

Safety evaluation of using ammonia as marine fuel by analysing gas dispersion in a ship engine room using CFD

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ABSTRACT

This paper seeks to address the question that each stakeholder in the maritime industry has about ammonia's potential as a marine fuel, *How safe is it to use ammonia as a fuel onboard vessel?* The principle aim of this paper is to quantify the exposure limits to which crew working onboard can get subjected to in a confined space onboard a vessel. It was achieved by simulating gas leaks at different locations inside an engine room of a hypothetical ammonia fuelled carrier similar to a 114,000 GWT LNG tanker using CFD. The transient nature of dispersion is analysed and compared for various scenarios. The results are promising and prove that ammonia does have a high risk due to its toxicity but a low risk in terms of flammability. Research findings also demonstrate that the gas dispersion depends on numerous factors such as position, area of leak, direction of leak, pressure and temperature of ammonia gas, obstruction due to placement of machinery and decks, ventilation, and the temperature gradient of surrounding material. The novelty of the paper lies in the problem it addresses and will contribute to the industry in a better understanding of the risk involved in operating an ammonia-fuelled vessel.

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Introduction

Background

The political and economic response to what is termed as the “climate crisis” is inclining all the major stakeholders in the maritime industry to adopt a sustainable approach towards building, operating and maintaining marine vessels. IMO, in line with the UN Climate Change Conference 2015 and targets set by United Nations Sustainable Development Goals, has adopted a strategy aiming to reduce GHG emissions to half by 2050. The use of low carbon fuels like LNG, LPG, and biofuel have already penetrated their way into the shipping industry and zero carbon fuels, hydrogen, and ammonia are considered as the next step in the evolution. An article published in *Journal of Cleaner Production*, 2021 (Al-Breiki and Bicer 2021) shows that hydrogen and ammonia when derived from renewables will have the least overall GHG emissions compared to other alternative low carbon fuels (Figure 1). Each alternate fuel that is considered to replace the conventional marine fuel has its own advantages and challenges. These have been studied in detailed in various academic works and have formed the basis for this paper. In author's opinion, ammonia is seen as the best alternative marine fuel and this paper contributes to accessing safety concerns and challenges to its adoption.

Ammonia has been used as a motor fuel from the early 1800s. NASA in 1962 used ammonia as a fuel in the X-15 rocket. Since late 1900s many other demonstrations have been carried out around the world illustrating ammonia's ability as a fuel. In maritime sector, ammonia is not new as a product onboard. It is transported globally through gas carriers similar to LPG carriers. However, as a marine fuel, ammonia is new and different projects and research are going around the world to harness its true potential. Some of the key advantages of ammonia over other alternatives are summarised for a better understanding.

Ammonia can be stored under ambient temperature (20°C) at a pressure as low as 10 bar. This eradicates the need for any cryogenic system required for storage, unlike hydrogen and LNG which require –253°C and –162°C to stay in liquid form.

Ammonia's low flammability range (15–27%), high auto ignition temperature (651°C), and slow flame propagation make it a safer fuel than LNG, LPG, and hydrogen in terms of risk by fire.

Its combustion produces no CO₂ and SO_x emission. NO_x emission produced can be easily reduced to nitrogen by exhaust gas after treatment technology (SCR system) and uses ammonia itself as a reducing agent.

Ammonia is the second largest chemical produced globally and chemical industry has more than 100 years of experience in producing, storing, handling, and

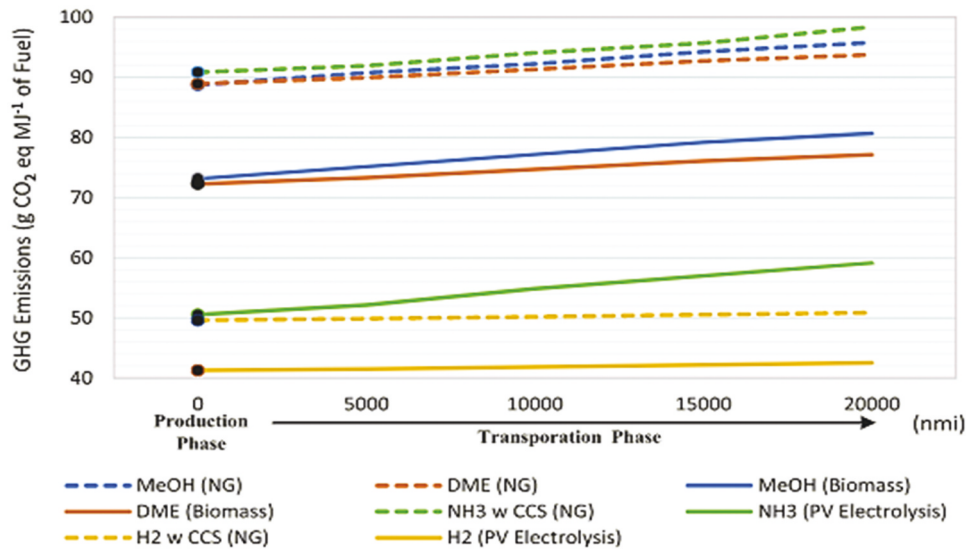


Figure 1. Life cycle GHG emissions for fuels derived from renewables and natural gas.

transporting. The regulations related to ammonia have evolved with time in the chemical industry and this can be a starting point for establishing rules for ammonia as marine fuel. The technologies, materials, and procedures for handling ammonia as a cargo are already in place, needing to be adopted and developed for designing ammonia bunkering and fuel systems.

