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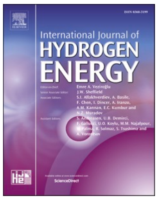

Safety evaluation on ammonia-fueled ship: Gas dispersion analysis through vent mast

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ABSTRACT

The maritime industry is exploring ammonia as an alternative fuel to reduce greenhouse gas emissions. However, the high toxicity of ammonia poses significant safety challenges for onboard handling and storage. This study investigates ammonia dispersion and toxicity levels from vent mast releases on ships, aiming to enhance safety measures for future ammonia-fueled vessels. Using CFD analysis on a 31,000-dwt general cargo ship model, the research examines various release scenarios, considering regulatory requirements, vent mast design, and environmental conditions. Results show that direct ammonia release from the vent mast poses fatal risks to the crew in the accommodation area and on adjacent ships, regardless of current regulatory stipulations. The study recommends installing an ammonia-catching system to reduce concentrations to safe levels of 30 ppm before release. These findings offer crucial insights for improving the safety of using ammonia as marine fuel through risk assessment and management.

Nomenclature

ABS	American Bureau of Shipping
AEGL	Acute Exposure Guideline Levels
B	Breadth
B.L.	Base Line
BV	Bureau Veritas
CAD	Computer-aided Design
CCC	Carriage of Cargoes and Containers
CFD	Computational Fluid Dynamics
CO_2	Carbon Dioxide
DNV	Det Norske Veritas
DWT	Deadweight Tonnage
GHG	Green House Gas
H_2	Hydrogen
HAZID	Hazard Identification
IBC Code	International Code for the Construction and Equipment of Ships Carrying Dangerous Chemicals in Bulk
IDLH	Immediately Dangerous to Life or Health
IGC Code	International Code of the Construction and Equipment of Ships Carrying Liquefied Gases in Bulk
IGF Code	International Code of Safety for Ship Using Gases or Other Low-Flashpoint Fuels
IMO	International Maritime Organization
ISO	International Organization for Standardization
KR	Korean Register
LR	Lloyd's Register
MAN	Maschinenfabriek Augsburg-Nurnberg
MEP	Model Evaluation Protocol
MP	Monitor Point
MSC	Maritime Safety Committee
MVR	Rules for Building and Classing Marine Vessels
NH_3	Ammonia
PRV	Pressure Relief Valve
QRA	Quantitative Risk Assessment
RINA	Registro Italiano Navale
TWA	Time Weighted Average

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US-NIOSH	US-National Institute for Occupational Safety and Health

1. Introduction

1.1. Hazards of ammonia and requirement of vent mast

The maritime industry plays a vital role in global trade, but its reliance on conventional fuels poses significant environmental challenges. In response to combat climate change and to adhere to the International Maritime Organization's (IMO) greenhouse gas (GHG) reduction targets for 2030 and 2050 [1], there is an urgent need to explore alternative fuel options.

Ammonia has emerged as a promising carbon-free energy carrier for marine fuel, having gained significant attention due to its potential as a sustainable marine fuel, and is projected to be classified as useable shipping energy in about three to four years [2].

As a marine fuel, ammonia presents several compelling benefits. When combusted, it produces only nitrogen and water, thus emitting no carbon and making it an optimal alternative fuel to mitigate climate change [3]. Its higher energy density compared to hydrogen makes it more suitable for long-distance shipping, addressing one of the key hurdles in alternative fuel adoption. Additionally, the existing global infrastructure for ammonia production, storage, and transportation can be adapted for maritime use, potentially easing the transition [4]. Moreover, the established safety protocols and experience from using ammonia in industrial applications, like fertilizers, can be applied to its use as a marine fuel.

However, the use of ammonia as a marine fuel presents various design and operational challenges. For instance, Fig. 1 shows the different hazards stemming from ammonia used as marine fuel such as dispersion, fire, explosion, and structural integrity.

In particular, the most significant challenge, and the focus of intense scrutiny, is the toxicity of ammonia. Ammonia exposure can cause severe health effects, including respiratory issues, eye irritation, and skin burns, with high concentrations potentially being fatal [5]. To comprehend the severity of ammonia's toxic effects on ship crew and passengers, it is essential to analyze the relationship between exposure time, concentration levels, and resultant health impacts. Table 1 provides an overview of how varying levels of ammonia exposure influence human health, where the term AEGL (acute exposure guideline levels) denotes acute exposure threshold levels to ammonia and delineates risks across three levels, with level 3 representing fatality. For instance, exposure to a concentration of 1600 ppm for approximately 30 min may result in life-threatening effects. Moreover, at concentrations of 5000 ppm or higher, there's a risk of respiratory arrest regardless of exposure duration, while concentrations exceeding 10,000 ppm may cause immediate skin burns upon contact [6]. This data is vital for identifying potential risks and formulating effective safety measures for the utilization of ammonia as a marine fuel.

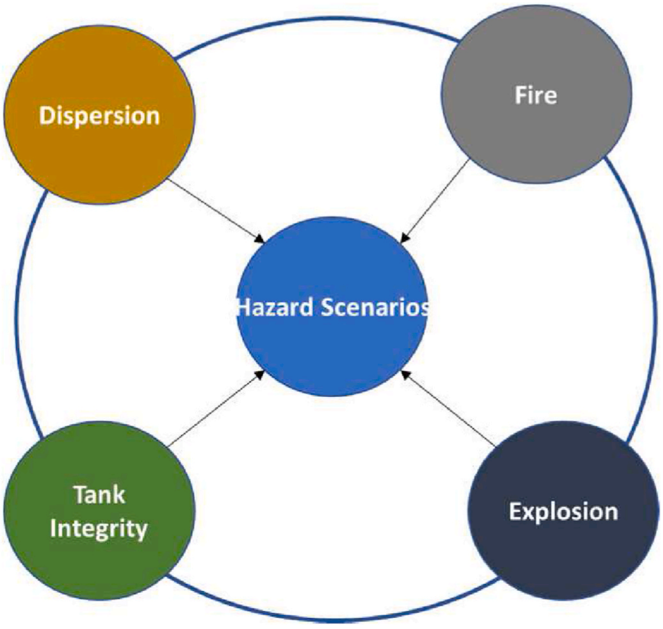


Fig. 1. Major hazards associated with ammonia-fueled ships.

Hence, the high toxicity of ammonia necessitates additional crew training requirements, port infrastructure, and emergency response planning. Crew members need extensive training to handle ammonia safely and respond to potential emergencies. Ports must develop specialized facilities and procedures for handling ammonia-fueled vessels, and coastal communities need to establish specific emergency response plans for potential ammonia releases. The public perception of ammonia's toxicity may also pose challenges, particularly in densely populated port areas. Addressing these concerns through education, stringent safety measures, and transparent communication will be crucial for widespread acceptance [7].

Furthermore, the toxic and corrosive nature of ammonia necessitates specialized materials and equipment for onboard storage and handling, adding complexity to ship design and operation [8]. The industry is working on developing comprehensive safety regulations, improving material selection for fuel systems to prevent leaks, and enhancing bunkering operations to ensure safe fuel transfer [9].

In comparison to traditional hydrocarbon fuels, ammonia has lower reactivity, a higher auto-ignition temperature, a slower laminar flame speed, and requires higher ignition energy, all of which limit its application in engines. Significant research and development are underway to create efficient engines for various types of vessels. For instance, studies by Yan et al. [10,11]; Yang et al. [12], and [13] explored methods to enhance combustion efficiency in internal combustion engines using alternative fuels. Further, recent investigations have significantly advanced the understanding of ammonia as a fuel for internal combustion engines, emphasizing its potential as a zero-carbon alternative and addressing the substantial challenges it presents. Junheng Liu and Liu [14] review ammonia combustion and emission control strategies, emphasizing from experimental studies the need to improve the ammonia in-cylinder combustion quality and develop effective after-treatment systems of ammonia and NOx capture. Jinlong Liu and Liu [15] use CFD models, validated with methane data, to analyze ammonia combustion and emissions. Liu et al. [16] explore converting heavy-duty engines to ammonia, recommending advanced spark timing and higher compression ratios for better combustion. While all studies address the potential and challenges of ammonia as a fuel, they differ in focus. These studies collectively highlight the multifaceted approach required to optimize ammonia combustion for practical use in internal

Table 1
The ammonia risk level for different exposure durations and ammonia concentrations.

Risk level	Exposure duration (in min)			Effect on humans
	10	20	30	
AEGL-1	30 ppm	30 ppm	30 ppm	Discomfort, irritation, or asymptomatic numb effect
AEGL-2	220 ppm	220 ppm	160 ppm	Irreversible or other serious and long-lasting adverse health effects or impaired ability to escape
AEGL-3	2700 ppm	1600 ppm	1100 ppm	Life-threatening health effects or death

combustion engines.

Despite these challenges, ongoing research, technological advancements, and regulatory developments are focused on mitigating the risks associated with ammonia as a marine fuel. Considering the safety of crew and passengers to be of paramount importance, compared to conventional-fueled ships, the ammonia-powered ship requires the installation of a vent mast connected to the ventilation systems, for the safe release into the atmosphere such as in case of accidental leakage [17]. In addition, the safe release and installation of the vent mast at an appropriate location on the ship becomes critical in the design process. This study aims to evaluate ammonia dispersion from the vent mast for the different release scenarios and provide design recommendations to enhance safety.

1.2. Ammonia accident statistics

To understand the potential risks in terms of ammonia toxicity and associated fatalities when using ammonia as a marine fuel, lessons from existing ammonia-fueled ship accidents would be ideal. However, with no ongoing operation of ammonia-fueled ships and limited usage in the automobile industry, there is insufficient historical data related to accidents to evaluate their safety. An alternative approach involves analyzing accidents in onshore ammonia production/consumption plants to indirectly assess the risks of ammonia-fueled ships. Certain insights can be gained from accidents involving ships carrying ammonia as cargo, particularly due to the lack of experience in ammonia-fueled ships.

Numerous accidents related to ammonia have been reported on land, particularly in the fertilizer and food industries. For instance, in a closed refrigerator workshop in Shanghai on August 31, 2013, 41 out of 58 employees suffered chemical burns due to anhydrous ammonia leakage [18]. A Canadian government report documents 59 ammonia leak incidents in British Columbia between 2007 and 2017, with 14 resulting in casualties. Fig. 2 illustrates the annual trend of accidents in ammonia facilities in the region, showing a consistent increase over the years [19], indicating that ammonia accidents are no more of a temporary problem in the past, but are still an ongoing problem. This illustrates the safety requirements for ammonia capture and release to the atmosphere within a safe level.

In summary, there is a need for preventive measures when handling ammonia at all stages of its operations, as ammonia transport is expected to increase in the future, combined with a lack of effective regulation, operational experience, training, and potential corruption at sea. Further, this necessitates the need for a proper mechanical ventilation system, and a safe release via vent mast could mitigate the toxic release of ammonia levels and reduce the fatality risk. In other words, the potential for utilization of ammonia as a ship fuel poses added safety concerns in terms of fatality, and mitigation measures in terms of ammonia capture and safe release become of paramount importance compared to traditional ships.

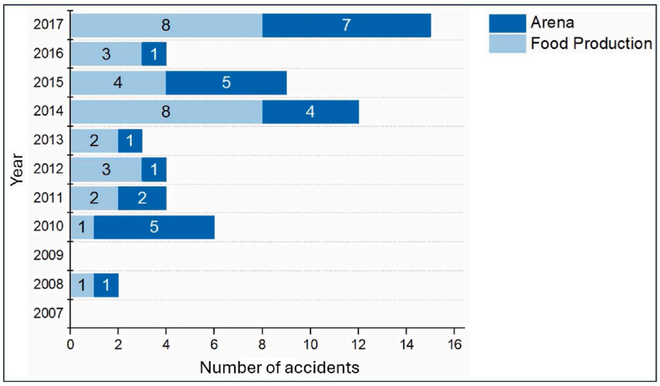


Fig. 2. Ammonia leakage accident statistics recorded in British Columbia [19].

