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Model-driven scope 3 upstream (procurement) CO_2 emission calculation for the design space exploration of maritime vessels

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ABSTRACT: The marine industry is increasingly adopting platform and modular design strategies while facing growing sustainability regulations and emission constraints. This paper proposes an approach that integrates scope 3 upstream CO2 emissions (i.e., procurement) into a Decision Support Environment (DSE) for design space exploration of alternative modular ship design concepts. The DSE, deployed in the conceptual design stage, enables simultaneous testing of various cruise ship configurations regarding CO2 emissions using a bottom-up approach with parametric CO2 models. It leverages data-driven models from existing databases or AI-generated data exemplified in a case study on the hotel system of a cruise ship illustrates how parametric design variables influence CO2 emissions, demonstrating a preliminary result of a prescriptive study in collaboration with a major international ship manufacturer

KEYWORDS: decision making, sustainability, early design phases

1. Introduction

The ship construction industry is a historically conservative field in embracing new technologies due to perceived risks (Bash, 2008) requiring the need for large upfront investments with narrow profit margins and featuring large concurrent engineering efforts where design and production are often overlapping (Abal et al., 2005). However, recent data from the ship construction industry after the COVID-19 pandemic highlights some criticality of the way the industry is operating (Kalosh, 2024; Taylan, 2022; The Marine Executive, 2022). There is a shift from a supply-driven to a demand-driven structure, emphasizing the importance of understanding and catering to specific customer needs, especially for what concerns the design and development of ad hoc solutions for different customers (Yip et al., 2023). Such evolution is pushing the ship construction industry into embracing concepts such as platform design and modular design, setting the need for increased capability to predict costs and the impact of new design concepts (Erikstad, 2019).

While in other fields, such as aerospace engineering, research literature often addresses such challenges by set-based concurrent engineering and value-driven design approaches, with a limited contribution to using model-based engineering solutions (Page & Seering, 2023) is present in ship design and engineering. When focusing on the conceptual design stage, there is a lack of data-driven and simulation-driven approaches supporting the design space exploration of different ship designs, while the applicability of such approaches has been demonstrated in other fields, such as aerospace or construction equipment engineering (Bertoni et al., 2020).

While addressing this gap and the need for a transition toward a model-driven approach for ship design requires modeling capabilities encompassing heterogeneous design criteria, this paper focuses on proposing an approach that allows the utilization of data-driven and simulation-driven approaches to quantify the CO_2 emissions in the early design phases of ship concepts to aid design decision-makers makers inform design decisions considering emissions.

The relevancy of this aspect is given by the increasing regulation and sustainability challenges imposed on manufacturers and increases attention to the sustainability implication of a ship design. The Paris Agreement to climate crises, Greenhouse Gas (GHG) Protocol (Corporate Standard | GHG Protocol, 2004) categorized corporate ship emissions into three scopes: scope 1, which refers to the direct emissions from the sources that are owned or controlled by the company (e.g. emission from facilities, vehicles, and fuel burnt by ships during construction and sea trial) (Hertwich & Wood, 2018); Scope 2 involves the indirect emissions from the generation of purchased power (Roston, 2021), steam, heating, and cooling by the shipyard operations; and scope 3, considering the indirect emissions that occur in the shipyard's value chain. This includes an "upstream" perspective, focusing on procurement, and a "downstream" perspective, focusing on emissions in operation.

The difficulty in collecting the scope 3 upstream data is due to insufficient data available, and the loss of information on emissions along the supply chain (Fritsch et al., 2024). The lack of standardized calculation methods and data sharing among stakeholders also makes it challenging to quantify the emissions accurately (Bonelli & Coqueret, 2024).

To proactively design for sustainable transition in ship manufacturing, rather than reactively calculating impact, there is a need to integrate emission quantification and thus scope 3 upstream assessment, as a decision-making driver in the conceptual design of ships. Emissions need to be considered at the same level as other KPIs, such as engineering performances or costs, when the design space of new ship solutions is explored in conceptual design.

