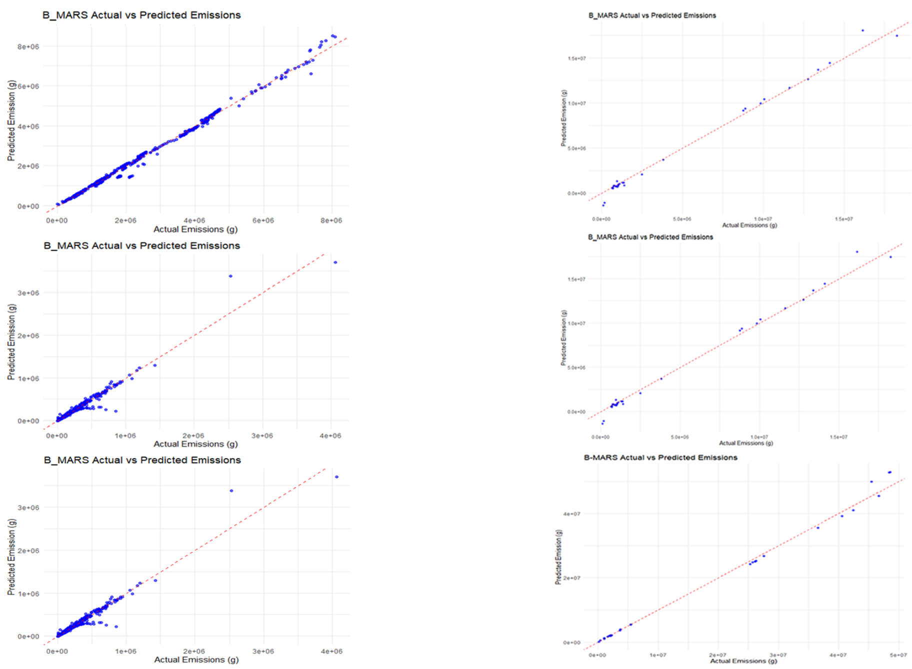
Ship type	Mode	Metric	MARS models					
			Log-Scale MARS	Original MARS	MARS Without Log	Log-Scale B-MARS	Original B-MARS	B-MARS Without Log
Cruise ships	C	RMSE	0.094	370984.728 g	587,208.1 g	0.397	294,2934 g	566,174.7 g
		R^2	0.997	0.996	0.990	0.920	0.74194	0.99269
		MAE	0.071	214953.697 g	420,379 g	0.156	871,928 g	360,756.3 g
	M	RMSE	0.190	535,904 g	844,628 g	0.130	384,456 g	872,822 g
		R^2	0.993	0.993	0.990	0.997	0.9977	0.984
		MAE	0.135	310,311 g	435,491 g	0.097	208,845 g	451,754 g
	H	RMSE	0.088	1300580 g	333946.000 g	0.090	1437849 g	290938 g
		R^2	0.997	0.995	1.000	0.997	0.9934	0.999
		MAE	0.056	733883.000 g	187609.000 g	0.058	749500 g	178251 g
Ro-Ro ferries	C	RMSE	0.070	74,100 g	100,525 g	0.062	78,208 g	80,749 g
		R^2	0.989	0.997	0.994	0.991	0.9963	0.9626
		MAE	0.025	41,076 g	54,154 g	0.027	46,851 g	47,2078 g
	M	RMSE	0.130	45,728 g	32,810 g	0.126	38,581 g	27,135 g
		R^2	0.991	0.910	0.955	0.991	0.9377	0.9694
		MAE	0.071	6,989 g	9,360 g	0.061	5,542 g	8,057 g
	H	RMSE	0.634	130,894.91 g	104,916 g	0.641	136,666 g	73,625 g
		R^2	0.852	0.997	0.996	0.832	0.9962	0.998
		MAE	0.176	41,719.50 g	37,042 g	0.270	41,021 g	17,496 g

Overall, log-normalised models generally performed better when handling skewed data, but performance varied by ship type and mode. Notably, B-MARS without log transformation achieved the lowest MAE and RMSE values in certain cases (e.g., Ro-Ro ships in mode M with an MAE of 17,459 g), suggesting that models based on raw values can outperform log-transformed ones when the data distribution is more balanced. These results showed that the most effective approach depends not only on the algorithm, but also on the nature of the emission data in different operational contexts.

However, since the B-MARS model, which was trained without log on average showed the most accurate prediction performance on average, it was implemented in the PrE-PARE system as the second module. Although the results generated by the chosen prediction module showed high accuracy, further validation was performed with unseen data. This was done to verify the module's ability to accurately predict emissions in different scenarios with unknown (first visit) ships and unpredictable changes in the operation of the included vessels. Therefore, a total of 15,930,840 AIS reference points and the corresponding technical details of the ships calling at the port in different periods of 2021, 2022 and 2023 were applied as unseen data for the extended validation of the results produced by the second module.

In this process, the non-log B-MARS module, trained on emission data from 2019, was used to predict emissions from Cruise ships and Ro-Ro ferries in all three modes which were then compared with the actual levels released by corresponding ship types in periods of 2021, 2022 and 2023, as shown in Figure 7 The graphs display cruising, manoeuvring and hoteling modes from top to bottom, with panels labelled (a) corresponding to Ro-Ro ferries and those labelled (b) representing Cruise ships. The blue dots in each scatter plot present emissions predicted by module, while the actual emissions based on real data are illustrated by red dotted line.