1.3. Regulatory gap in the design of vent mast for ammonia-fueled ship

1.3.1. International regulations

Currently, various international regulations govern the safe transport of ammonia on ships, including the IBC Code [20] for aqueous ammonia, and the IGC Code [21] for anhydrous ammonia. However, for utilizing ammonia as a shipping fuel, the relevant regulation is the IGF code [22], established in 2017. In 2020, the IMO approved the '*Interim Guidelines for the Safety of Ships Using Methyl/Ethyl Alcohol as Fuel*' (MSC.1/Circ.1621) [23]. International regulations in the form of Interim Guidelines for the safety of ships using ammonia as a fuel are currently under development within the IMO, falling under the purview of the IMO Sub-Committee on Carriage of Cargoes and Containers (CCC). Table 2 lists the documents containing the specific regulations for

Table 2
The ammonia risk summary of IMO regulation developments on using ammonia as a marine fuel.

Reference No.	Document title	Summary
MSC 104/15/9 [24]	Development of non-mandatory guidelines for the safety of ships using ammonia as fuel	Proposes a new output to develop non-mandatory guidelines for the safety of newly built ships using ammonia as a fuel
MSC 104/15/10 [25]	Hazard identification of ships using ammonia as a fuel	Provides the results of hazard identification of ships using ammonia as a fuel
MSC 104/15/30 [26]	Necessity of deliberations on operational safety measures and fire safety measures	Points out the necessity of careful deliberations on operational safety measures and fire safety measures for ammonia-fueled ships
CCC 7/3/9 [27]	Report from the correspondence group and proposal for developing guidelines for the use of ammonia and hydrogen as a fuel	Provide comments on the progress made in the report from the correspondence group on the development of technical provisions for the safety of ships using low-flashpoint fuels and propose to include the development of two separate guidelines for the safety of ships using ammonia and hydrogen as fuel in the work plan of the CCC Sub-Committee
CCC 7/INF.8 [28]	Forecasting the alternative marine fuel: ammonia	Introduces the outline of the outlook of ammonia as green ship fuel
CCC 8/13/1 [29]	Development of guidelines for the safety of ships using ammonia as fuel	Provides information on possible issues to be considered for developing guidelines for the safety of ships using ammonia as fuel and proposes the way forward
CCC 8/13/2 [30]	Comments on document CCC 8/13	Proposes a review of the environmental effect which will be considered in future discussions
CCC 8/13 [31]	Report of the Correspondence Group (safety information for the use of ammonia)	Provides the report of Correspondence Group on the development of technical provisions for the safety of ships using low-flashpoint fuels, regarding the collection of the safety information for the use of ammonia.
CCC 9 [32]	Amendments to the IGF code and development of guidelines for alternative fuels and related technologies (report of the working group)	Discussed overarching principles and directions for the further development of the draft interim guidelines for ships using ammonia as fuel towards finalization.

ammonia. These Interim Guidelines have been closely aligned with the IGF Code, as adopted by resolution MSC 391(95).

In the absence of specific regulations governing ammonia use on vessels, the IGF code, initially designed for natural gas applications at sea, serves as the primary regulatory framework for integrating ammonia systems onto ships. As per the IGF code, vent exits are recommended to be positioned at a height not less than $B/3$ or 6 m, whichever is greater, above the weather deck, and at least 6 m above working areas and walkways. Additionally, the IGF code stipulates that vent mast outlets must be situated at a minimum radius of 10 m away from accommodation, service, or other non-hazardous spaces. These design values, however, need to be examined against different ship types using gas dispersion analysis.

Further, IGC regulation 8.2.10.1 [21] recommends that "*the discharge will be unimpeded and directed vertically upwards at the exit*", preventing the installation of any components which restrict the free flow, or create counterpressure, in the venting pipe after the valve. In other words, filters, reactors or selective catalytic oxidizers should not be installed to reduce ammonia in its gaseous phase. Due to these serious limitations, ammonia-fueled ships should be built with the aim of zero leakage or release with a very low concentration.

1.3.2. *Class rules and guidelines*

To further identify the relevant rules and guidelines specific to the design and safety of the vent mast, the following list of documents (along with the year of publication) from the major classification societies developed for ammonia-fueled ships is used.

- LR – '*Rules and Regulations for the Classification of Ships using Gases or other Low-flashpoint Fuels*' [33]
- ABS - '*Requirements for Ammonia Fueled Vessels*' [34,35]
- ABS – '*Guide for Ammonia Fueled Vessels*' [36]
- ABS – '*Rules for Building and Classing Marine Vessels (MVR) - Part 5C, Specific Vessel Types (Chapters 7–18)*' [37].
- BV - '*Ammonia-Fuelled Ships*' [17]
- DNV - '*Part 6 additional class notations - Chapter 2 Propulsion, power generation and auxiliary systems*' [38]
- KR - '*Guidelines for Ships Using Ammonia as Fuels*' [39]
- NK – '*Guidelines for Ships Using Alternative Fuels*' [40]
- RINA – '*Amendments to the "Rules for the Classification of Ships"*' [41]

Although most of these class rules are broadly consistent with the IGF code, there are currently no international standards applicable to ammonia-fueled ships [42]. As per ABS [34], where venting of ammonia is necessary for safety reasons, systems are to be designed to minimize the accumulation of gas released to the open space and to facilitate dispersion into the atmosphere so that minimum safe flammable and toxic levels can be maintained within acceptable distances from the vent mast or riser location.

Furthermore, different classification societies have slightly varying thresholds for detecting ammonia gas levels. Methods for setting these thresholds include Time Weighted Average (TWA) and Immediately Dangerous to Life or Health (IDLH) levels of the US-National Institute for Occupational Safety and Health (US–NIOSH), considering that crew members might be repeatedly exposed to ammonia during ship operations. For example, KR follows a TWA of 25 ppm as the allowable concentration on ships. Similarly. ABS and NK adhere to the 25 ppm threshold, while BV and DNV recommend 30 ppm, and RINA suggests 50 ppm. In these toxic areas, gas dispersion simulation studies can be used to obtain design approval and verify vent mast arrangements.

ABS, BV, and DNV class mandates that the vent mast outlet be positioned at least 25 m (or B, whichever is less) away from any air intake opening, outlet, or opening to accommodation spaces, service spaces, control stations, or other non-hazardous areas. Further, gas dispersion analysis is recommended by class societies, especially when ensuring the safety of smaller vessels (less than 90 m in length) in toxic areas is of primary concern. On the other hand, KR stipulates at least 15 m apart toxic area in the horizontal direction.

Reflecting this need for fuel management, BV classification established regulations such as prohibiting direct venting under normal conditions and venting for tank pressure control, ensuring emission concentration of less than 30 ppm from the vent mast, requiring a dilution device before venting through combustion/water/air and so on, and permitting direct venting only in case of fire [17].

1.4. *Research gap*

In the literature, numerous experimental and CFD studies on ammonia dispersions are available in the application to onshore facilities. For instance, Bouet et al. [43] conducted large-scale ammonia release to the atmosphere in industrial applications to understand ammonia dispersion patterns. Nielsen et al. [44] conducted field experiments on liquified ammonia and validated 27 different release rates and concentration measurements. Min et al. [45] focused on chemical processing plants, exploring the efficacy of water curtains as a novel mitigation strategy. Salamonowicz et al. [46] delved into the critical role of ventilation in ammonia engine rooms in industrial plants, offering insights into the management of ammonia dispersion in enclosed spaces. Labovský and Jelemenský [47] broadened the scope to include storage and manufacturing plants, enhancing simulation precision with dynamic boundary conditions.

Even with the ongoing active development of ammonia as a marine fuel, research on ammonia dispersion in marine applications remains limited. For instance, Duong et al. [48] compared the dispersion characteristics of ammonia and LNG (liquefied natural gas) during bunkering operations, noting significant impacts from ground geometry, weather, and traffic conditions on dispersion characteristics and distance in bunkering areas. Ammonia displayed broader dispersion and longer dispersion periods than LNG under equivalent conditions, necessitating larger safety zones. Ng et al. [49] investigated ammonia dispersion behavior in Singapore during bunkering operations under various operational and weather conditions. Yadav and Jeong [50] analyzed the safety evaluation of ammonia dispersion in a ship engine room using CFD and demonstrated that the ammonia dispersion depends on numerous factors such as position, area, and direction of leak, pressure, and temperature of ammonia gas, and ventilation. Yang and Lam [51] performed a risk assessment for different ammonia releases during bunkering operations and concluded that wind speed is the most critical factor in small and large releases, while large release is dominated by the hose diameter. Jeong et al. [52] performed a risk assessment on the LNG bunkering operations and established safety zones for LNG-fueled ships. Cao et al. [53] assessed potential risks associated with LNG leakage from the vent mast of an Aframax oil tanker, emphasizing heightened vent mast positions to enhance ship design safety, with the minimum height for LNG storage surpassing tank height (10 m). Further studies on the LNG gas dispersion studies can be found, for instance, Ref. [48,54–60]. Blaylock and Klebanoff [61] conducted a hydrogen (H_2) gas dispersion analysis from the vent mast releases and found that despite the buoyancy of hydrogen, wind affects strongly hydrogen speed exiting the vent mast. In summary, there is currently a lack of available studies on ammonia gas dispersion in shipping, especially concerning the need for ammonia catching and examining the safe release of ammonia from vent masts with the prevalent regulations.

1.5. *Motivation and novelty*

Currently, no existing studies are addressing the safe release of ammonia from vent masts during ship operations. This is particularly significant due to the low energy density of ammonia, which necessitates more storage space and increases the likelihood of potential leakage, especially when stored at high pressures. Recently, the NH3CRAFT (2022) project [62], focusing on the safe and efficient storage of ammonia within ships, clearly underscores the necessity for a dedicated study on ammonia dispersion from vent masts during HAZID (Hazard Identification) workshops, as well as an examination of the adequacy of current rules and regulations. Therefore, this study aims to fill these gaps through numerical simulations to comprehend dispersion behavior and ammonia concentrations under varying environmental conditions, vent mast positions and heights, and release rates and ultimately to provide design safety recommendations for the safe release of ammonia from the vent mast.

2. Research methodology

Fig. 3 illustrates the flowchart outlining the various steps entailed in the research methodology adopted in this study.

- In Step 1, the scope of the study is defined, utilizing an ammonia retrofit general cargo ship as the demonstrator vessel.
- Step 2 entails the definition of different dispersion scenarios, encompassing the selection of various parameters such as vent mast locations, release heights, wind speed and direction, and release rates from the vent mast.
- Step 3 involves conducting CFD modeling for the developed scenarios, which includes CAD modeling of the ship, establishing appropriate boundary conditions, mesh convergence criteria, and selecting the solver. Further, a grid convergence study is performed to determine the optimal grid size for running the scenarios with sufficient accuracy.
- Step 4 involves post-processing the scenarios, which includes generating 2D and 3D plots to measure ammonia concentrations, vapor cloud size, and dispersion patterns. The results are then compared with existing rules and regulations regarding vent mast positioning and release, as discussed in Section 1.3.
- In Step 5 based on the aforementioned findings, necessary safety recommendations are provided to enhance the safety of ammonia release via vent mast. The subsequent sections elaborate on each step using a case study approach.

The following sections elaborate on each step using a case study approach.