Based on such premises, the paper proposes an approach integrating the assessment of scope 3 upstream CO_2 emissions into a Decision Support Environment (DSE) for the design space exploration of alternative ship concepts. The DSE is meant to be deployed in the conceptual stage of ship design, serving as a tool for design space exploration through which potentially hundreds of different ship configurations could be simultaneously tested for feasibility, production cost, and emissions. The logic of the approach is based on a bottom-up model structure in which different ship modules are imported in a parametric global ship model (similar to the Ship Synthesis model described by (Vernengo & Rizzuto, 2014), which sets the boundaries and conditions for the module selection. To address the lack of availability of data, AI is used to generate data related to the overall physical constraints of maritime vessels, specifically in areas where traditional design relationships may not be directly applicable. For instance, to populate regression models where two physical quantities do not have a straightforward, linear relationship.

The proposed approach is exemplified in a case study, focusing on the design of the cabin area of a cruise ship. The case study shall be seen as a simplification of a real case, whose details are covered by an industrial secrecy agreement, and it has the intent to demonstrate the role of modular selection and parametric modeling in CO_2 emission calculation, as well as show a prototype of a visual computer-based interface for the decision-making environment.

2. Research approach

The research presented in this paper is the result of a 10-month research project in collaboration with one of the major companies worldwide operating in the ship design and construction industry, a consulting company working on modular product development, a consulting company working on meta modeling for systems engineering, and another university partner. The research can be framed into the design research methodology (DRM) by (Blessing & Chakrabarti, 2009), encompassing research clarification, descriptive study, and an initial prescriptive study. In the frame of DRM, participatory action research (PAR) by (Avison et al., 1999) has been the main research approach for problem identification and for the development of the intended support as part of the initial prescriptive study. Data collection happened through meetings and workshops both online and on-site at the company facilities and university premises during the whole period of the project. Besides the close collaboration with practitioners, research clarification has also been performed through a literature review and analysis of official published documents. The implementation of the proposed approach in the case study was based on modeling and simulation activities performed by the authors supported by access to industrial data sources. In cases where data were missing, AI-generated inputs were utilized, primarily using GPT-4o and o1 models. The validation and verification of the approach happened through a 6-hour prototyping and testing sessions run at the ship manufacturer facilities in the presence of a consulting company and the other university partner. The purpose of the validation activity was to receive feedback about the applicability and usability of the method, validate the results obtained in the example case, and set up a plan for the further development of the approach and its integration into larger decision support systems. The results of such phase are described in the discussion session of this paper.

3. CO_2 estimation in ship design

The estimation of CO_2 emissions in ship design is experiencing a transition from operational-centric estimations to comprehensive, design-integrated approaches. It is driven by increasing regulatory pressures and general awareness amid global decarbonization targets. Traditionally, CO_2 estimation primarily focused on operational emissions, particularly those related to fuel consumption for ship propulsion and hotel load (Moreno-Gutiérrez et al., 2019).

Life Cycle Assessment (LCA) has emerged as a critical methodology for evaluating the environmental impacts of ships across all stages of their life cycle. Early studies applied LCA to quantify emissions during ship operation, but recent efforts now encompass all other aspects of the cruise ship lifecycle. For example, (Perčić et al., 2021) conducted a comprehensive LCA of battery and diesel-powered ferries which assessed the environmental impact of battery and diesel-powered ferries across multiple life cycle stages. The study did not limit its analysis to operational emissions alone and included emissions linked to the design and construction phases as well. Another significant development in CO_2 estimation is the incorporation of DSE which assists in making decisions regarding optimal configurations. Along similar lines, (Koronakos et al., 2023) presented a decision support system (DSS) called Optiship that compares design configurations that correspond to the three main LCA dimensions criteria, on economic, environmental, and social KPIs. However, DSS is devoted to the assessment of the ship's operation and the end-of-life phases. The integration of LCA into the design phase is further supported using life-cycle performance assessment framework. It enables simultaneous evaluation of lifecycle cost and life-cycle emissions (Gualeni et al., 2019).