In all modes and for both ship types, the predictions closely match the reference line, indicating that the model generalises well beyond its original training dataset. Strongest alignment is observed in the cruising and hoteling modes, where the predictions show minimal deviation from the actual values. Even though some over or underestimation can be observed for outliers with high emissions, especially in manoeuvring and hoteling operations done by cruise ships, the overall performance indicates that the B-MARS model trained on 2019 data is able to produce robust and accurate predictions of ship emissions in different scenarios and future trends.



(**a**) (**b**)

Figure 7. Comparison of ship emissions based on real data and values predicted by non-log B-MARS module for Ro-Ro ferries (a) and Cruise Ships (b) in C, M and H modes placed from top to bottom.

3.3. Third module – ship emissinons metric, scaling, classification and ranking module

Although the second module demonstrated effective predictive performance for ship exhaust gasses even under new conditions, the modelled results always reflect the emission-related attributes of a specified period, as determined by analysing the outputs generated by the first module. Spatial, temporal, technical and operational aspects vary with the intervals considered, which limits the broader interpretability and comparability of the results. Furthermore, the repeated generation, examination and comparison of results is time-consuming and requires both computational and expert resources. Therefore, adapting a standardised system for evaluating air pollution risk in ports, ranking emission intensity and assessing the potential for ship emission optimisation would be a more efficient and scalable solution. That is why, in this research, novel methods integrated within the third module were applied on outputs produced by the analytical component of PrEPARE system.

3.3.1. Standardised and interpretable measurement of ship emissions efficiency and impact based on novel metric and scaling methods

As a central method to universally determine the emission efficiency and performance of individual ships, the VAPOR as novel metric system was established and applied in this research. Therefore, processed datasets of all ships recorded in 2019 were used to calculate the baseline VAPOR (VAPOR-b), which quantifies the hourly emissions production in grammes (g) per unit of working capacity in different modes of operation. For all types of cruise ships, high-speed vessels, pleasure craft, sailing ships and excursion vessels, the working capacity was defined based on passenger capacity. In the case of Ro-Ro ferries, both passenger and vehicle capacity were considered. For tugboats, the bollard pull was used as a measure of working capacity, while for fishing vessels the net volume of cargo space was applied. These results where aggregated to derive average VAPOR-b for each ship type, as illustrated in Figure 8 for APSs (SOx, NOx, PM10, PM2.5, NMVOC, and CO) as emissions with local impact. It must be clarified that the maximum working capacity has been used as a static value, independent of the actual utilisation of the ships, to create a static reference point that can be compared with the actual emission production, optionally considering the actual workload of the individual ships. Furthermore, in the context of port visits, which include arrival, stay and departure, the mentioned capacities have been doubled for all vessels as they are able to embark/load and disembark/unload passengers/goods during a single voyage, as defined in this research. The exceptions are Tugs, as their working capacity is defined by the bollard pull, and Fishing vessels, that use their capacity at sea and do not overturn the goods in both directions. When comparing all three modes of operation, Pleasure crafts exhibited the highest hourly rate of exhaust production per unit of work capacity, reaching 763 g in cruising mode. This highlights the correlation between small work capacity and relatively high-demand engines. In contrast, Ro-Ro ferries, which are often equipped with similarly powerful engines but with large work capacity, demonstrated the overall lowest emission rates per working unit, despite being the largest annual polluters and the second in total emissions on the observed day. In addition, Sailing ships showed a high emission rate of 640 g in cruise mode, due to the assumption of continuous engine usage, thus the analysis in this study reflects the worst-case operational scenario for this ship type.