3. Case study

3.1. Target ship

For the case study, a real full-scale A-class general cargo ship, with a deadweight tonnage of 31,000 dwt and a cargo hold capacity of 39,700 cubic meters is used, as depicted in Fig. 4 (a). It measures approximately 194 m in length, has a breadth of about 28.2 m, and a maximum draught of 11.20 m (see Table 3). Designed for efficient cargo operation, the vessel features two deck cranes located on the centerline at both the fore and aft sections of the cargo deck, complemented by another pair of cranes on the port side of the cargo deck. For the case study, this ship is used to retrofit the ammonia fuel storage and handling system for running an ammonia/diesel dual-fuel engine.

Fig. 4 (b) shows a CAD model of the key components of the ammonia-fueled ship considered for the study which includes the potential installation location of the storage tanks, fuel preparation room, accommodation area, and the vent mast on the deck. In addition to the two metallic tanks installed on the upper deck, Cargo Hold No. 5 space has been allocated to store fuel tanks in containerized solutions, to explore scalability options (refer to Fig. 5 in the drawings). This arrangement is intended to ensure that the total capacity, approximately 750 m^3 of ammonia, is sufficient to power the engine for at least a single ship voyage.

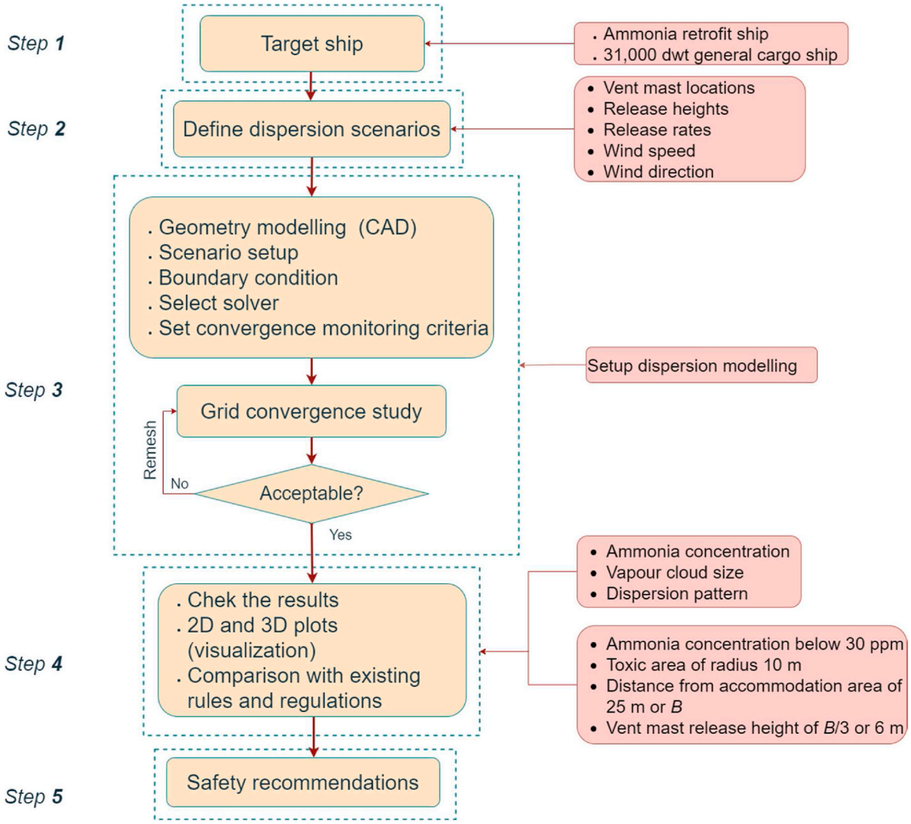


Fig. 3. Research methodology

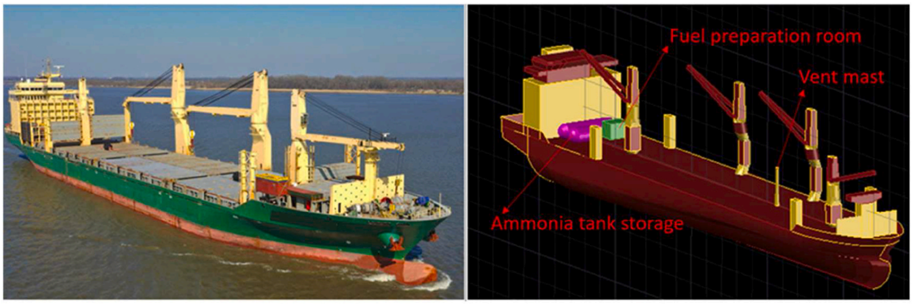


Fig. 4. (a) Target ship - 31,000 dwt A-class general cargo ship (left), (b) CAD model of the ammonia retrofit ship showing ammonia storage tank and its auxiliary components (right).

Table 3
Main ship particulars of the ammonia-retrofit ship.

Sl No.	Unit	Characteristics
Type of ship		General Cargo
Length overall	m	194
Breadth (molded)	m	28.20
Depth (molded)	m	15.6
Draught (molded)	m	11.20
DWT	ton	31,000
Cargo capacity	m^3	39,700

3.2. *Vent mast design scenarios*

Fig. 5 presents the general arrangement of the ship, illustrating the three best possible locations (scenarios) of the vent mast for the target ship considered in the study.

In addition, the chosen locations comply with the IGF code and class rules, as detailed in the introduction section (Section 1.3). Scenario 1 features a vent mast installed at a baseline (B.L.) distance of 40 m and release height of 6 m, adhering to the minimum release height requirements of the IGC and class rules. In Scenario 2, the vent mast remains at a B.L. distance of 40 m but with a higher release height of 10 m. Scenario 3 situates the vent mast 108 m from the aft side of the vessel at a release height of 10 m, adhering to the requirements set by some classification societies - ABS, BV, and DNV. Scenario 1 benefits from the vent mast's proximity to the storage tanks on the deck, facilitating the rapid release of any potential ammonia leaks. However, its closeness to the accommodation area poses a heightened risk of toxicity, particularly under unfavorable environmental conditions. Conversely, in Scenario 3, the vent mast is positioned as far as feasible from the accommodation area (B.L. 108 m), aiming to mitigate toxicity risks. However, the greater distance may lead to pressure drop issues during ammonia release. Additionally, given the ship's proximity to the crane operation area, a vent mast in Scenario 3 may be susceptible to potential damage from crane collisions.

3.3. *Ammonia release and environmental parameters*

For the three above-mentioned vent mast installation scenarios, several CFD simulations were performed under varying environmental conditions and leak properties to capture worst-case scenarios. Table 4

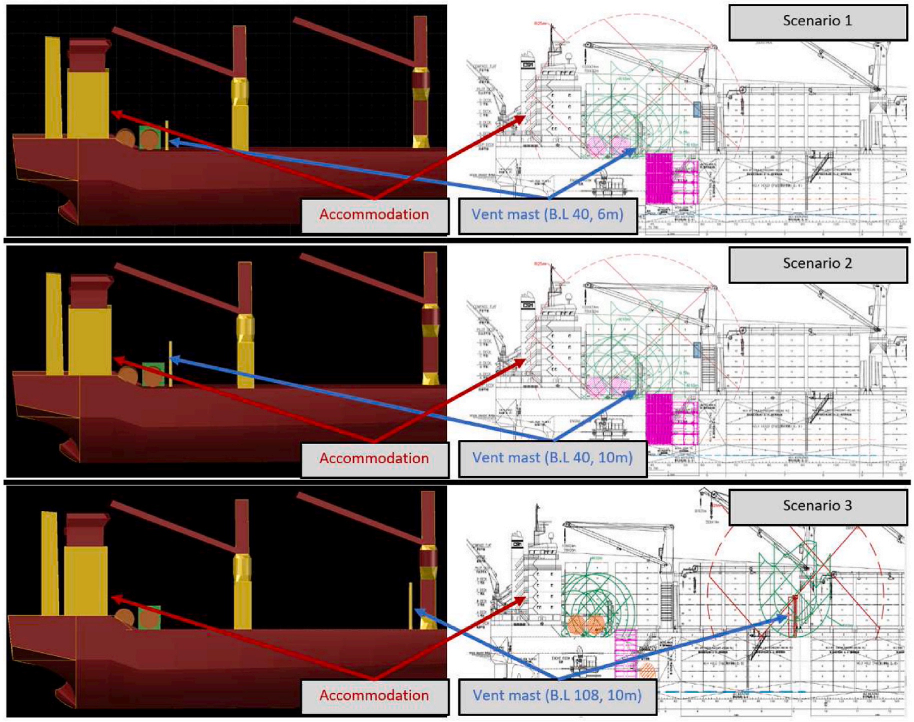


Fig. 5. Comparison of simplified CAD models (left) with general arrangement drawings (right) depicting vent mast and accommodation locations across three dispersion scenarios

summaries the different parameters considered in this study. In the study, leakage from the largest tank with a capacity of 290 m^3 was examined. The pressure and temperature were set to match the pressure relief valve (PRV) settings (17.8 bara and 45 °C); beyond this threshold, the PRV triggers and releases ammonia via the vent mast. Adhering to IGC regulations, all releases were assumed to occur in a vertically upward direction. Additionally, the study accounted for three wind speeds—calm (0.1 m/s), light air (1 m/s), and gentle breeze (5 m/s)—and three wind directions: 180°, 225°, and 270°, with an ambient temperature of 20 °C and pressure of 1 bara, where Fig. 6 shows the definition of wind direction used in the study.

4. Numerical modeling of ammonia Gas dispersion

Accurate dispersion modeling is crucial for assessing the potential consequences associated with ammonia release from the vent mast. To address this critical need, FLACS (Flame Acceleration Simulator) software was chosen to conduct this simulation. Developed by Gexcon AS in 1980, FLACS is a specialized CFD tool designed for process safety applications. Unlike general CFD tools, it is tailored to simulate complex scenarios in large-scale 3D geometries, such as gas dispersion, explosions, blast wave propagation, and fires - critical concerns in industries where the majority of major property losses involve such incidents. FLACS-CFD offers more accurate predictions than simpler analytical models by solving conservation equations with actual initial and boundary conditions [63].

This advanced capability makes it particularly well-suited for simulating ammonia releases and their potential impacts. Given its specialized nature and importance in safety assessments, it is crucial to understand the underlying models used in FLACS. This section presents briefly the dispersion model involved in CFD simulations using the FLACS tool.

4.1. Governing equations

The flow of ammonia as it disperses into the atmosphere was calculated through the ideal gas equation of state based on the Reynolds-averaged Navier-Stokes (RANS) equation and the standard k-ε model with the standard set of constants for turbulence, considering the buoyancy effects [64]. The numerical model utilizes a 2nd-order central difference scheme for resolving diffusive fluxes and a 2nd-order kappa scheme for resolving convective fluxes. The RANS approach addresses the Navier-Stokes equations for mean flow variables and focuses exclusively on calculating large-scale motions. Its simplicity and low computational demands make it particularly suitable for the ammonia gas dispersion study. While the use of temporal averaging in the RANS method typically limits temporal resolution, it can still provide good spatial resolution.

Table 4
Key parameters considered for vent mast location scenarios.