Ammonia is highly toxic, but the odour of ammonia gas can be detected when present in air with a concentration as low as 5 ppm. This acts as an early warning for the personnel in vicinity of a leak and is one of the most advantageous properties of ammonia.

Challenges in adopting ammonia as marine fuel

Production

While grey ammonia (produced by steam reforming of natural gas) is currently cost competitive to the conventional fuel and global production quantity and scale can meet the maritime fuel requirements, the carbon footprint is almost 48% higher than VLSFO. An article in International Journal of Hydrogen Energy, 2018 (Bicer and Dincer 2018) demonstrates that even if ammonia is partially utilized in the engines of ocean tankers as dual fuel (with heavy fuel oils), overall life cycle greenhouse gas emissions per tonne-kilometre can be decreased to about 27%. Whereas it can be decreased to about 40% when hydrogen is used as dual fuel. Blue ammonia which is produced in the same manner as grey ammonia but the CO₂ produced is captured using CCS, reduces life cycle emissions to almost 57%. However, the greatest reduction in carbon footprint (83%) is seen when ammonia is derived using electrolyzers powered by renewable energy (ABS 2021). The biggest producers of ammonia have already started

their journey, in replacing grey ammonia production with blue and green ammonia. But since the transition has started only over this decade, the prices of green and blue ammonia are higher than grey ammonia. With the cost of renewable energy and electrolyzers decreasing dramatically over the next decade, it is right to say that blue and green ammonia will be as cost competitive as the conventional fuels.

Corrosivity

Ammonia is incompatible with various industrial materials, and in presence of moisture corrodes copper, brass, zinc, and various alloys forming a greenish/blue colour. Ammonia is an alkaline reducing agent and reacts with acids, halogens, and oxidizing agents. Stress corrosion cracking is induced and proceeds rapidly at high temperatures in steel when oxygen levels of more than a few ppm in liquid ammonia are introduced. Therefore, materials are to be carefully selected when ammonia is used onboard marine vessels. Iron, steel, and specific non-ferrous alloys resistant to ammonia will be useful in manufacturing tanks, pipelines, and structural components. The IGC Code outlines the requirements for piping components, cargo tanks and equipment in contact with ammonia liquid or vapor. Engine manufacturers also have to study the effect on corrosion on engine components before making engines commercially available. The challenge of corrosivity can be overcome with design considerations and proper material selection and is not seen as a big hurdle.

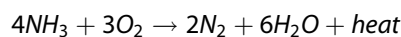
Flammability

The auto-ignition temperature of ammonia is around 650°C under atmospheric conditions and has a narrow flammability range (15.15%-27.35%).

Table 1. Concentration, duration, and effect of ammonia exposure without protective clothing.

Concentration/Time	Effect
10,000 ppm	Promptly lethal
5,000–10,000 ppm	Rapidly fatal
700–1700 ppm	Incapacitation from tearing of the eyes and coughing
500 ppm for 30 minutes	Upper respiratory tract irritation, tearing of the eyes
134 ppm for 5 minutes	Tearing of the eyes, eye irritation, nasal irritation, throat irritation, chest irritation
140 ppm for 2 hours	Severe irritation, need to leave exposure area
100 ppm for 2 hours	Nuisance eye and throat irritation
50–80 ppm for 2 hours	Perceptible eye and throat irritation
20–50 ppm	Mild discomfort, depending on whether an individual is accustomed to smelling ammonia

Ammonia also has a low burning rate (four times less than methane) and thus poses lower fire risk when compared to other gaseous fuels like LNG, LPG and biogas. On combustion it yields nitrogen gas and water, with a stoichiometric AFR of 6.06 by weight. Nitrous compound formed in the process has a direct impact on ozone depletion. However, these are currently considered as negligible and SCR technology is readily available to convert NO_x emissions to nitrogen gas.



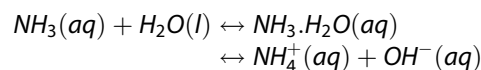
Nonetheless, with the right conditions there exists a potential for ammonia to ignite. Thus, in principle ammonia is required to be isolated from any ignition source onboard vessel when used as a marine fuel. Small fires involving ammonia can be extinguished with dry chemicals or CO₂ and large ammonia fires can be extinguished through water spray, fog, or foam. However, it is never safe to direct water jet straight on liquid ammonia or source of leakage. Protective clothing with oxygen supply should be used by responders even if the concentration of ammonia detected is as low as 25 ppm.