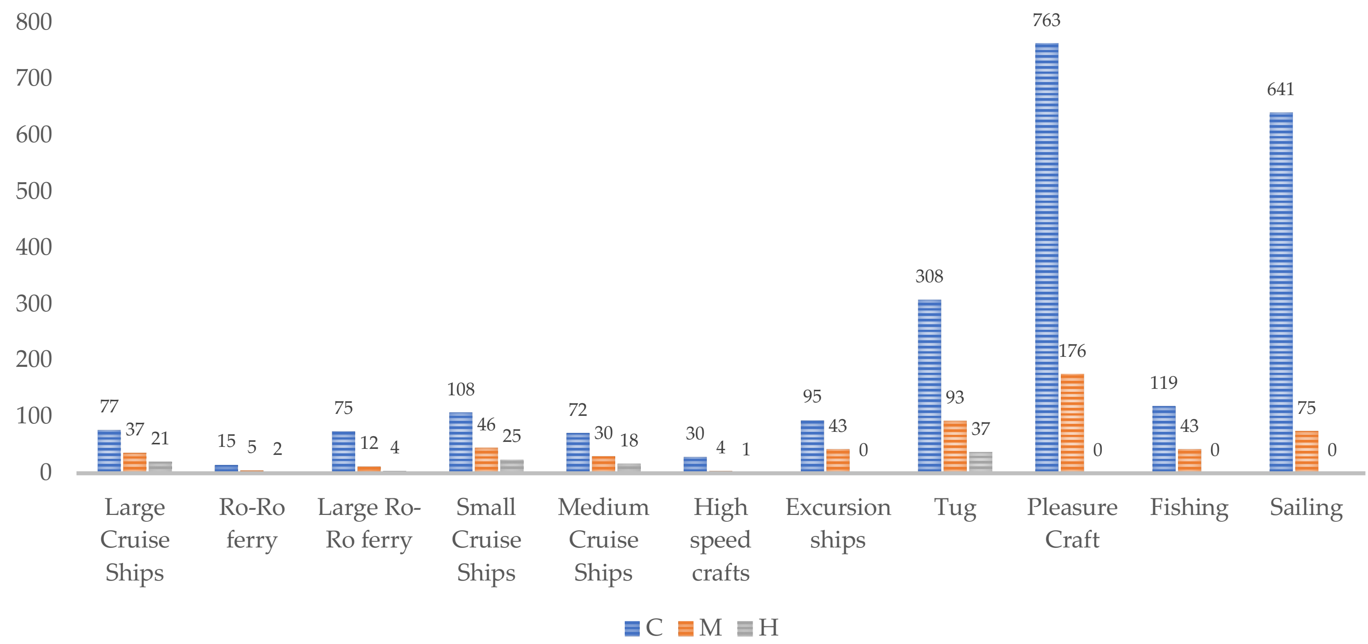
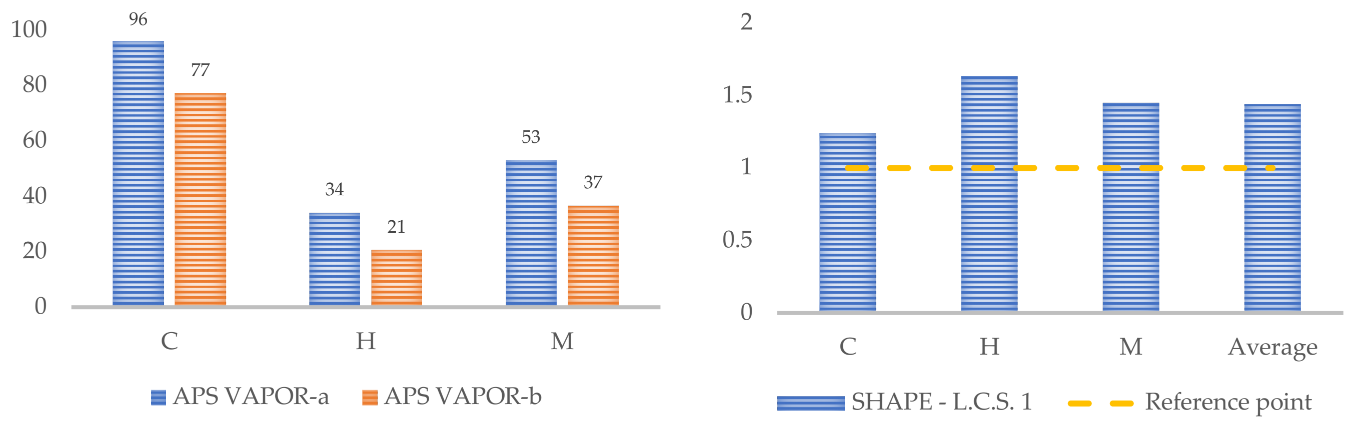


Figure 8. Overview of hourly rate of APS production in g per work capacity (APS VAPOR-b) in each mode across all ship types calling at Port of Split in baseline year 2019.

These baseline values were then applied in a scaling process, where they were compared to the actual VAPOR (VAPOR-a) calculated for vessels calling at the port on 2 July 2019. It is important to note that the work capacities used for calculating VAPOR-a were treated consistently with those applied to the VAPOR-b. By correlating mentioned values, the SHAPE metric was derived for each operational mode of every ship recorded on the observed day. The SHAPE values greater than 1 indicate reduced emission efficiency (higher actual hourly emission rate per capacity), whereas values below 1 reflect better efficiency. Given that the Large cruise ships were recognised as the most significant contributors to emissions on stated day, Figure 9 presents the APS results from both the metric and scaling perspectives for one representative vessel from this category. The left-hand panel (a) displays a comparison between the calculated VAPOR-a and the reference VAPOR-b across operational modes. For example, Large cruise ship 1 (L.C.S. 1) in hoteling phase on hourly basis produced 13 g of APSs per unit capacity more than ships with similar characteristics. The right-hand panel (b) illustrates the corresponding SHAPE values, normalized against the baseline. The bars represent the ship's actual efficiency, while the yellow dashed line indicates the reference point (SHAPE = 1). These results show that L.C.S. 1 was on average less efficient in all operating modes.

The application of VAPOR and SHAPE to the case of a L.C.S. 1 clearly demonstrates the ability of the metrics to provide transparent and pragmatic insights. As can be seen in Figure 8, both the raw (VAPOR) and normalised (SHAPE) results are intuitively visualised across all operating modes, enabling easy identification of inefficiencies in this example. The standardised calculation method, which is based on available operating and emissions data, ensures that the results are not only objective but also directly comparable with ships of similar features. The simplicity of interpretation, particularly through the SHAPE values relative to the baseline, makes these metrics highly effective for communicating emissions performance as they do not require high expert or computational resources. In addition, as the metric is based on available operational data, it provides more realistic results and can be used universally to monitor the emission efficiency of ships at an international level.