	Parameters		Scenario 1	Scenario 2	Scenario 3
Ammonia storage tank	Volume	m^3	290	290	290
	Pressure	barg	17.8	17.8	17.8
	Temperature	°C	45	45	45
Atmospheric conditions	Temperature	°C	20	20	20
	Pressure	bara	1.0	1.0	1.0
	Wind speed	m/s	0.1, 1, 5	0.1, 1, 5	0.1, 1, 5
	Wind direction	°	180, 225, 270	180, 225, 270	180, 225, 270
Release properties	Release rate	kg/s	10, 30, 50	10, 30, 50	10, 30, 50
	Release position (B.L)	m	40	40	108
	Release height	m	6	10	10
	Release direction	–	Vertically up	Vertically up	Vertically up

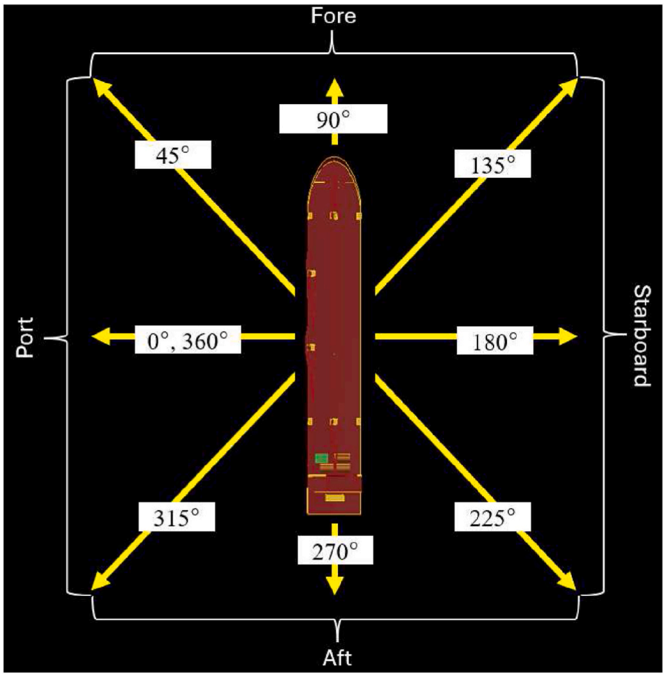


Fig. 6. Definition of wind direction used in the study.

To address the complex behavior of ammonia in the atmosphere, where variations in atmospheric density are prevalent, the governing equation was extended to include the Favre average concept. This modification required the utilization of the Favre mean compressible flow equation, a grid arrangement based on Cartesian coordinates, and a comprehensive set of essential parameters. These adjustments were meticulously implemented through the finite volume method [65].

The process of ammonia leakage was thoroughly elucidated using fundamental principles, including the conservation of mass, energy, momentum, and species transport equations [48], as provided below:

Conservation of mass:

$$\frac{\partial}{\partial t}(\beta_v \rho) + \frac{\partial}{\partial x_j}(\beta_j \rho u_j) = \frac{\dot{m}}{V} \tag{1}$$

where, β_j, β_v and u denote porosity, volume porosity, and velocity component (m/s), respectively. $\dot{m}$, ρ, and V represents mass rate (kg/s), density of the fluid (kg/m^3), and volume (m^3), respectively.

Conservation of momentum:

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial}{\partial x_j}(u_i \rho u_j) = -\frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial u_i}{x_j}\right) + \rho g + F_i \tag{2}$$

where, F_i = resistant by walls, t = time (s), g = gravitational acceleration (m/s^2), p = pressure (kPa), x_j = the general Cartesian coordinate, and μ = dynamic viscosity of the fluid (Pa·s)

Conservation of energy:

$$\frac{\partial \rho h_s}{\partial t} + \nabla(\rho u h_s) = \frac{Dp}{Dt} - \nabla \dot{q}'' + \tau \nabla u \tag{3}$$

where, h_s = specific enthalpy (kJ/kg), $\dot{q}''$ = rate of heat transfer per unit area per unit time (J/s), and τ = stress tensor in the fluid (Pa)

Standard k-ε model transport equation:

$$\frac{\partial}{\partial t}(\rho K) + \frac{\partial}{\partial x_j}(\rho K u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{u_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_b \tag{4}$$

where, K = kinetic energy turbulent (m^2/s^2), G_b = production of kinetic energy turbulent by buoyancy, G_k = production of kinetic energy turbulent by velocity gradients, S_b = values defined by the user, σ_k =

turbulent Prandtl-Schmidt number for k, and u_t = eddy viscosity.

In addition, the ammonia leakage rate is modeled using the Bernoulli equation:

$$Q = C_d \times A \times \sqrt{2 \times \rho \times \Delta P} \tag{5}$$

where, Q = ammonia leakage rate (kg/s), C_d = discharge coefficient (a dimensionless constant that depends on the shape and size of the hole), A = area of the leakage hole (m^2), ρ = density of ammonia (kg/m^3), ΔP = pressure difference between the inside and outside of the container (Pa)

Wind inlet profiles are imposed according to the Monin–Obukhov length (L) and the atmospheric roughness length (z_0) for the given atmospheric stability class.

4.2. FLACS software validation

The computer program FLACS is mainly used in study, which is a well-established, validated, and approved CFD code for toxic gas dispersion scenarios. The validation of FLACS for simulating gas dispersion scenarios, particularly for ammonia, has been the focus of several key studies.

For example, Hansen et al. [57] and Hanna et al. [66] provided foundational evidence for FLACS's reliability in vapor dispersion modeling. Hanna et al. [66] reported that approximately 86% of FLACS predictions fell within a factor of two of observed values, demonstrating a median relative bias of 20% underprediction and a median relative scatter of about 50%. Hansen et al. [57] utilized the Model Evaluation Protocol (MEP) database to simulate 33 tests across various scales and found that FLACS met or exceeded statistical performance measures for most test groups.

Further validation of FLACS has been demonstrated in studies focusing on large-scale flammable cloud dispersion. Dasgotra et al. [67] used FLACS to model the dispersion of propane and octane in real-scale storage facilities, finding that the predicted cloud sizes corresponded well with observations from recent accidents. Their work highlighted FLACS's capability to provide detailed information on possible worst-case scenarios, which is crucial for risk assessment and safety planning.

Zhang et al. [68]proposed a new equivalent method to obtain stoichiometric fuel-air clouds from inhomogeneous clouds based on FLACS-dispersion simulations. This method, which considers turbulent burning velocity, offers a more accurate representation of explosion loads in risk analysis.

Specific to ammonia dispersion, the works of Tan et al. [69]and Tan et al. [70] offered valuable insights. These studies, validated against small-scale wind tunnel experiments and field studies, revealed that ammonia concentration varies significantly with release rate, wind speed, and release height. Also, these studies observed that ammonia tends to concentrate along the central axis near the release source and exhibits upward movement due to its lower density compared to air. Notably, they found that obstacles can lead to higher ammonia concentrations due to windward side effects and aggregation. These findings emphasized the importance of immediate evacuation from the symmetric plane to the sides in the event of a release.

Building on these studies, Duong et al. [48] conducted a comparative analysis between ammonia and LNG. This research, validated against experimental data and existing literature, revealed that ammonia exhibits a greater dispersion range and longer dispersion time compared to LNG under equivalent operational conditions. These characteristics necessitate more extensive safety zones for ammonia.

The validation methodologies employed across these studies were comprehensive, encompassing comparisons with experimental data, the use of statistical performance measures, comparative analyses, and detailed examination of concentration and velocity fields.

Additionally, Bleyer et al. [71]compared FLACS explosion simulations with experiments conducted in a Pressurized Water Reactor (PWR) Steam Generator casemate scale down with hydrogen gradients, further demonstrating FLACS's capability in modeling complex combustion scenarios.

This multi-faceted approach to validation has solidified the position of FLACS as a reliable tool for simulating gas dispersion scenarios, including the complex behavior of ammonia under various conditions.

4.3. Computational domain and boundary conditions

In the FLACS-CFD simulation, the computational grid is modeled with cubic or rectangular cells separated by both vertical and horizontal grid lines, essentially forming a unified 3D Cartesian grid, where the complex models are represented by a porosity concept. The simulation was executed within a 3D computational domain using a full-scale ship model, with an overall dimension of 390 m × 200 m × 287 m along the X, Y, and Z axes, respectively. This domain was refined using a total of 610,242 grid cells, with the smallest grid cell size measuring 0.6 m in all planes. FLACS employs both macro and micro-sized gids, along with stretched grid domains to effectively capture the dispersion while simultaneously reducing the computational time [72]. Grid cells expanded outward in all directions from the point of leakage. Fig. 7 shows the computational domain, grid details, and boundary conditions employed. Inlet boundary conditions included specified wind profiles, and stability classes were applied to compute turbulence kinetic energy and turbulence dissipation rate profiles. Further, it was assumed that the vessel was situated in an extensive open water body rather than a confined area.

The simulation was set up to represent a vessel in a vast open-water environment. To accurately model this scenario, the sea surface and the ship's stern were designated with a "NOZZLE" boundary condition. This condition effectively simulates the sea surface and allows for the outflow of wind. The remaining surfaces of the ship, including its bow, starboard, port, and upper sides, were assigned a "WIND" boundary condition. This setup enables the model to account for the interaction between these surfaces and the surrounding air. By implementing these boundary conditions, the simulation aimed to replicate the desired environmental conditions, with a particular focus on recreating wind flow from the ship's bow towards its stern. To ensure a comprehensive dispersion study, the model incorporated stable wind conditions, utilizing a Pasquill stability class F and setting the ground roughness parameter to 0.0002 m. These specifications allowed for a more precise representation of the atmospheric conditions affecting the vessel in its open-water

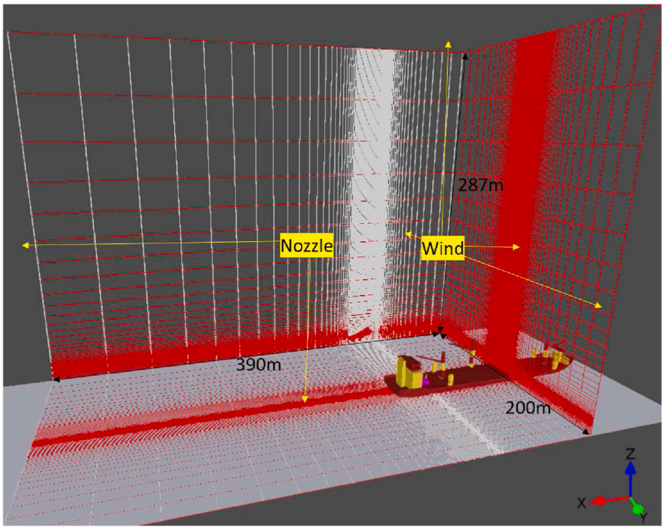


Fig. 7. Details of grid domain, modeling, and boundary conditions used in the simulation.

setting.

A steady-state solver is utilized to investigate dispersion patterns and concentration profiles of ammonia during continuous or prolonged releases, with the expectation that the ammonia plume emanating from the vent mast will attain a stable condition.

4.4. Installation of the monitoring points

To capture the concentration of ammonia gas after a leak at key locations, a total of seven ammonia gas monitoring points (MPs) were positioned around the exterior of the ship, as depicted in Fig. 8 for the scenarios considered. The first three MPs, located near the vent mast, are capable of detecting increased ammonia levels during a leak. The primary area of focus in this study was the placement of detectors 4 to 7. These were strategically placed close to the areas essential for the crew's work and living spaces. The exact locations of these MPs, in alignment with the coordinate system of the ship shown in Fig. 8, are provided in Table 5.

4.5. Model verification

The dispersion of ammonia is influenced by various factors, encompassing the physio-thermal properties of ammonia, external environmental conditions, the rate of leakage, and the position and complexity of the vent mast in the given scenarios. As such, the chosen grid resolution must be sufficient enough to capture all these gradients and therefore a grid independence analysis is performed, as shown in Fig. 9, for two different MPs.