For the estimation of scope 3 upstream CO_2 emissions, LCA-based methods are frequently employed (Chatzinikolaou & Ventikos, 2014) using bottom-up or top-down approach. Bottom-down approach starts with a higher-level view of the system and breaks it down into its components. On the other hand, the bottom-up approach starts from the sub-system or low-level view of the systems and builds up to form the overall system. (Tran & Lam, 2024) and (Jang et al., 2024) use the bottom-up approach in LCA, leveraging operational data such as ship routes, fuel consumption, and port activities to create detailed emissions inventories. These inventories often highlight the spatial and temporal distribution of emissions, emphasizing the impact of specific regions and operational modes (Yu et al., 2024). Other methodologies include predictive models based on ship speed and engine characteristics, which are compared with LCA simulations to validate their accuracy (Jang et al., 2024). Overall, the quantification of CO_2 emissions in the shipping industry is an intricate process that involves detailed modeling of various lifecycle phases and operational conditions to provide a comprehensive understanding of the environmental impact. However, the primary focus of research lies in the estimation and optimization strategies during the operational phase of the existing ships as the operation phase is typically identified as the most significant contributor to CO_2 emissions (Quang et al., 2020). However, due to the sheer scale and material intensity of cruise ships, incorporating scope 3 upstream emissions associated with the production, transportation, and processing of materials used in shipbuilding can have a significant impact on overall CO_2 emissions (Mathew & Kumar, 2024).

4. Data-driven CO_2 emission calculation in ship design: the proposed approach

4.1. Results from the descriptive study

The first results of the research focused on the identification of the gaps and problems in the current state of practice when integrating CO_2 assessment in the conceptual design stage of ship design. The descriptive study results in this stage were obtained both from literature and with interaction with industrial partners during meetings and workshops. The study revealed that there exist several critical challenges in utilizing emissions as a key decision-making KPI during a conceptual stage in complex maritime products. Existing methodologies primarily focus on economic and engineering KPIs and often marginalize environmental KPIs, i.e., emissions. This marginalization creates a gap as early design decisions strongly influence the long-term carbon footprint of the ship. A limitation is due to the lack of models identifying dependencies between engineering design choices and impact on emissions, the latter often calculated on parameters with a much lower level of granularity, with no direct correlation with a single change in the design. Without being capable of aligning the level of granularity between design choices and CO_2 emissions impacting variables, the consideration of emissions as a critical KPI alongside economics and engineering becomes highly challenging. The results from the descriptive study converge into the definition of a set of requirements to be addressed in the prescriptive study (in alignment with the DRM), those requirements were defined as follows:

- Emission models must be integrated into the decision-support environment with the same level of granularity as economic and engineering KPIs. These models shall be at a level of detail that a change in a design feature will trigger a change in the emission model results, as it would happen for economic and engineering KPIs.
- Dependency models are necessary to capture the relationships between the input and output of economic and engineering models with the emission models to ensure cohesive integration in a decision-support environment.
- To capture an appropriate level of detail in emission, the approach shall be developed considering a bottom-up approach, where modular sub-system-level models concur in creating the overall ship model.
- A top-level modular modeling structure is essential to accommodate the diverse range of ship types, allowing modules to be added or removed depending on the vessel's purpose, such as cargo, cruise, or ferry. For such reason, the top-level modeling structure shall be based on the parametric variables used to set the boundaries and conditions for sub-system module selection.
- To address the usability challenge, emission models shall not only be at the same level of detail as economic and engineering models but their output shall also be visualized and communicated in the same fashion and format, better if in the same interface.
- Given the extremely large variety of potential design solutions, emission models need to be linked to external data sources providing emission data for different materials or products. To allow the exploration of radically new solutions, the model should encompass the possibility of accessing AI-generated content, accepting the risk of reduced accuracy of data.

These findings form the foundation for the subsequent prescriptive study, ensuring sensitivity to design changes, equitability and interconnectivity of emissions KPI with economic and engineering ones, sub-system integration using the bottom-up approach, adequate granularity, modularity, and adaptability with external and AI-generated data sources.

4.2. Results of the initial prescriptive study: logic of the proposed approach

The approach proposed as a result of the initial prescriptive study consists of the integration of a parametric CO_2 emissions quantification model into a decision-support environment where different concept configurations are assessed, analysed, and visualized based on their economic engineering, engineering, and CO_2 emission performances. The decision support environment (DSE) is visualized in Figure 1 in the area marked with number 1. The decision support environment consists of a GUI to prompt the user to input design parameters to visualize various design configurations. Some parameters are used to set the higher-level boundary of the system such as the overall size of the cruise ship (internal enclosed volume and dimensions). That does not affect the material composition of the sub-systems. DSE runs the design of experiments and comparisons by executing the parametric CO_2 emission model and visualizes various design configurations against the baseline design for decision-making purposes. The iterative design space exploration process continues until the optimal configuration is identified, supporting informed decision-making.