(**a**) (**b**)

Figure 9. (a) Comparison between actual VAPOR-a and reference VAPOR-b values across different operational modes; (b) Normalized SHAPE values for Large Cruise Ship 1. The bars represent the calculated SHAPE for each mode, while the yellow dashed line marks the reference efficiency (SHAPE = 1), indicating that Large cruise ship 1 performed less efficiently across all modes.

To complement the technical metrics with a more accessible perspective for the wider port community, the SEIL was applied on the day analysed. As a simplified and intuitive indicator, the SEIL expresses the total emissions released by each ship during its port visit relative to the emissions of a "generic" ship, whose value is derived by aggregating the total emissions and voyages of all ships recorded on that day. This allows a clear comparison of individual ship impacts on a standardised scale. As illustrated in Figure 10, SEIL provided a visual ranking of ships based on their emissions per voyage on a selected day, highlighting those that contribute more than average to air pollution in the port area. The introduction of this metric supports greater transparency and enables informed discussions on emissions accountability among port stakeholders and the general public.

The SEIL results clearly reveal the disproportionately high environmental impact of certain ships. In particular, Large Cruise Ship 1 emitted over 17 times more air pollutants than the average ship during a single voyage on the examined day. This straightforward contrast emphasises the magnitude of emissions caused by high-consumption ships. Furthermore, the results show that while Ro-Ro ferries as a group make the second largest contribution to emissions, a typical Ro-Ro ferry would have to make approximately 23 separate voyages to match the emissions generated during a single port visit by the Large Cruise Ship 1. These results highlight the extent to which such ships contribute to local air pollution and emphasise the importance of differentiated emission management strategies in port operations.

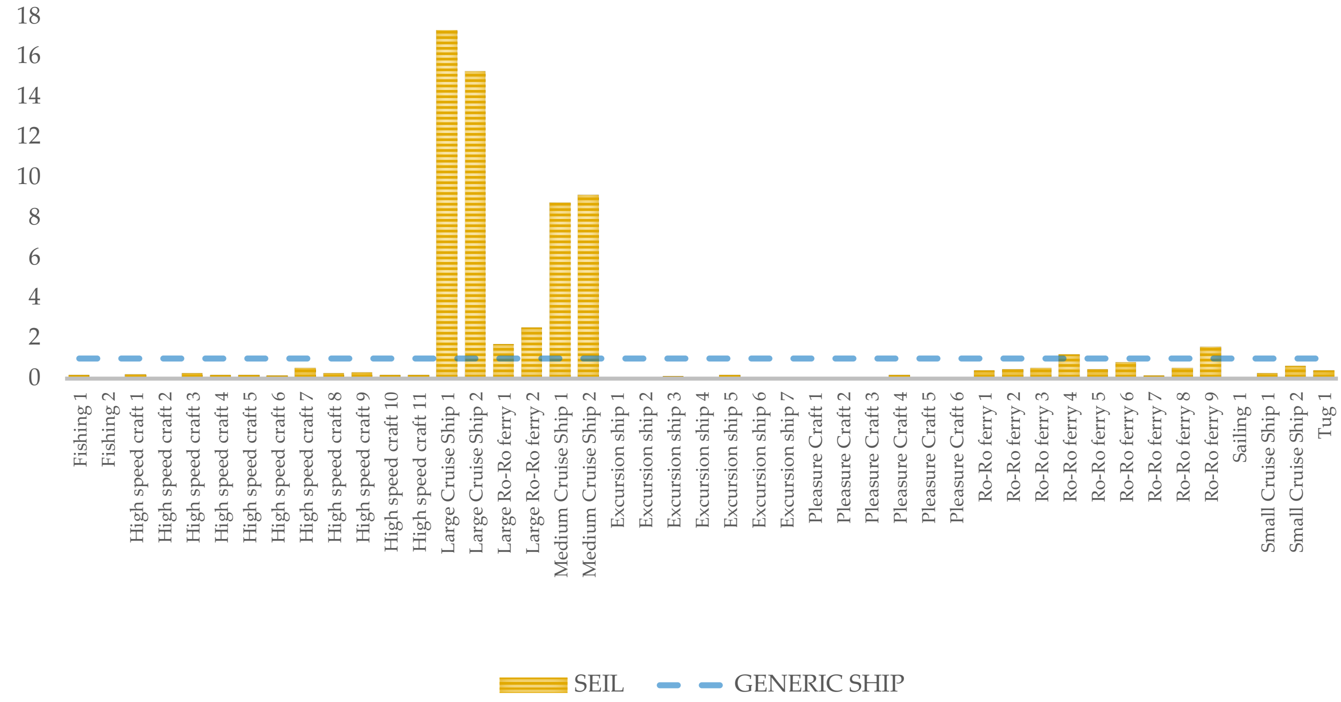


Figure 10. The Ship Emissions Impact Level (SEIL) of vessels calling at the port on the 2nd July 2019. The SEIL metric expresses the emissions per port visit (voyage) in relation to a standardised "generic ship" represented by the dashed line (value = 1). Notably, the Large Cruise Ship 1 emitted over 17 times the average, while most ships, including Ro-Ro ferries and High speed crafts, were below or close to the reference point. This visualisation illustrates the significant differences in the impact of emissions between individual ships.