Three mesh sizes were selected - coarse, medium, and fine. The coarse mesh is comprised of 416,208 cells, while the medium mesh has 610,242 cells, and the fine mesh includes 1,174,932 cells. The sensitivity study examined if the ammonia concentration at MP2, located near the vent mast, and MP6, close to the accommodation area, reached a steady state with different mesh sizes. The findings show that at steady state, the ammonia concentration measured for the two mesh sizes is more or less the same, revealing that the performance of coarse and medium meshes closely matches that of fine meshes. Consequently, considering higher accuracy, a medium-mesh with a grid size of 0.28 m was selected for the actual simulations. The subsequent sections present the results of the sensitivity analysis conducted on release rates, wind direction, and wave direction concerning ammonia gas dispersion from the vent mast.

Table 5
Description of MP installed for different scenarios (refer to Fig. 8 for 2D visualization of MP location).

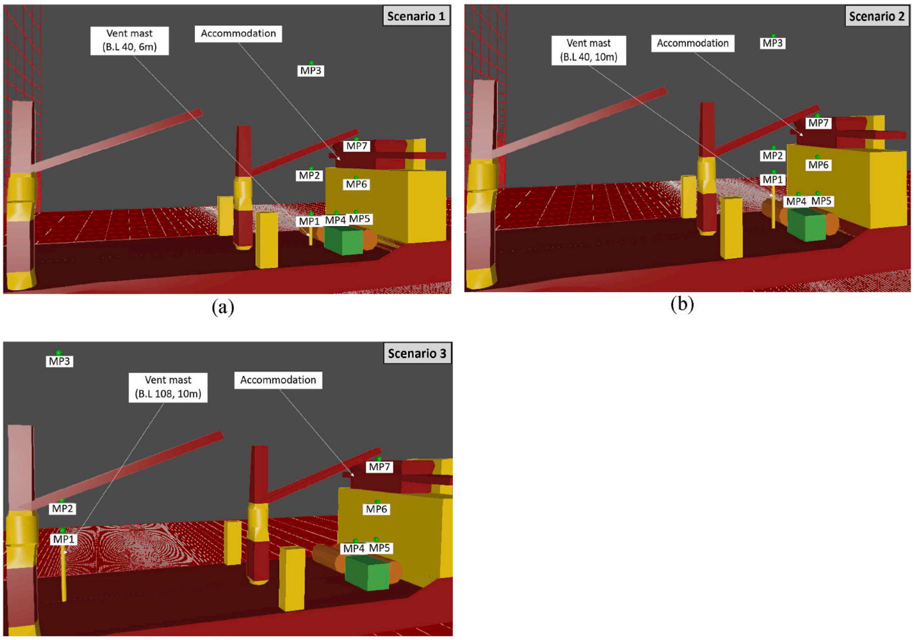
MP ID	Description	Scenario 1 (x, y, z) (in m)	Scenario 2 (x, y, z) (in m)	Scenario 3 (x, y, z) (in m)
MP1	At release point	−13.3, 0, 26	−13.3, 0, 30	−64.3, 0, 30
MP2	Above vent mast, at accommodation level	−13.3, 0, 35	−13.3, 0, 35	−64.3, 0, 35
MP3	Above vent mast, 23.3 m above accommodation area	−13.3, 0, 58.3	−13.3, 0, 58.3	−64.3, 0, 58.3
MP4	Storage tank on the deck	−7, 0, 25	−7, 0, 25	−7, 0, 25
MP5	Lower level of accommodation area	−1.9, 0, 25		
MP6	Mid-level accommodation area	−1.9, 0, 32.8		
MP7	Upper level of accommodation area	−1.9, 0, 41.7		

4.6. Scenario assumptions

The study considers several key assumptions in developing the scenarios for ammonia leakage simulation. Based on the equation for the ammonia leakage rate described in Section 4.1, the area of the leakage hole (*A*) is identified as a critical variable in determining the leak rate. To select realistic leakage hole sizes, potential PRV systems on ships were considered. The assumed ammonia release hole diameters range from 20 mm to 50 mm.

Using these hole sizes, along with typical values for other parameters in the equation, a range of representative leak rates was calculated. Specifically, the discharge coefficient (C_d) is set at 0.85, the density of liquid ammonia (ρ) is 681 kg/m^3, and the pressure difference (ΔP) is 17.8 bar. From these calculations, three representative leak rates were selected.

- 10 kg/s: representing a smaller leak scenario



(a) (b) (c)

Fig. 8. Location of different MPs around the vent mast and accommodation area across three scenarios: (a) scenario 1, (b) scenario 2, (c) scenario 3.

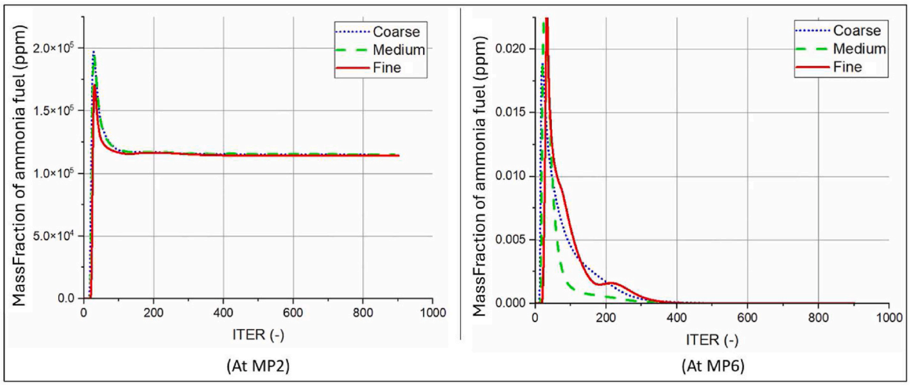


Fig. 9. Grid independence analysis of ammonia dispersion at MP2 (left), at MP6 (right)

- 30 kg/s: representing a moderate leak scenario
- 50 kg/s: representing a larger leak scenario

These three flow rates were chosen to cover a spectrum of potential leak severities, allowing for the analysis of dispersion patterns and safety implications across different scenarios.

Wind variability plays a crucial role in ammonia dispersion, and accurately modeling wind patterns in maritime environments presents challenges due to their inherent variability and complex interactions with ship structures. The geometric complexity of maritime settings, including intricate structures such as vent masts, accommodation spaces, and other ship features, may introduce uncertainties in the FLACS model, particularly regarding their effects on gas flow and dispersion patterns.

The level of detail in the computational grid, especially around complex ship geometries, could potentially influence the simulation results. This aspect has been addressed well within computational constraints. However, given the specific nature of ammonia releases in maritime settings and the limited availability of real-world data for thorough validation of the simulation results, the approach relies on the established validation of FLACS for similar gas dispersion scenarios and the recommended values and parameters provided in the FLACS manual [63].

This study focused on specific scenarios considering a limited set of parameters, including wind directions, wind speed, leakage rate, and constant ammonia leak from the vent mast. While this simplification was necessary for practical reasons, it may introduce uncertainties when extrapolating to more complex real-world conditions. These factors

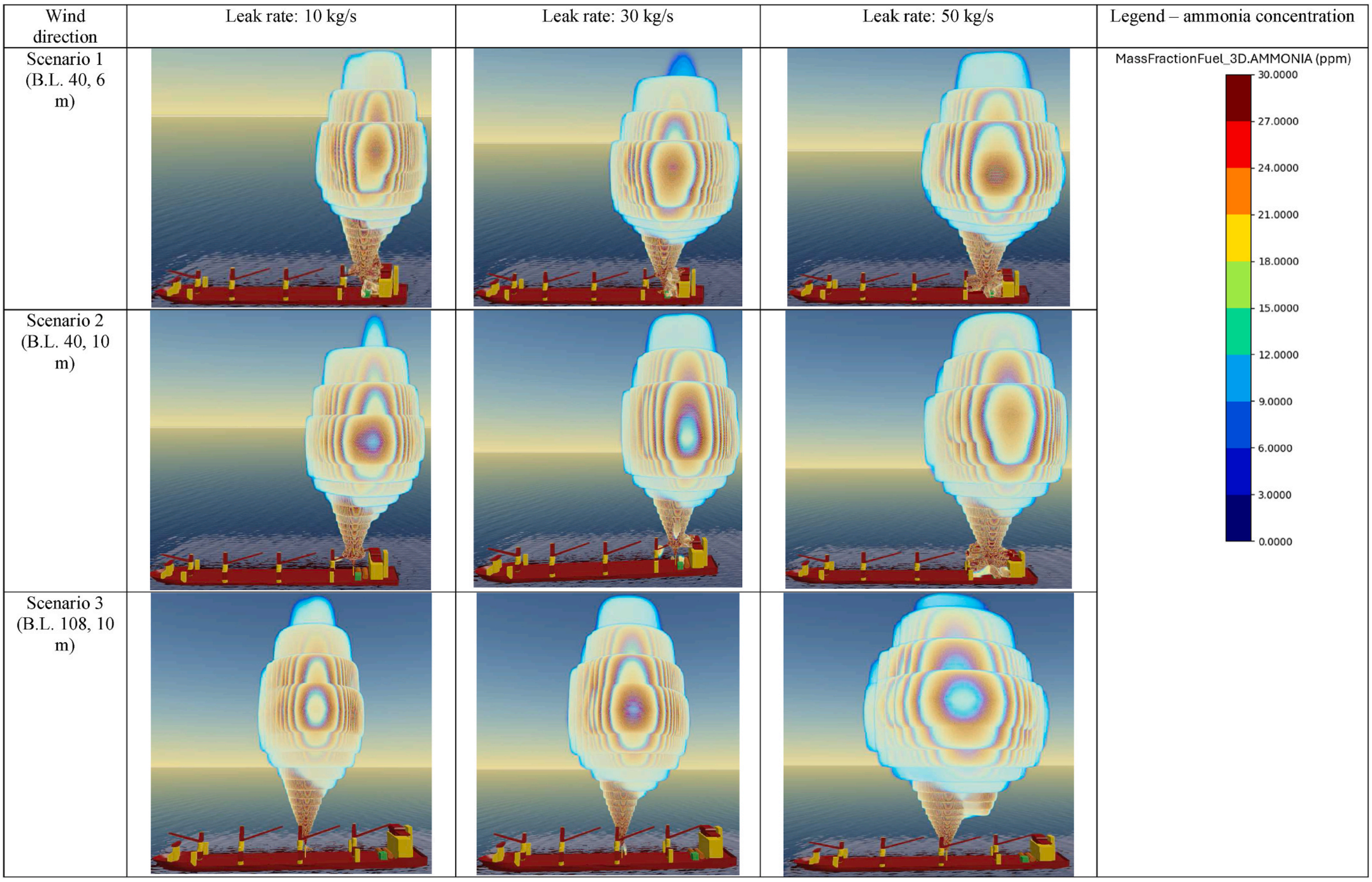


Fig. 10. 3D view of different release rate scenarios showing the development of ammonia vapor clouds

collectively contribute to the overall uncertainty in the modeling approach and should be considered when interpreting the results and applying them to real-world scenarios.

5. Results and discussion

5.1. Effect of release rate on the ammonia dispersion

Fig. 10 illustrates the 3D plot results for three scenarios with varying release rates from the vent mast, conducted under calm sea conditions (wind speed of 0.1 m/s). Generally, across all scenarios, the vapor cloud initially takes on a cyclone shape and widens significantly at a distance above the ship. Notably, the developed dense vapor cloud extends above the ship's upper deck and accommodation area. With the increase in the release rate, the lateral dispersion of ammonia also increases with the formation of a dense vapor cloud above the ship.