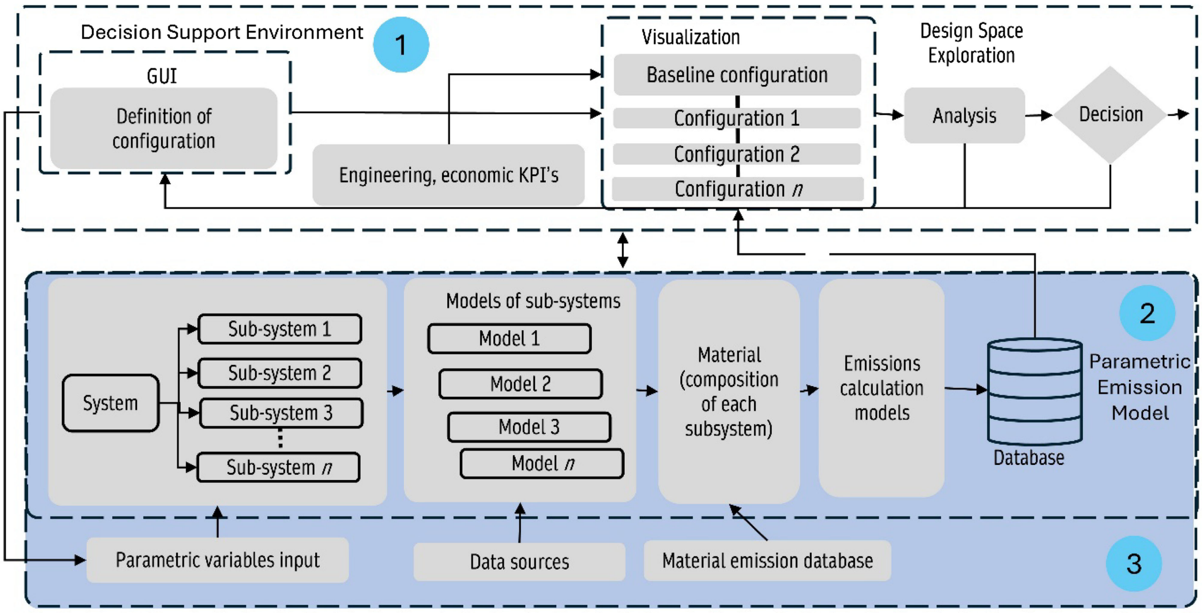

Figure 1. Visual depiction of the logic of the approach applied in the demonstrative case study

The approach utilizes the LCA method for the estimation of materials emission combined with the bottom-up approach that starts from the sub-system or low-level view of the systems and builds up to form the overall system, as shown on the left side of the parametric emission model (marked with number 2). The rationale behind the bottom-up approach is that it allows more freedom in making design decisions (Crespi et al., 2005) where there is an increasing need for modular and platform-based design.

The parametric emission models take parametric variables input from the GUI and utilize it in a bottom-up approach where the starting point is the sub-systems of a larger system which adds up to the higher-level system. In the same figure, number 3 represents the input layer. It shows the type and the stage where the input has been given to the emissions parametric model.

The parametric emission model allows the quantification of scope 3 upstream emissions using LCA and a bottom-up approach. Each subsystem is represented by one or more parametric models. As the subsystems are closely linked together. There exist material, structural, and computational dependencies which are shown in the figure through bi-directional connections among models of sub-systems. Data used in the development of regression models were sourced from publicly available literature and company reports. Where no available data existed, synthetic data was generated using a large language model-based AI model. The generated data was subjected to screening and sanity checks to ensure plausibility and accuracy. However, the results would be more accurate using verified and validated company data. To ensure flexibility, the model allowed for the seamless replacement of AI-generated data-based regression models with validated and trusted models as they become available.

The output of the models is the material composition in terms of the mass of each sub-system. The material composition is fed into models that calculate the emission based on the material type and the procurement channel. The procurement channel includes the transportation mode and the geographical zone from where the material is transported to the manufacturing site. Each configuration is then stored in the database and is called into the decision support environment to be visualized and compared for design space exploration purposes. Further decisions are made to include additional configurations as needed. The overall approach allows the modeling of indirect contributions from the value chain through a specific focus on material procurement and transportation. The CO_2 emission factors associated with producing different materials were obtained from industrial and literary databases which considers the material-specific environmental impacts.