3.3.2. Classification of Air Pollution Risk and Ranking of Ships Based on Emission Intensity, Optimisation Potential, and Performance in Port Areas

To effectively evaluate and manage ship emissions in the port areas, a top-down system for determining air pollution risk, intensity and performance was developed and applied to real operational data. As a first part of three-step process, the PERIL classification algorithm was implemented on daily emission totals quantified by the first module for the baseline year 2019. This approach, based on statistical distribution, segments daily emissions into five categories by using standard deviation and the mean value as central reference points. These categories are visualised in Figure 11, where thresholds are defined from the annual average of daily exhaust gases and their variability: Very Low (dark green) spans from 0 kg to 60,081 kg, Low (light green) from 60,081 kg to 120,163 kg, Moderate (yellow) from 120,163 kg to 180,246 kg, High (orange) from 180,246 kg to 240,327 kg, and Very High (red) that includes all values above 240,327 kg.

Although the Moderate zone begins above the average, it encompasses values within one standard deviation and can thus be considered as a part of the statistically normal range. This classification methodology avoids arbitrary thresholds and supports meaningful distinction between typical and extreme emission events, enabling targeted emission control, particularly in the High and Very High categories. According to the PERIL classification, 13 out of 360 days were categorised as Very High risk and 50 as High risk, with the events distributed between April and November. This finding indicates that overall, only a minority of days have a significantly increased risk.

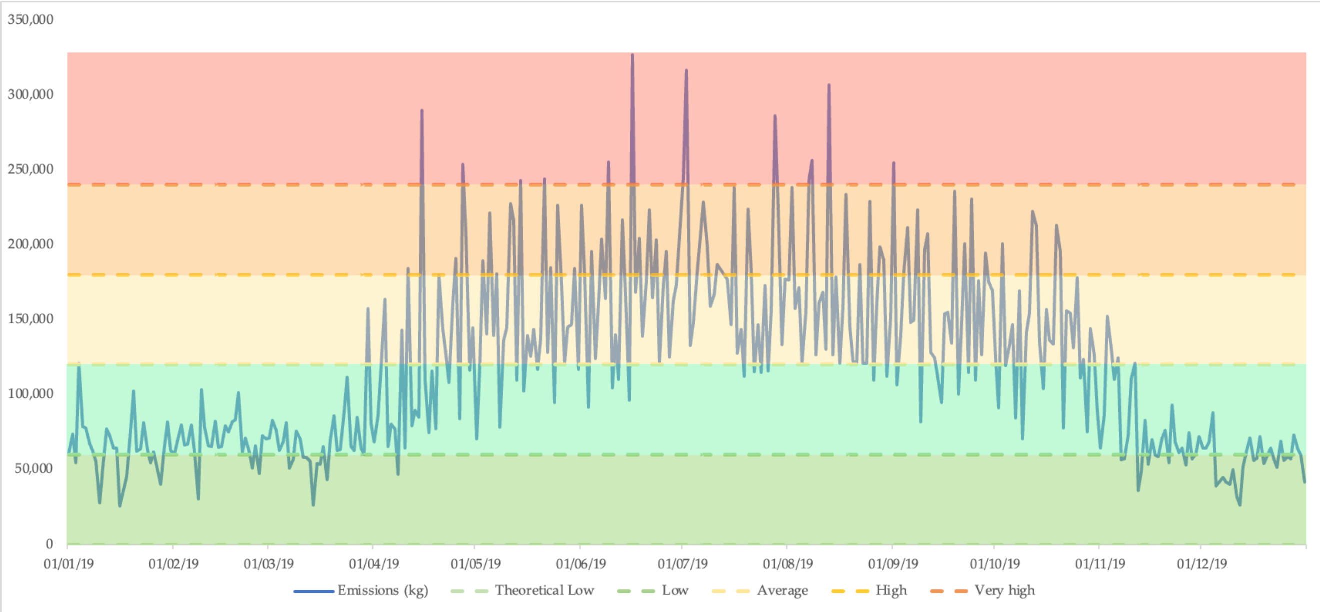


Figure 11. The Port Emissions Risk Level (PERIL) classification algorithm appled on daily ship emissions qunatified by the fisrt module for the basile 2019 in are relevan to Port of Split.

Due to total ship emissions reaching 317,214 kg on 2 July 2019, corresponding to 2.6 standard deviations above the annual mean, the day was clearly classified in the Very High risk category. This result prompted further analysis aiming to categorically identify the sources of high ship-emissions.

To determine the distribution of emissions among the various ship groups, the ST-EI method was applied in a second step of the bottom-down approach. This measure compares the quantified emissions per voyage for each ship type with the overall average for the fleet in the period analysed and thus highlights categories with significant intensity.

As can be seen in Figure 12, Large Cruise Ships exhibited the highest APS intensity of all ship types on the day observed, indicating that they had the most significant impact per port call. This result served as the basis for further analysis of the individual vessels first within this group and assess their optimisation potential.