The initial cyclone shape of the vapor cloud is likely due to the combined effects of buoyancy, release momentum, and air entrainment. Ammonia vapor, being less dense than air at ambient temperatures, naturally ascends upon release. This upward movement is further propelled by the initial release velocity from the vent mast. As the plume rises, it draws in surrounding air, causing it to expand. The calm conditions, with a wind speed of only 0.1 m/s, allow this buoyancy-driven flow to dominate, resulting in a more symmetrical, cyclone-like shape.

The significant widening of the vapor cloud at a distance above the ship can be attributed to several factors. As the plume ascends, its vertical momentum diminishes, while continued air entrainment encourages lateral spread. Additionally, temperature equilibration with the surrounding air may further contribute to this widening effect.

This cyclone shape characteristic signifies several important aspects of the ammonia dispersion. It indicates how the ammonia vapor is likely to spread in calm conditions, initially rising and then expanding outward. The extension of the cloud above the ship's upper deck and accommodation area suggests that even elevated areas on the ship could be exposed to ammonia vapor. The shape implies that ammonia concentrations will vary both vertically and horizontally from the release point, which is crucial for assessing exposure risks at different locations on the ship.

Understanding this cyclone's shape and its implications is essential for designing effective safety measures and optimizing vent mast positioning on ships using ammonia as fuel. It provides valuable insights into potential exposure risks and helps in developing strategies to mitigate these risks in maritime settings.

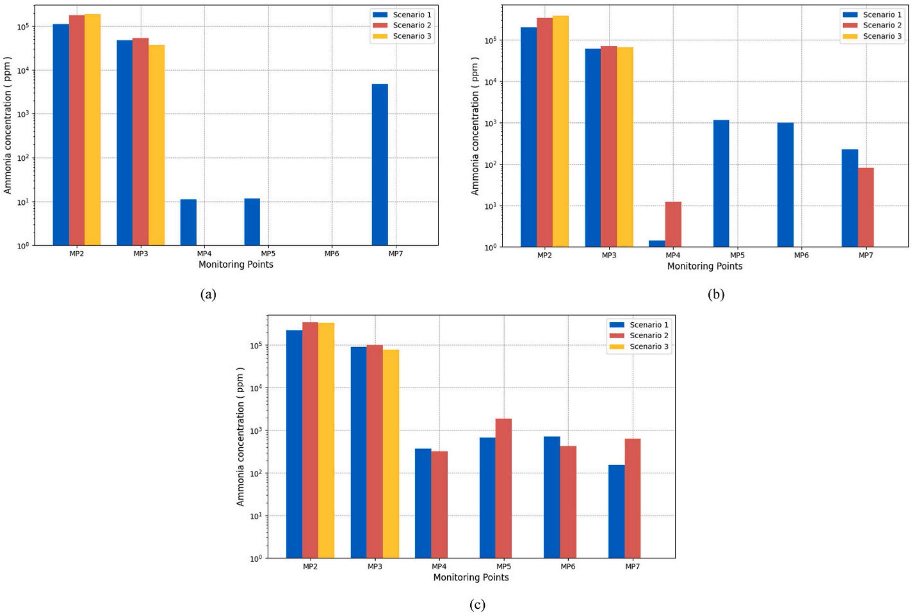
In Fig. 11, ammonia concentrations measured at specific MPs on the upper deck for various release rates and scenarios are compared. In Fig. 11(a), depicting a leak rate of 10 kg/s, all scenarios (1, 2, and 3) show very high ammonia concentrations near the vent mast, where ammonia is directly released (at MP2 and MP3). However, ammonia concentrations around the accommodation area (at MP4-MP7) are only observed in Scenario 1, where the vent mast is located at B.L. 40 and a height of 6 m, with the concentration exceeding 30 ppm at MP7. In contrast, Scenarios 2 and 3 show no ammonia concentrations in the accommodation area.

As the leak rate increases to 30 kg/s and 50 kg/s, shown in Fig. 11(b) and (c) respectively, Scenario 1 shows increased ammonia concentrations around the accommodation area, with MP5 and MP6 exceeding 30 ppm. Additionally, Scenario 2 begins to show some ammonia concentration around the storage tank on the deck and the accommodation area. Only Scenario 3, where the vent mast is positioned at B.L. 108 and has a height of 10 m, shows no ammonia concentration around the accommodation area, regardless of the leak rate. The results demonstrate that ammonia concentrations around the accommodation area increase with higher leakage rates and closer vent mast positions.

Comparing the different scenarios, Scenario 3, with the vent mast positioned at a 108 m distance, proves to be more effective at protecting the accommodation space. This increased effectiveness likely results from the greater distance allowing more time for the ammonia to dilute and mix with the air before reaching inhabited areas. In contrast, Scenarios 1 and 2, with closer vent mast positions, exhibit higher concentrations in the accommodation area, indicating insufficient distance for adequate dispersion and dilution.

According to IGC regulation 8.2.10.1 mentioned in Section 1.3.1, it is important to note that when ammonia is released from the vent mast, it is under high pressure. This high-pressure release creates a strong initial dispersion effect, preventing significant accumulation of ammonia in the immediate vicinity of the vent mast. As a result, in scenarios where the vent mast is positioned far from the accommodation area, such as in Scenario 3, there is often an absence of ammonia detection in the accommodation area. This phenomenon contributes to the enhanced safety of configurations with greater separation between the vent mast and accommodation areas.

The effect of vent mast height on dispersion patterns is significant.



(a) (b)

(c)

Fig. 11. Effect of different ammonia release rates for the three scenarios at: (a) 10 kg/s, (b) 30 kg/s, (c) 50 kg/s.

Lower release heights, such as 6 m, result in higher concentrations at the top of the accommodation space, likely because the plume stays closer to the ship's structures. Conversely, higher release heights, like 10 m, result in lower concentrations at the top level but higher concentrations at lower levels, suggesting the plume rises higher before descending.

Regarding toxicity levels, the analysis reveals that in many scenarios, especially those with higher release rates, ammonia concentrations exceed the 30 ppm threshold in inhabited areas, indicating significant safety concerns.

In conclusion, the effectiveness of different configurations depends on several factors, including distance from inhabited areas, release height, and release rate. The most effective configuration appears to be a vent mast positioned far from accommodation spaces, with a release height optimized to allow maximum dispersion before the plume descends to inhabited levels. However, the study demonstrates that even with optimized configurations, high release rates can still pose significant safety risks, emphasizing the need for comprehensive safety measures beyond just vent mast positioning.

5.2. Effect of wind speed on the dispersion

Fig. 12 displays the 3D ammonia dispersion results, illustrating the impact of different wind speeds (calm, light air, and gentle breeze) on various release scenarios. Each scenario maintains a consistent ammonia leak rate of 30 kg/s with a wind direction of 180°. Overall, it is observed that as wind speed increases, the lateral dispersion of ammonia also increases.

Fig. 13 presents a comparison of ammonia concentration measured at different MPs for varying wind speeds and scenarios. In calm sea conditions, scenario 3 shows no impact on the accommodation area, while scenarios 1 and 2 exhibit significant ammonia concentration, with scenario 2 showing lower severity at MPs 5 and 6 and slightly lower concentrations at MP 7 compared to scenario 1. This suggests that increasing the release height can potentially reduce toxicity levels in calm seas. Additionally, even with a slight wind speed of 1 m/s or higher, ammonia concentrations near accommodation areas increase significantly.

Under light air conditions, scenario 3 is mostly affected, with ammonia levels exceeding safety thresholds, albeit with lesser severity as the maximum concentration measured is less than 100 ppm. Conversely, under gentle breeze conditions, scenarios 1 and 2 are deemed unsafe for the accommodation space, with concentrations exceeding 1000 ppm, while scenario 3 exhibits lower concentrations, with the maximum measured within the safe level at 25.3 ppm.

These findings underscore the critical role of wind speed in managing the risks associated with ammonia leaks. Moreover, the study highlights the importance of integrating wind factors when developing safety protocols and emergency responses for ships powered by ammonia.

5.3. Effect of wind direction on the dispersion

Fig. 14 illustrates the effect of three wind directions (180°, 225°, and 270°) (see Fig. 6 for the definition of wind directions) on ammonia gas dispersion for three vent mast scenarios, with a wind speed of 1 m/s and a leakage rate of 30 kg/s. With the wind direction increasing from 180° to 270°, the accommodation space becomes increasingly exposed to ammonia release.

A detailed examination of ammonia concentration measured at MPs from Fig. 15 reveals that for a wind direction of 180° (port to starboard), the accommodation area remains safe, with only minor concentrations recorded for scenarios 1 and 2, well within the threshold value. A similar trend is observed for the 225° wind direction. For a wind direction of

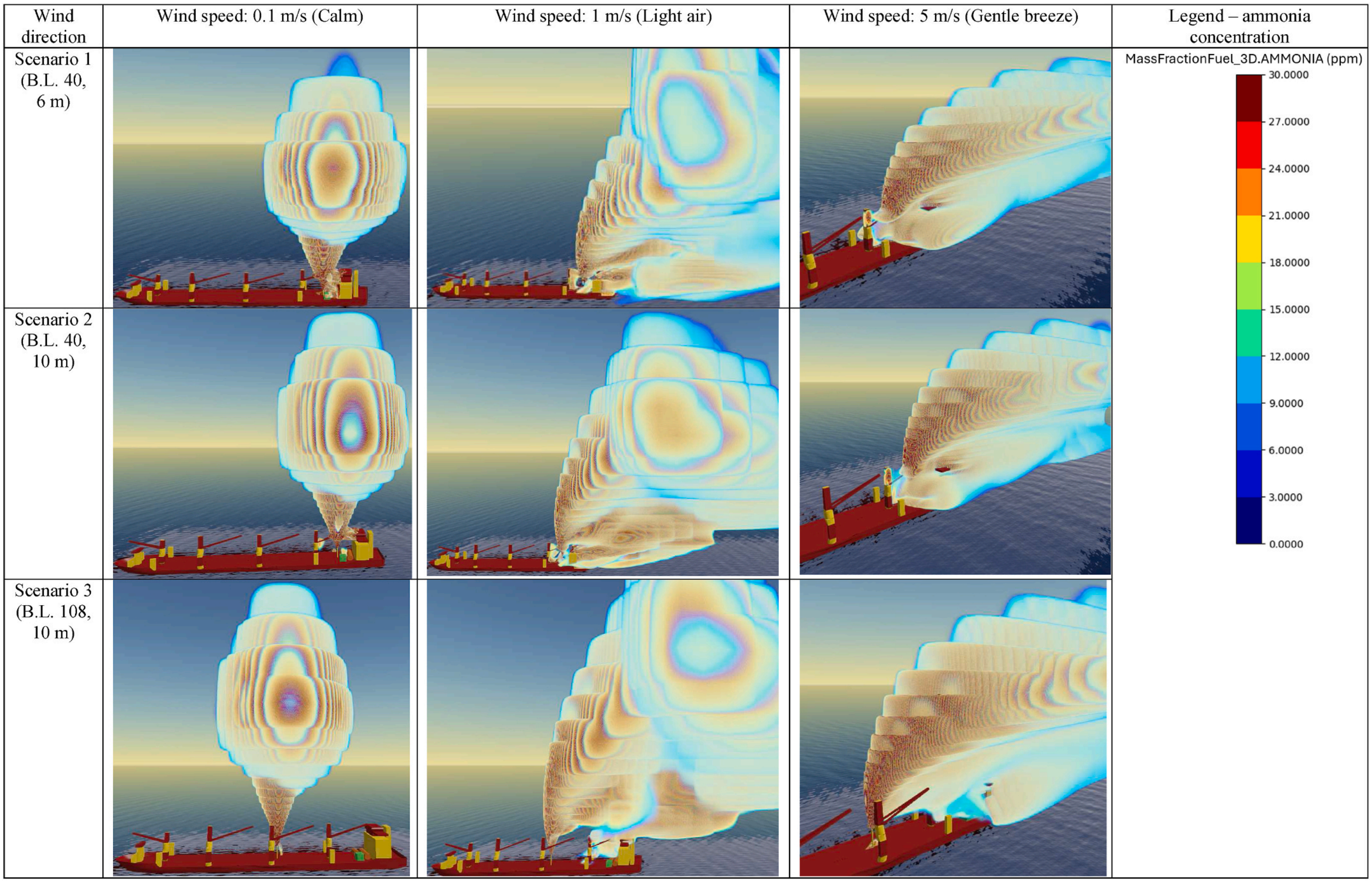
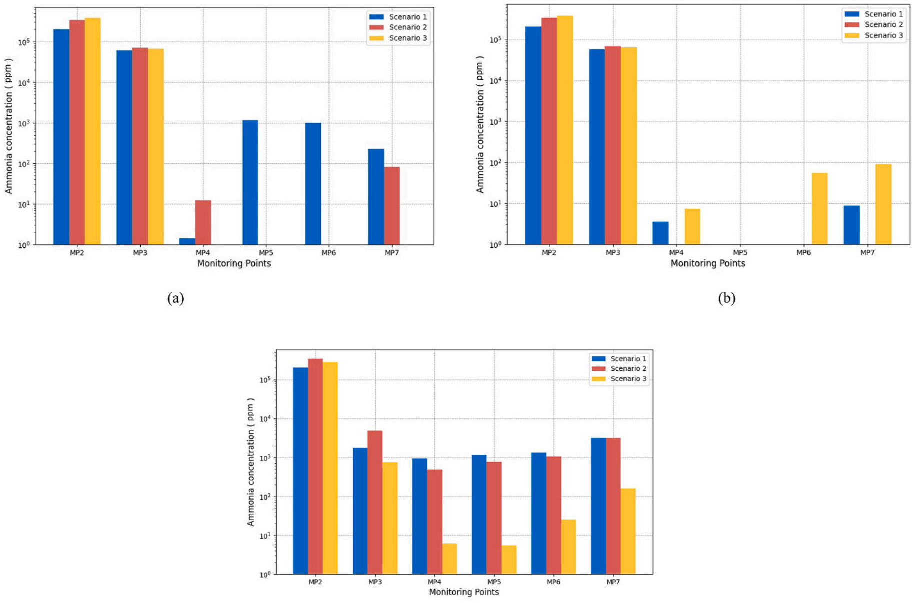