The model estimated CO_2 emissions from transporting those materials from suppliers to the shipyard. Mode of transportation (sea, rail, air, road) and geographical distance from procurement to shipbuilding site were considered. All material and transportation emissions were stored in a central repository. This dataset was then fed into a Decision-Support Environment (DSE), allowing for the visualization and comparison of different design configurations in terms of CO_2 impact.

4.2.1. Example usecase: hotel system of cruise ship

The approach presented in Figure 1, is described in this section through its application in a case study focusing on the hotel section of a cruise ship. Cruise ships typically consist of seven sub-systems, each with unique characteristics depending on how they are classified. The example use-case places particular emphasis on the hotel system, as it is one of the most material-intensive sub-systems of the cruise ship. Figure 2 highlights the sub-systems within the hotel system, each playing an important role in designing modular solutions.

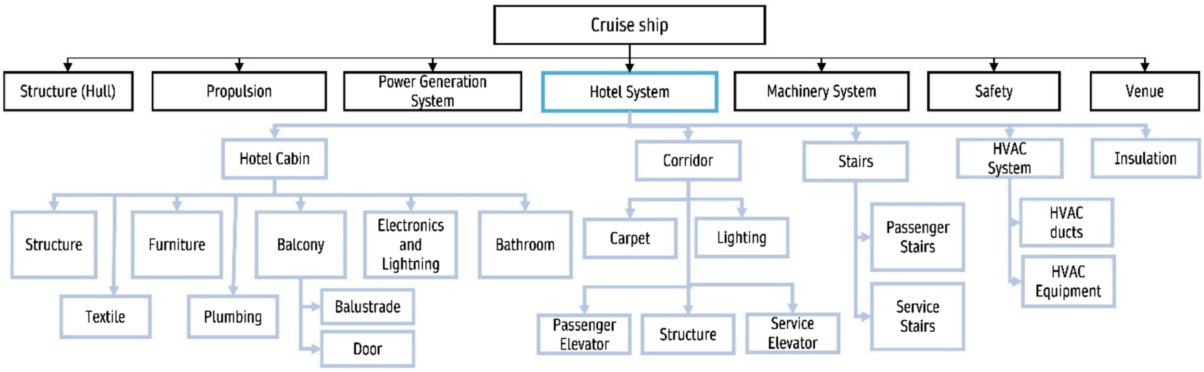

Figure 2. Hierarchical breakdown of cruise ship with a focus on the hotel system components

The application of the approach began with defining the high-level boundary of the cruise ship by defining the overall size in terms of gross tonnage (GT). GT represents a nonlinear measure of a ship's overall internal volume. Space ratio is a measure of a ship's comfort, calculated by dividing its GT by the number of passengers onboard. It establishes a high-level boundary upon which the bottom-up approach is developed. The overall length of the cruise ship was calculated using equations proposed by (Schwarzkopf et al., 2021) respectively as follows:

$$L = \sqrt[b]{\frac{GT}{a}} \quad (1)$$

For cruise ships, (Schwarzkopf et al., 2021) set $a = 0.0129\ m^{-1}$ and $\mathbf{b} = 2.8$ in Eq. (1), and $a = 24.6\ m^{-1}$ and $\mathbf{b} = 3.9$. To calculate the total number of decks the height of the ship is taken as input which is often dictated by constructional and operational limits. The internal enclosed volume of the cruise ship is calculated using the following equation (Eyres & Bruce, 2012):

$$GT = (0.2 + 0.02 \log_{10} V) \times V \quad (3)$$

Eq. (3) requires the use of numerical methods or the use of iterative techniques to approximate internal enclosed volume (V). Volume facilitates the calculation of the number of decks and the area of Main Vertical Zones (MVZs) per deck. MVZs are vertical sections separated by bulkheads along the ship's length, with fireproof insulation between them to meet fire safety requirements stipulated by the Safety of Life at Sea (SOLAS) regulations. Each MVZ per deck represents a distinct area that is populated with cabin rooms, stairways, elevators, corridors, and service rooms, such as HVAC rooms and other service-related areas.