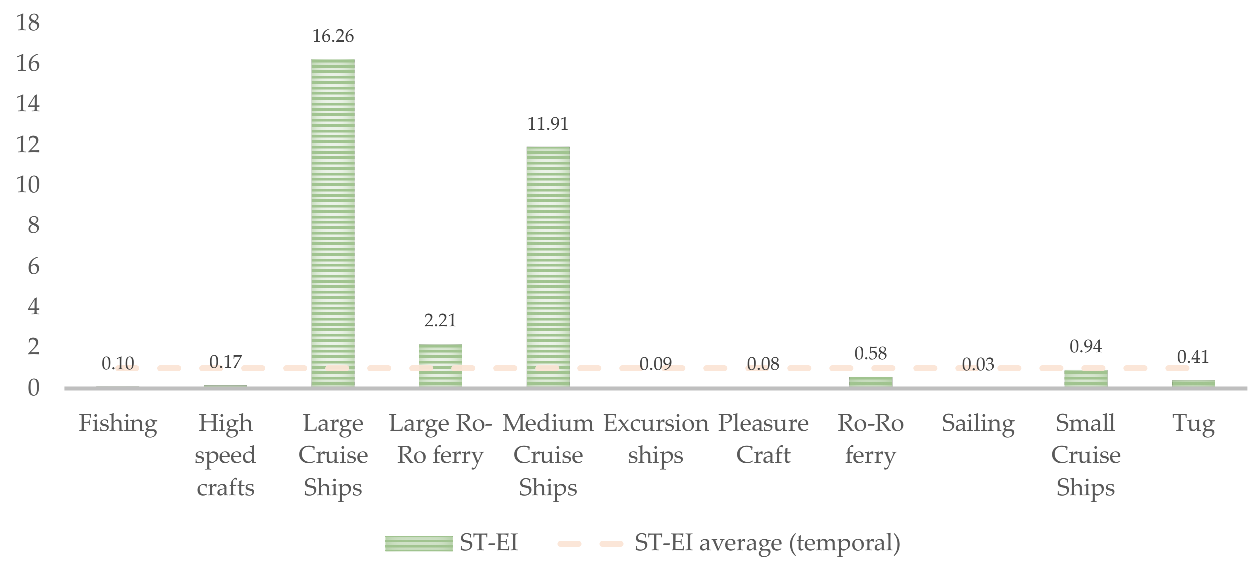


Figure 12. The Ship Type Emission Intensity (ST-EI) method for measuring the degree of air pollutants released in all ship types compared to temporal total ships emissions per all voyages, applied for APSs on examied day, 2nd July 2019.

In the final stage of the process, the EOP was calculated to determine the quantity of emissions that could realistically be reduced. This was initially performed for the two ships that comprise the entire Large Cruise Ship category by comparing their actual emission per work capacity (S-EI a) through the entire voyage with their historical baseline (S-EI b), which reflects the average emissions released per work capacity during all previous port visits.

In contrast to VAPOR, which is a universal metric method that quantifies the hourly production of emissions per capacity, the S-EI used in the EOP focuses on the total emissions during a complete voyage. It integrates the total time spent in each mode and is thus sensitive to the temporal and spatial differences specific to operational pattern of individual ships. Due to these variations, the S-EI cannot be used for a direct and clear comparison between ships. Instead, it enables intra-ship performance evaluation by comparing each voyage with the vessel's own operational history.

As shown in Figure 13, Large Cruise Ship 2 exhibited lower-than-expected emissions in all voyage segments, indicating overall efficient operation. In contrast, Large Cruise Ship 1 demonstrated higher emission outputs in hoteling by 20% and by 5% in manoeuvring operations, while cruising was slightly below average, suggesting the concrete potential for improvement. The EOP values were then combined with SHAPE, a metric that reflects universal emissions efficiency of each ship, to calculate the Ship Emissions Performance Indicator (SEPI). By integrating emission efficiency and optimisation potential, the SEPI enables a fair and balanced ranking of vessels.

In the end, all ships recorded on the analysed day were automatically categorised first by the ST-EI and then by SEPI, with the corresponding SHAPE and EOP values, what is displayed in Table 4 for the top 10 ranked ships. This layered classification enables not only targeted emission control for the most intensive vessel types, but also identifies specific vessels that should be prioritised for further optimisation interventions, ensuring a fair and data-driven basis for port emissions management.