Fig. 12. 3D view of the impact of different wind speeds on the ammonia gas dispersion



(a)

(b)

(c)

Fig. 13. Effect of different wind speeds for the three scenarios at: (a) 0.1 m/s, (b) 1 m/s, (c) 5 m/s.

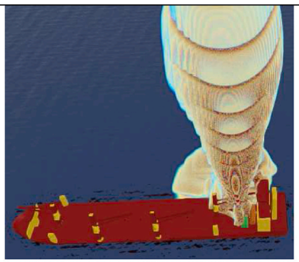
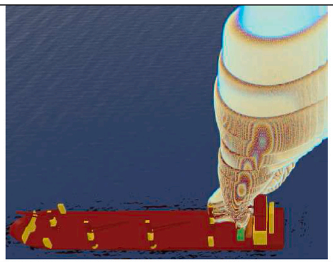
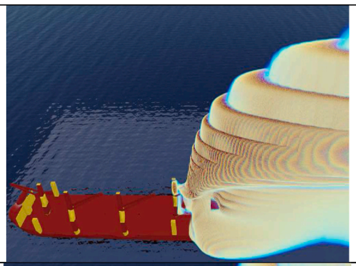
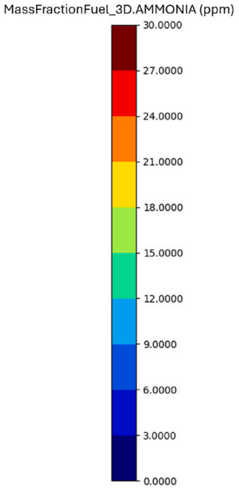
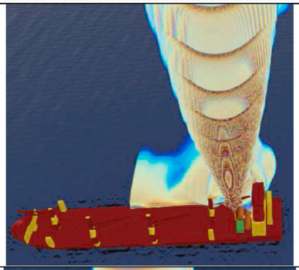
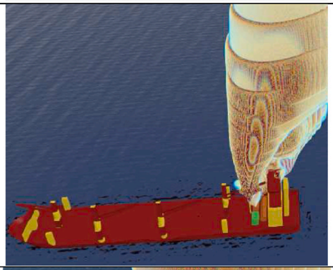
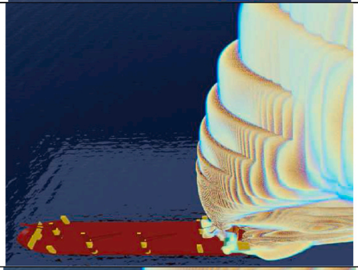
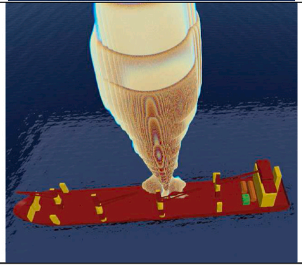
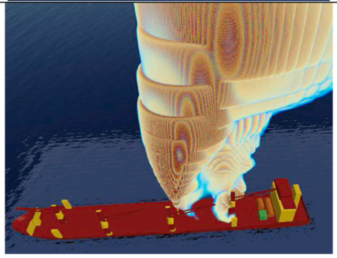
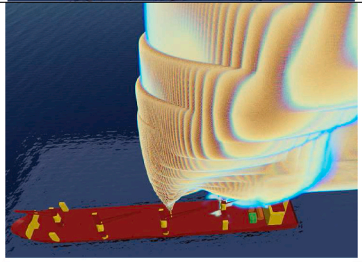
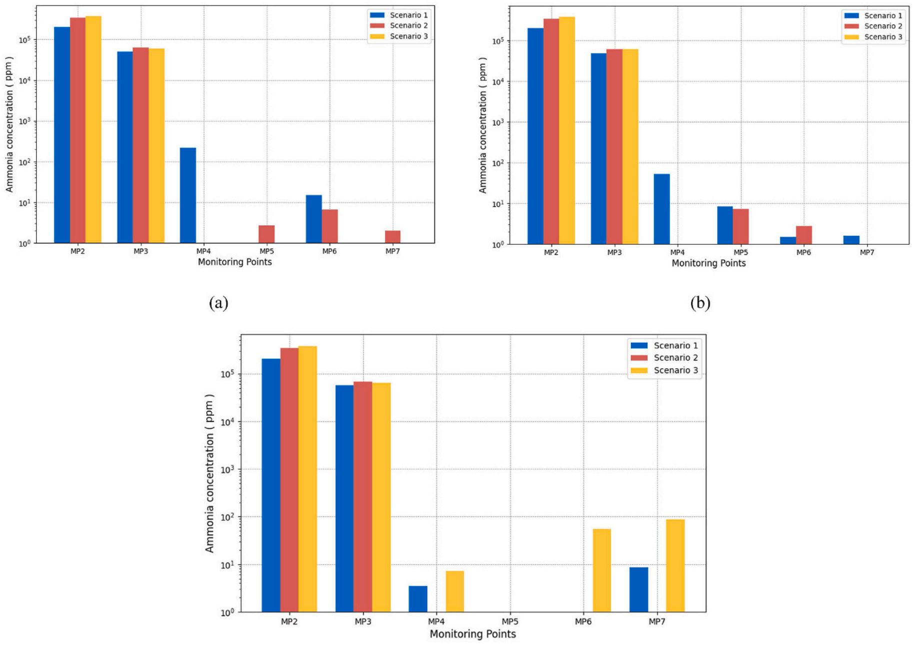
Wind direction	Wind direction: 180° (From port to starboard)	Wind direction: 225°	Wind direction: 270° (From bow to stern)	Legend – ammonia concentration
Scenario 1 (B.L. 40, 6 m)				
Scenario 2 (B.L. 40, 10 m)				
Scenario 3 (B.L. 108, 10 m)				

Fig. 14. Impact of different wind directions and vent mast location scenarios on the ammonia gas dispersion.

270° (bow to stern), no ammonia presence is observed for scenario 2, where ammonia is released at a height of 10 m close to the accommodation space. Conversely, minimal ammonia concentration is measured at the accommodation space for scenario 1, while scenario 3 exhibits concentrations higher than 30 ppm.

This indicates that placing the vent mast far away from the accommodation space does not always guarantee safety, necessitating risk mitigation actions to limit ammonia concentration.

The study concludes that wind orientation significantly influences ammonia levels in residential zones, indicating that heightened



(a)

(b)

(c)

Fig. 15. Influence of wind directions for the three release scenarios at wind directions: (a) 180° (b) 225° (c) 270°.

ammonia concentrations could pose safety risks. In addition, this analysis underscores the critical role of wind direction and speed in the assessment of safety and design considerations for ventilation systems aboard vessels powered by ammonia.

In addition, Fig. 16 presents the 2D view of the ammonia vapor cloud observed at the accommodation level for various wind directions. The figure also outlines the 10 m radius of the toxic safety zone around the vent mast and the 25 m radius from the vent mast. Generally, the

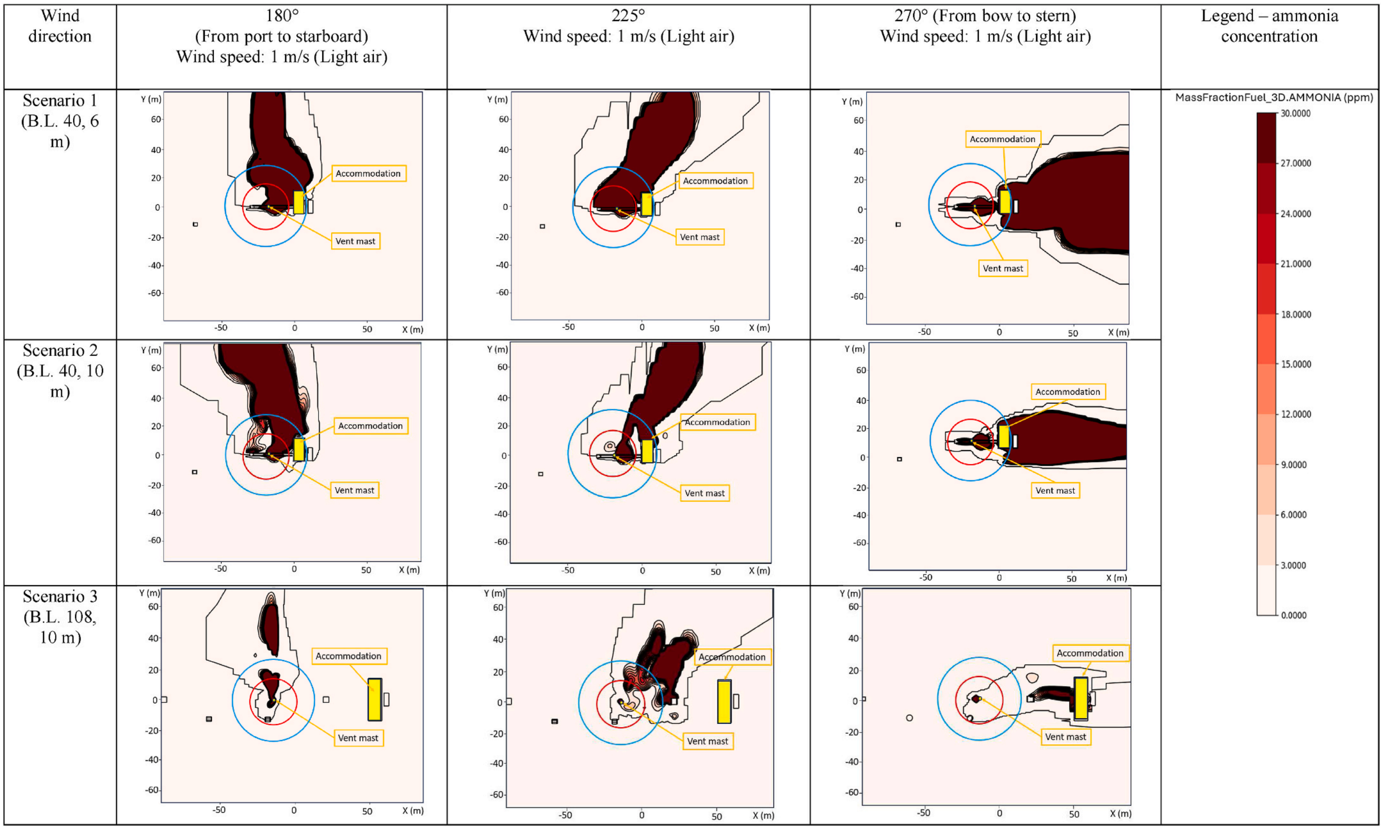


Fig. 16. Dispersion patterns of ammonia vapor cloud from vent mast to accommodation area: 2D visualization across various scenarios and wind directions (red circle: 10 m radius, blue circle: 25 m radius). (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