For the sake of simplicity, cabin rooms were categorized into four main types, although further sub-classifications exist. The model required users to input the percentage of hotel system space allocated to

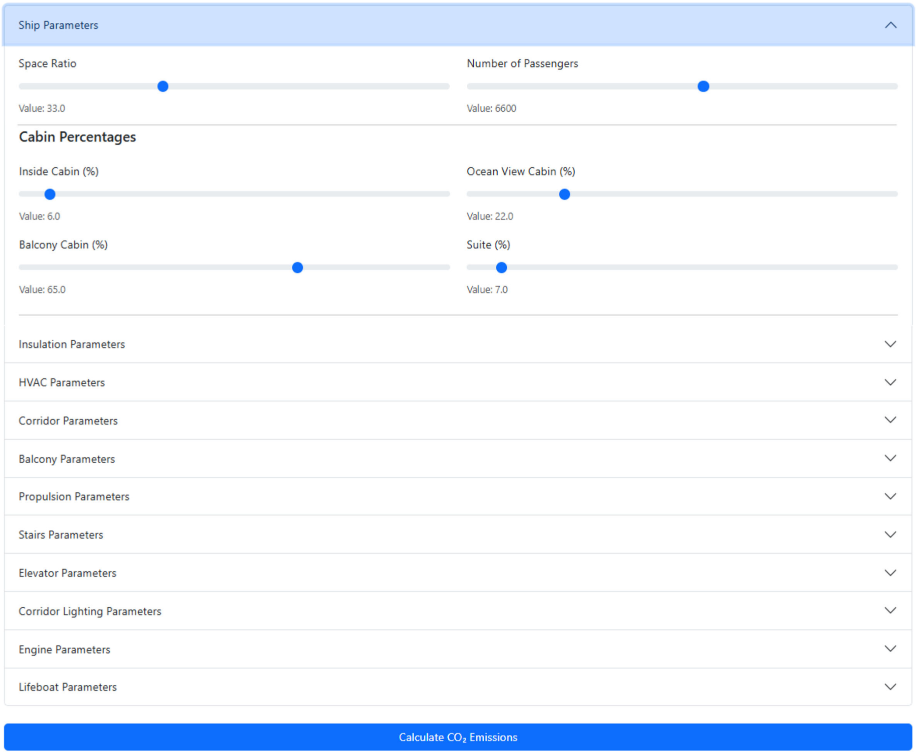

Figure 3. Web-based Interactive GUI DSE form for setting up various design configurations

cabin areas and the percentage of each type of cabin per MVZ per deck as shown in Figure 3.
The total number of cabins per MVZ per deck was calculated to determine the mass of cabin room components, which depends on luxury level due to material variations. Cabin components include structural panels, doors, furniture, electronics, flooring, bathroom ceramics, and plumbing fixtures. Mass estimation used kg/m^2, with mass proportional to the cabin area. Balcony cabins and suites included additional calculations for balustrades and doors. The model accommodated various cabin types per MVZ per deck, outputting material composition and area data.
Corridor areas were calculated based on the cabin type they serve, as more luxurious cabin types require wider corridors. The calculation of corridor areas informs the material requirements for sidewalls, flooring, and ceilings. Flooring materials consist of leveling compounds and carpet finishes, which vary according to the cabin's luxury level. The model computed total mass, with lighting design based on illumination needs.
Stairways within the hotel system were classified into passenger stairs and service stairs. Passenger stairs facilitate passenger mobility between decks, while service stairs support crew movements and enable emergency evacuation in the event of fire or other emergencies. The model allowed the selection of different configurations of stairs based on the requirements. The material required was calculated for stairs fabrication. Area requirements were also calculated, considering the width of stair flights and landing areas. Elevators were divided into two categories: passenger elevators and service elevators. Passenger elevators were typically grouped in banks while service elevators operated alongside service stairways to facilitate crew operations and had material determined using manufacturer data.
The HVAC system, accounting for up to 16 kg/m^2, included equipment and air ducts, with each MVZ requiring a separate system. Mass calculations were stored for analysis. The model's output presented material composition in kilograms, with CO_2 emissions calculated using:

$$C_m = \sum_{i=1}^{n} (M_{mi} \times EF_{mi}) \quad (5)$$

Where C_m is the manufacturing CO_2 emission of material, M_{mi} is the total amount of type i material required and EF_{mi} is the CO_2 emission factor of type i material. Eq. (5) allowed to calculate emissions by multiplying the material mass by the emission factor for each material type. Calculation of CO_2 emission due to transportation from specific procurement channels for each material was performed using the following equation:

$$C_{tr} = \sum\nolimits_{i=1}^{n} (M_{mi} \times TF_i \times D_i) \tag{6}$$

Where C_t is the CO_2 emission due to the transportation of the material. M_{mi} is the total amount of type i material to be transported, TF_i is the CO_2 emission factor of the transport mode i (sea, train, road, or a combination) and D_i represents the transportation distance of the material i based on geographic location. The model revealed that transportation emissions account for approximately 5% to 8% of the total CO_2 emissions associated with the cruise ship's hotel system, underscoring its significant contribution to overall environmental impact. The material and transportation CO_2 emission data was stored in a central repository and fed to a decision-support environment as shown in Figure 1.

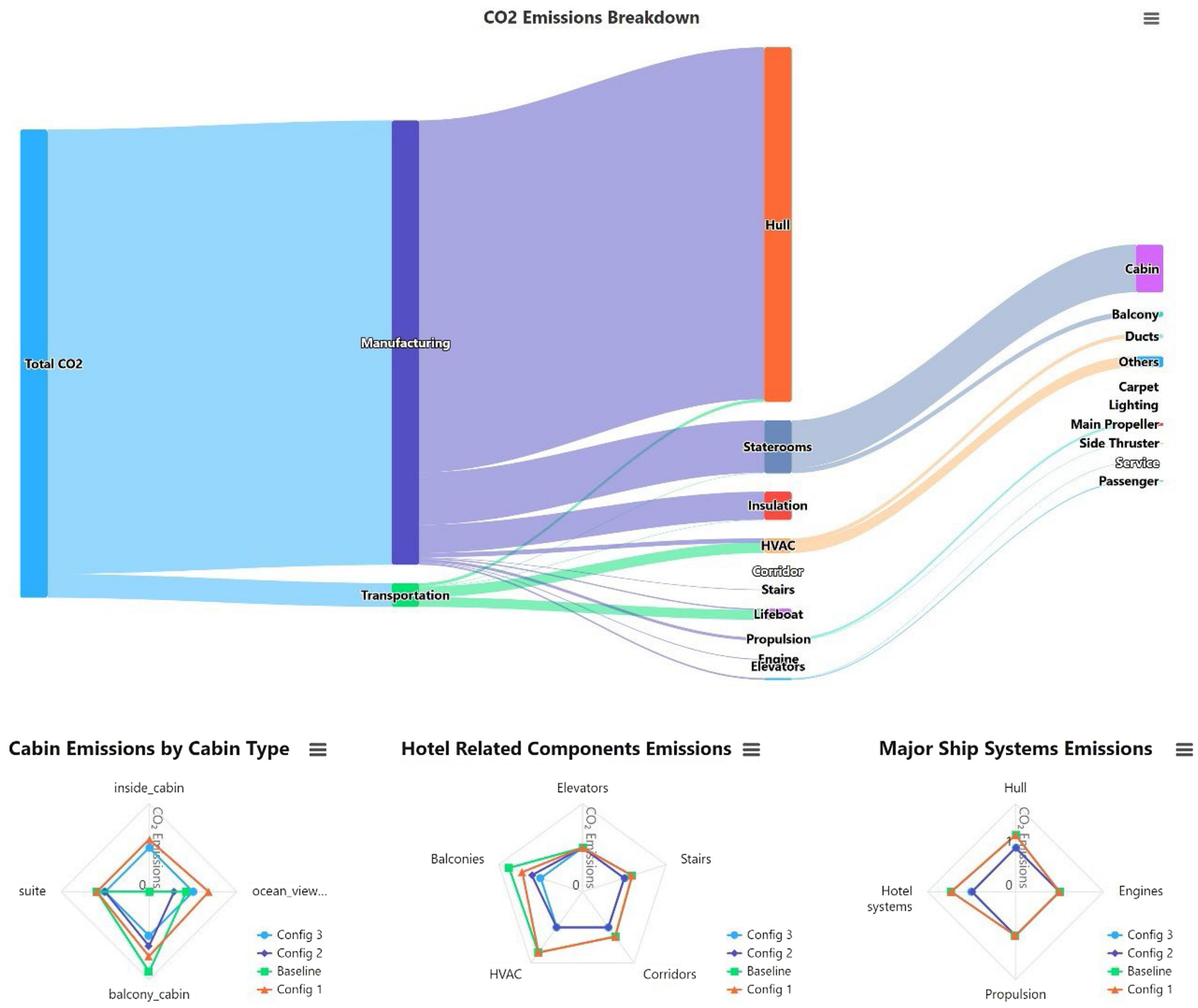

Figure 4. CO_2 Emissions breakdown and comparison of different configurations with baseline

In Figure 4, four different configurations were simulated. A baseline was selected having a space ratio of 33 and for a total of 6600 passengers with typical distribution of cabin. Config 2 has the same high-level parameters, yet the cabin distribution was altered, and two-thirds of the cabin rooms were selected as balcony rooms. Similarly in Config 3 and 4, the high-level parameters were the same (space ratio 50 and for 8000 passengers), the only difference was the cabin distribution. The results showed that increasing balcony cabins resulted in more CO_2 emissions as there were no balconies for ocean view and inside cabins. So, overall material utilization increased. Similarly, the DSE visually depicted the information in the Sankey diagram for CO_2 contribution of each component of the hotel cabin systems. The DSE allowed to store multiple configurations and visually compared them against a pre-selected baseline configuration.

5. Discussion and conclusion

The primary challenge that the approach addresses, identified in the descriptive study, is the ability to perform quick parametric calculations of CO_2 emissions. The capability is particularly valuable in the early design stages, where rapid exploration of alternatives is essential in making informed design decisions. While the approach has the potential to be further generalized, the current stage of research does not yet allow broader generalization. However, it is more utilizable for passenger-carrying ships, where there is significant design freedom and a multitude of design decisions to be made. In contrast, cargo ships are often more constrained and primarily focused on structure benefiting less from this approach. Nevertheless, similar methodologies can be employed to facilitate CO_2 emissions calculations in cargo ship design.