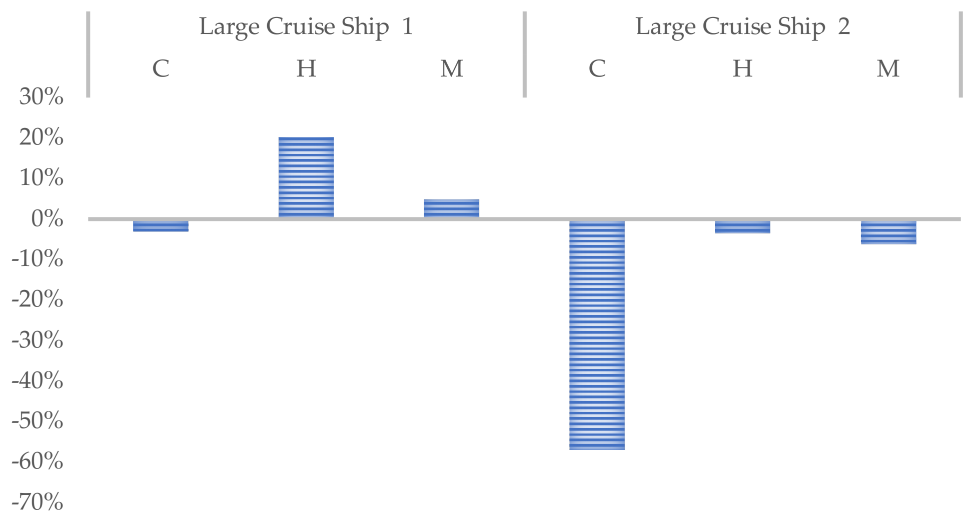


Figure 13. Emission Optimisation Potential (EOP) results for APSs of Large Cruise Ship 1 and 2, presented as percentages. Large Cruise Ship 2 demonstrated better performance across all operational modes, while Large Cruise Ship 1 showed notable optimisation potential, particularly in hoteling and manoeuvring, where emissions exceeded typical values

Table 4. Ranking of the top ten ships in the Port of Split on 2 July 2019, based first on the ST-EI, and SEPI indicators for the entire voyage, including the SHAPE and EOP values for each operating mode.

Ranking	Name	ST-EI	Mode	SHAPE	EOP	SEPI voyage
1	Large Cruise Ship 1	16.26	C	1.24	0.97	1.56
			H	1.64	1.20	
			M	1.45	1.05	
2	Medium Cruise Ship 1	11.91	C	0.96	0.70	1.16
			H	1.17	0.95	
			M	1.04	1.62	
3	Ro-Ro ferry 9	0.58	C	1.21	1.11	2.37
			H	1.20	3.37	
			M	0.99	1.75	
4	Ro-Ro ferry 4	0.58	C	1.49	0.90	1.92
			H	1.61	0.67	
			M	1.49	2.23	
5	Ro-Ro ferry 4	0.58	C	1.76	1.06	1.52
			H	1.61	0.11	
			M	1.31	1.92	
6	Ro-Ro ferry 6	0.58	C	0.99	1.14	1.22
			H	0.76	2.10	
			M	0.64	1.44	
7	Tug 1	0.41	C	0.99	1.11	1.05
			M	2.16	0.47	
8	High speed craft 1	0.17	C	0.93	1.09	1.50
			M	0.85	2.35	
9	High speed craft 7	0.17	C	1.81	1.56	1.37
			H	1.18	1.07	
			M	0.00	0.86	
10	High speed craft 8	0.17	C	1.02	0.18	1.30
			H	1.07	1.59	
			M	1.05	1.93	

3. Discussion

The results generated by the PrE-PARE model demonstrate that by applying methodologies integrated within its three modules to the extensive technical and operational data, ship-sourced emissions in port areas can be effectively quantified, analysed, predicted, evaluated, and categorised in a clear, comparable, and standardised manner. Although each module can operate separately and produce function-specific outputs, their compatibility and shared reliance on structured shipping data support the control of port-related air pollution by simplifying the complex relations between the different aspects of ship emissions as a final outcome. As demonstrated in this and previous studies, technical, temporal, spatial and operational factors vary in relation to the area and period considered, leading to inconsistencies in the interpretation of their influence on port-related air pollution. This variability complicates the analysis and prevents a meaningful comparison of the results in different contexts. The combination of novel metric, scaling, classification and ranking methods with quantified emissions-related data therefore enabled an effective interpretation of the various implications crucial for analysing and managing ship emissions in ports throughout changing conditions. In practical terms, the PrE-PARE model provides tangible answers to the critical management questions: What level of emissions should be considered high for a given port? Which ships perform efficiently in terms of emissions? And which vessels should be prioritised for operational optimisation?

The introduction of the VAPOR and SHAPE as central metric methodologies addressed the need for a universal, data-driven measure of ship emission efficiency. In contrast to conventional regulatory indicators such as EEDI, EEXI, or CII, which are primarily based on theoretical design parameters and emissions per NM, overlooking time spent in port, the VAPOR reflects hourly emissions per ship-specific unit of work capacity across all operational modes, including cruising, manoeuvring, and hoteling, by relying on available operational data. Moreover, while the referenced IMO indicators are limited to assessing CO2 emissions, the metrics presented in this research encompass a broader range of air pollutants, offering a more comprehensive evaluation of a ship's environmental footprint. Additionally, the application of SHAPE facilitates comparability by normalising and comparing calculated values against category-specific baselines, thereby enabling clear and consistent performance monitoring. The practicality of using the PrE-PARE metrics is demonstrated by comparing Ro-Ro ferries and Large Cruise Ships, both of which contribute significantly to emissions in the Port of Split. While Large Cruise Ships were the dominant emitters on the analysed day, Ro-Ro ferries accounted for the highest annual totals. However, across all operational modes, Ro-Ro ferries emitted approximately 5 to 10 times less APSs than Large Cruise Ships on the VAPOR-b. This contrast emphasises the value of applying standardised metrics that account for a work capacity of a ship and apply a consistent time unit, such as hourly output, allowing a meaningful assessment of performance for different ship types and timeframes in all operating modes.