dispersion cloud is notably wider for scenarios 1 and 2 compared to scenario 3. Additionally, it is evident that, across all scenarios, the toxic dispersion extends beyond the threshold safety zones.

Only in scenario 3, with wind directions of 180° and 225°, there is no observed impact on the accommodation site. However, areas just outside the safety zones are deemed unsafe as well. In conclusion, there is only a slim possibility that the accommodation space will be safe and ammonia dispersion is significantly influenced by the wind directions.

In conclusion, wind direction plays a crucial role in ammonia dispersion. For the 270° wind direction (bow to stern), scenario 3 exhibited concentrations higher than 30 ppm at the accommodation space, while scenarios 1 and 2 showed lower or no concentrations. This counterintuitive result demonstrates that distance alone does not guarantee safety in gas dispersion scenarios.

The structure of the ship may create wind corridors that channel the ammonia plume toward the accommodation area, even from a greater distance. Paradoxically, the lack of obstructions between the distant vent mast and the accommodation space might allow the ammonia to travel further without significant dispersion or dilution.

Plume behavior is influenced by the release height and momentum, combined with wind direction. These factors may cause the ammonia plume to travel further before descending to the accommodation level.

The study emphasizes that wind direction significantly influences the ammonia release direction. Fig. 14 clearly illustrates how the ammonia dispersion pattern changes with different wind directions, highlighting the importance of this factor in safety assessments.

This observation underscores the complexity of gas dispersion in maritime settings and the need for comprehensive risk assessments. It reveals that safety design and planning must consider a multitude of factors beyond simple distance, including wind patterns, ship geometry, release characteristics, and atmospheric conditions. The interplay of these elements can lead to unexpected and potentially hazardous dispersion patterns, emphasizing the need for sophisticated modeling and careful safety considerations in ammonia-fueled ship designs.

6. Safety recommendations

The results of ammonia dispersion under various release rates and environmental conditions found that the speed and direction of the wind are critical factors affecting the dispersion of ammonia to the accommodation area. Independent of the vent mast position or height, the wind speed and direction strongly suggest a high likelihood of ammonia reaching the living quarters at concentrations exceeding well above 30 ppm upon release from the vent mast. While continuous and prolonged exposure of the crew to such concentrations may vary based on factors like the vent mast ammonia output, duration of emission, and wind conditions, there is still a risk of potentially lethal exposure.

This underlines the danger of human exposure to ammonia concentrations above the critical 30 ppm threshold. Elevated levels of ammonia present considerable health hazards and could be severely harmful. Thus, managing ammonia levels and enforcing strict safety measures is crucial.

Based on the aforementioned findings, it is recommended to implement measures for capturing and treating ammonia to maintain its concentration below 30 ppm before its release into the vent mast. Presently, the IGF code lacks specific guidelines regarding acceptable concentration levels. On the other hand, various classification societies offer slightly different thresholds for detecting ammonia gas levels: 25 ppm, 30 ppm, and 50 ppm, irrespective of ship type. However, for large passenger ships, a more stringent toxicity threshold, such as 5–10 ppm, could be considered.

Recently, MAN Energy Solutions conducted a 2-stroke ammonia engine test at their research center in Copenhagen, limiting the maximum released ammonia concentration to below 5 ppm [73]. As depicted in Fig. 17 (a), MAN's ammonia engine test also showcases a simplified ammonia catch system, by considering the maximum

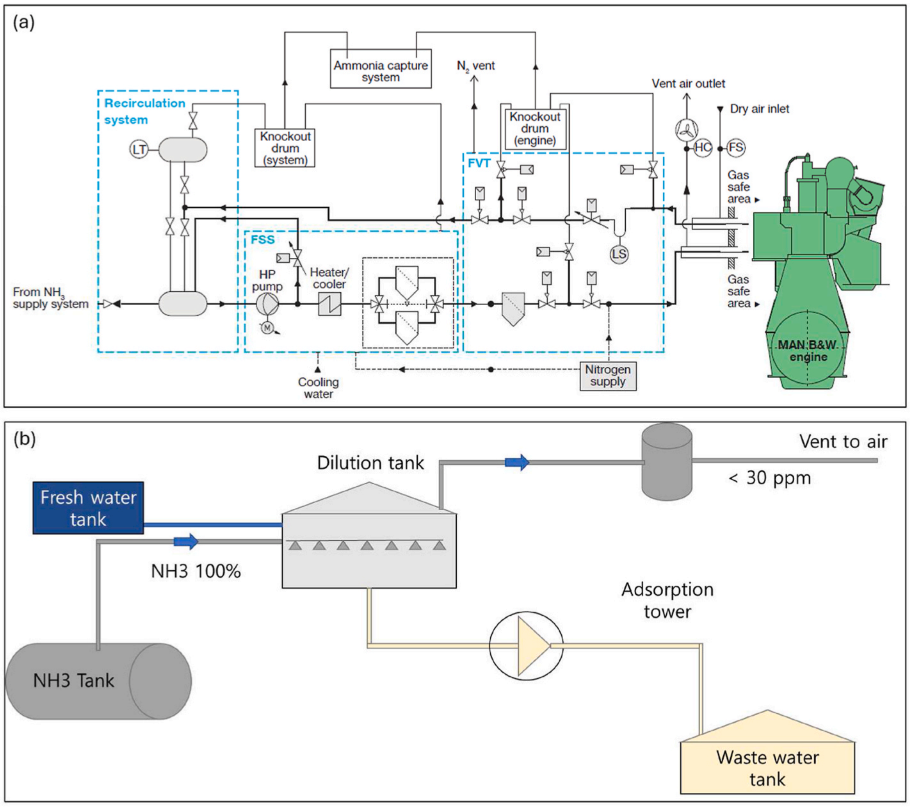


Fig. 17. (a) Process flow with ammonia catching system used in the MAN B&W ammonia engine test [73], (b) different equipment involved, and process flow in the ammonia catching system.

ammonia concentration released limited to below 5 ppm. Fig. 17 (b) provides an example of a simple catching system that employs a dilution tank to reduce leaked ammonia concentration collected from different spaces such as tank connection spaces, ventilation ducts, and PRV to below 30 ppm using fresh water. The diluted ammonia is then vented to the air via the vent mast while the resulting wastewater accumulates in a dedicated wastewater tank via an adsorption tower.

7. Conclusions

The novel objective of the study is to establish the technical groundwork necessary for the formulation of science-driven regulations ensuring the safe utilization of ammonia technology onboard vessels. In particular, this paper highlights the safety of ammonia dispersion from the vent mast in an ammonia-fueled ship and is considered to be the first to carry out this task. The following are the main conclusions derived from the study.

- Though current regulations require the direct release of leaked ammonia via vent mast without any obstruction at high pressure, however, from a safety perspective and based on the findings from the numerical simulations under varying environmental conditions and leak rates, the direct release of untreated ammonia from the vent mast is well above the standard toxicity limit of 30 ppm and toxic safety zones of 10 m and 25 m, thus prove to be fatal to the human.
- To mitigate these hazards, regulatory bodies must urgently consider revising these standards. The establishment of unified regulations is critical, as current class rules stipulate slightly varying toxicity limit levels for ammonia. Consistent and stringent thresholds are necessary to ensure the safety of human exposure to ammonia, thereby preventing fatal outcomes.
- The vent mast location is found to have little or no effect in reducing the ammonia concentration measured near the accommodation area.
- Thus, for large vessels, it is recommended to implement emission control technologies such as ammonia-catching systems and reduce the concentration of ammonia to an industry-acceptable toxicity level before released into the atmosphere.
- Overall, the release of liquefied ammonia into the air should be prevented and minimized through proper handling, storage, and containment measures to prevent health hazards, environmental damage, and potential safety incidents. Advanced sensing technologies for rapid detection of ammonia gas need to be developed and real-time monitoring systems with emergency response protocols should be integrated.
- The study highlights the ability of QRA to support the design of ships involving toxic gases. Therefore, it is recommended that the shipping industry adopt QRA to assist with the next-generation ship design involving ammonia release via vent mast.
- Further research is required to ensure that the catching system should not compromise the pressure at which ammonia gas is released during the emergency and should account for the effective safe storage and disposition of the resulting aqueous ammonia.
- Currently, various class rules stipulate slightly different toxicity limit levels for ammonia. Consequently, further efforts are necessary to establish a unified regulation regarding the toxicity threshold deemed safe for human exposure to ammonia.

In the present investigation, our focus centers on the assessment of ammonia leakage originating from the storage tanks of a general cargo ship. However, forthcoming inquiries will examine the potential discharge emanating from auxiliary systems, including the fuel preparation room, engine room, and various pressure relief valves, as well as the consequent mechanical ventilation leading to vent mast release across various ship types, notably large passenger ships, using probabilistic risk assessment. Additionally, the future study may explore the dispersion behavior of ammonia under high-humidity conditions.

In addition to these safety-focused aspects, we also recognize the importance of considering the potential environmental impact of ammonia release. While outside the scope of our current study, future work may include an examination of how ammonia releases could affect marine ecosystems and air quality. This broader perspective will contribute to a more comprehensive understanding of the implications of using ammonia as a marine fuel, helping to balance safety considerations with environmental concerns.

CRediT authorship contribution statement

Hayoung Jang: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis. **M.P. Mujeeb-Ahmed:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Haibin Wang:** Writing – review & editing, Writing – original draft, Validation, Project administration, Investigation, Conceptualization. **Chybyung Park:** Writing – review & editing, Data curation. **Insik Hwang:** Writing – review & editing, Investigation, Data curation. **Byongug Jeong:** Writing – review & editing, Validation, Supervision, Software, Resources, Methodology, Investigation, Funding acquisition, Conceptualization. **Peilin Zhou:** Writing – review & editing, Writing – original draft, Supervision, Software, Resources, Project administration, Methodology, Funding acquisition, Formal analysis. **Astrinos Papadakis:** Writing – review & editing, Supervision, Resources, Project administration, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Alexandros Giannakis:** Writing – review & editing, Resources, Project administration, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Konstantinos Sykaras:** Writing – review & editing, Resources, Project administration, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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