During the development of the approach, several workshops were conducted to perform preliminary verification. Hours-long prototyping sessions at the company's facilities were held which included participants from industrial partners, consulting firms, and researchers. Feedback was gathered on the applicability and usability of the approach. Verification efforts were focused on assessing the logic of the approach, the consistency of the models, and the dependencies between different models. Overall, the applicability of the approach was tested, while its usability was only partially validated, as it was demonstrated on the hotel system of the cruise ship. Some of the key takeaways were:

- The proposed approach advocates for the use of AI in CO_2 estimation and integration to facilitate quick sustainability assessments. While this introduces the risk of misjudgement due to unreliable data generated by AI, this practice was introduced to provide evidence of the potential of data availability in areas where data have historically not been collected, this was done to promote actions to collect real data to eventually substitute AI-generated data.
- The balance between quick simulation and accuracy. It was concluded that during the initial design stage, rapid simulations with relatively higher granularity are quite helpful and acceptance of uncertainty is acceptable because of prioritization of speed of execution and because models could be improved iteratively along the design process.
- AI is currently present and is expected to improve significantly. This will allow to have more accurate estimates for missing data in the future. Thus, reducing uncertainty in the early design process. AI as a tool, is anticipated to be more reliable for overcoming initial design inertia.

The work contributes to the broader discourse on DSS for cruise ship design by providing a more holistic framework that includes scope 3 upstream CO_2 emission. Through it, the approach emphasizes sustainability from the early stages of design, which is important as there is an ever-growing regulatory pressure to consider lifecycle emission in decision-making. Moreover, the research encourages the use of modular and platform-based design, which is becoming a key priority in the maritime industry, However, CO_2 emission integration is still a challenge. Methods and tools in other fields are needed to be adapted to ship design. A challenge in CO_2 assessment is that rarely data are available for exploring new designs quickly and efficiently.

Although the proposed approach includes the integration of engineering and economic KPIs with CO_2 emission at the same level, however, the use case is limited to an initial prescriptive analysis and does not yet integrate all KPIs into the DSE.

The work presented in the paper shall be regarded as a first step toward a more comprehensive approach for modeling and simulations to support value-driven design space exploration in the conceptual design stage of ship design.

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