Although the VAPOR was applied within the port area for this study, its calculation is not spatially limited. The model can be extended to evaluate emissions along the entire voyage, allowing a continuous analysis from port to port on sea and ocean passages. This flexibility makes the model suitable not only for port management, but also for regional policy development, transboundary environmental assessments and global monitoring of the efficiency of specific ships and related groups. In addition to these metrics, the SEIL indicator further simplifies the interpretation of a ship's air pollution during a single voyage making the results accessible to experts and inclusive for the broader community.

To evaluate the risk of shipping emissions in different timeframes, the PERIL classification algorithm was developed and applied, where aggregated averages and standard deviations are used to objectively classify overall port emissions into categories ranging from Very Low to Very High.In the context of this research, the algorithm identified only 13 Very High and 50 High emission days for the Port of Split, unevenly distributed throughout 2019, highlighting the need for improved management of port activities, particularly during expected peak emission periods.

Following the PERIL classification and continuing the top-down evaluation process, the ST-EI method was applied to identify and rank the ship types based on their emission intensity relative to their operational activity. On the analysed day, Large Cruise Ships were recognised as the ship type with the highest emission intensity. This result directed the subsequent evaluation of all recorded vessels, starting with those within high-impact group. The EOP and SEPI indicators were thus applied to determine both the emission performance and optimisation potential of individual ships. These indicators revealed clear distinctions in performance levels, enabling a fair and targeted ranking system that prioritises ships with the greatest room for improvement within relevant groups.

It is important to emphasise that by combining a predictive module based on the B-MARS machine learning approach with other components of the model, the system extends beyond current conditions and enables the modelling, prediction and evaluation of possible future pollution scenarios. This feature supports strategic planning and enhances port resilience against emerging operational and environmental challenges.

In this context, the modular structure of the PrE-PARE model ensures a high degree of flexibility that allows the possible integration of new methodological findings, regulatory requirements or additional emission-related factors without changing the basic architecture and logic of the system. This adaptability also enables the application in different areas, maritime transport structures and port operation contexts, regardless of size or local emission characteristics. At the same time, the outputs generated by the model remain consistent, comparable and easy to interpret as they are based on a relevant methodological foundation supported by extensive operational and technical data.

Ultimately, all the mentioned features support the future adaptation of the model as a decision support system for the control of ship-based emissions in ports, as well as a framework for the introduction of air pollution tariffs in the broader context of integrated environmental management in seaports.

5. Conclusions

The PrE-PARE model presented in this research demonstrated the capacity to model, analyse, predict and comprehensively evaluate port-related air pollution from ships by combining relevant methodologies with emission-related data. To perform these tasks effectively and in a standardised manner, the model comprises three interconnected modules:

- emissions quantification and analysis,
- emission prediction under different scenarios,
- emissions metric, scaling, classification and ranking.

All three modules with integrated methods were applied to extensive technical and operational data for all ships that visited the passenger basin of the Port of Split in 2019 and in different periods of 2021, 2022 and 2023.

The first module applied a bottom-up logic and energy-based approach to quantify the emissions of each voyage covering all operating modes for all recorded ships, providing a high-resolution emissions inventory for the Port of Split in 2019. This module was also used for the detailed analysis of technical, temporal, spatial and operational aspects for 2 July 2019 as a day with particularly high emissions.

In the second module, a B-MARS machine learning algorithm was applied to predict the emissions of different ship types. The module demonstrated strong predictive performance and was validated against unseen technical and 15,930,840 AIS records, confirming its consistency and capacity to forecast emissions in various scenarios.

The third module implemented novel metric tools such as VAPOR and SHAPE, which enabled standardised efficiency comparisons between ships, while classification systems such as PERIL and ST-EI identified high-risk emission periods and intensive ship groups. These methods were further supported by EOP and SEPI indicators, which offered a structured methodology for assessing operational optimisation potential and a fair vessel ranking. In addition, the SEIL metric provided a contextualised insight into the impact of individual ships on each voyage, improving interpretability and promoting awareness of air-pollution of ship-sourced air pollution for the wider port community.

Together, the components of the PrE-PARE model form a transparent and flexible system for the efficient and standardised monitoring of ship emissions, particularly within port areas. Its modular architecture allows for adaptability in diverse regulatory, spatial, and operational contexts. The results show that the PrE-PARE model is not only an effective tool for current emission control and environmental planning in ports, but also holds significant potential for application in broader maritime networks and future operational scenarios. As such, it represents a valuable foundation for sustainable port management and the development of emissions-based policy mechanisms within integrated environmental decision support systems.

Author Contributions: For research articles with several authors, a short paragraph specifying their individual contributions must be provided. The following statements should be used "Conceptualization, F.B.; methodology, F.B.; software, A.G.; validation, A.G., F.B.; formal analysis, F.B. and A.G.; investigation, F.B.; resources, F.B.; data curation, F.B. and A.G.; writing—original draft preparation, F.B.; writing—review and editing, F.B.; visualization, F.B. and A.G.; supervision, A.G. and R.B. All authors have read and agreed to the published version of the manuscript.

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