Toxicity

Ammonia is a highly toxic gas and has a strong odour characteristic. Acceptable exposure limits to humans are defined by legislation and is typically a function of concentration and exposure limits. The threshold for detection in odour by humans is between 5 and 50 parts per million (ppm). The industrial used ammonia sensors can detect concentrations as low as in the range of 0–50 ppm. In case of an enclosed ventilated space, often two sets of ammonia detectors are used, a low concentration detector (0–250 ppm) for emergency ventilation control and a high concentration detector (0–15,000 ppm) for electrical shutdowns. Various countries around the world have different regulations and guidelines on the exposure guidance related to ammonia. The Fertilizer Institute, which is an agriculture association in the United States, in their report “Health Effects of Ammonia” (TFI 2010) have provided a chart which brings shows the effect of various concentration exposure on the human body (Table 1). Being extremely soluble in water, ammonia is

absorbed by body fluids like sweat, saliva, tear and can cause severe chemical burns on skin, respiratory organs and damage to corneas in the eye. Exposure to ammonia in liquid form can cause swelling, redness, ulcer on skin, and frostbite.

Another important factor to be considered and related to ammonia’s toxicity is its effect in water if any spillage is reported. Ammonia is toxic even in water and forms ammonium (non-toxic) and hydroxide ions when it reacts with water.



The concentration of ammonia and ammonium shifts back and forth depending upon the water temperature and pH. At high concentrations, it is difficult for aquatic organisms to excrete the toxicant. With time due to toxic build-up in blood, internal tissue damage leads to death. A study by USEPA also prove that chronic effects of ammonia reduces hatching success, growth rate of aquatic organisms, and pathological changes in gill, liver, and kidney tissue. Thus, it is very important to also device containment plans if any spillage accident occurs, especially when ships are operating in freshwater bodies, closed waters and in port.

Ammonia as marine fuel

In order to analyse the feasibility of using ammonia as marine fuel on ships, four main aspects are discussed: the infrastructure related to fuel bunkering, storage onboard, engine and fuel systems, and regulatory requirements.

Bunkering infrastructure and operations

More than 120 ports are equipped with facilities to import and export ammonia. Most of these ports transfer and receive ammonia from ships in special isothermal storage tanks. The storage infrastructure at such ports can be revamped to address the initial transition to ammonia as fuel. Later, such storages can similarly be built at other harbours and ports. Other option would be to design and develop vessels that are capable of ship to ship bunkering. This would not be a difficult task, as such vessels are

already used for LPG and LNG bunkering. Ship to ship bunkering can also be preferred in densely populated ports to reduce the risk of exposure from any major accidental leakage. The bunkering operation include the handling, connection and disconnection of heavy bunkering hoses. In order to reduce the risk to people involved in bunkering of ammonia fuel, safety procedures and system need to be developed for preventing any accidental leak or spill. Lifting arrangements for heavy bunkering hoses, quick disconnecting couplings and break-away devices, remote control stations for overseeing operations, flushing and draining systems for residual removal, temporary mechanical shielding at connection points, automatic shutdown bunkering valves, etc. are few such examples that may be used for reducing the risk of exposure to personnel involved in bunkering operation. The personnel involved in ammonia bunkering will require professional training and will have to work with appropriate PPE. Emergency showers and eyewash should be available at convenient location outside bunkering station to provide first aid.

Storage onboard

Ammonia either needs to be compressed to 18 bars at 45°C or refrigerated to -33°C at 1 bar to be stored as liquid to increase the volumetric efficiency as ammonia takes almost 2.4 times more space than HFO to generate the same amount of energy. However, this is considering that the ship is only fuelled by ammonia. In dual-fuelled vessels, the tank size would be considerable. Two types of tanks can be used to store ammonia onboard, Type

A (fully refrigerated) and Type C (semi- or fully pressurised). Type C tanks would be preferred as it would eliminate the requirement of re-liquefaction equipment and standardise the bunkering process globally. Storing ammonia in pressurised form is also a less energy intensive process. The storage tanks can either be integrated into the ship's hull or tanks can be placed on the deck with suitable shielding. The IGC and IGF code provide a good guidance on minimum distance of gas fuel tanks from hull's shell to prevent risk of tank damage in case of collision or grounding, accommodation space, design and safety requirement, tank material requirements for high corrosive nature of ammonia, etc. Additional safety measures like boil-off gas management system for refrigerated tanks, secondary barrier and ventilation of void spaces between tanks will be required for ammonia storage onboard. The most important aspect would be to prevent any release of ammonia to the atmosphere and to the waters. Thus scrapping technology or re-collection system will need to be installed on vents heads to isolate leaks to the external environment. Japan's organisation MLIT with JSTRA has released a document with a conceptual design for an 80,000 DWT bulk carrier (MLIT 2020) fuelled by ammonia dual fuel engine (Figure 2). The design consists of a Type C tank at the stern of the ship, a machine room for handling ammonia and bunkering manifold on both sides of the stern with hose handling carne.

Engine technology and exhaust treatment

De Vries (2019) has investigated the feasibility of steam turbine, GT, ICE (SI and CI), and fuel cells (PEMFC, AFC, and SOFC) using ammonia as fuel and acknowledged

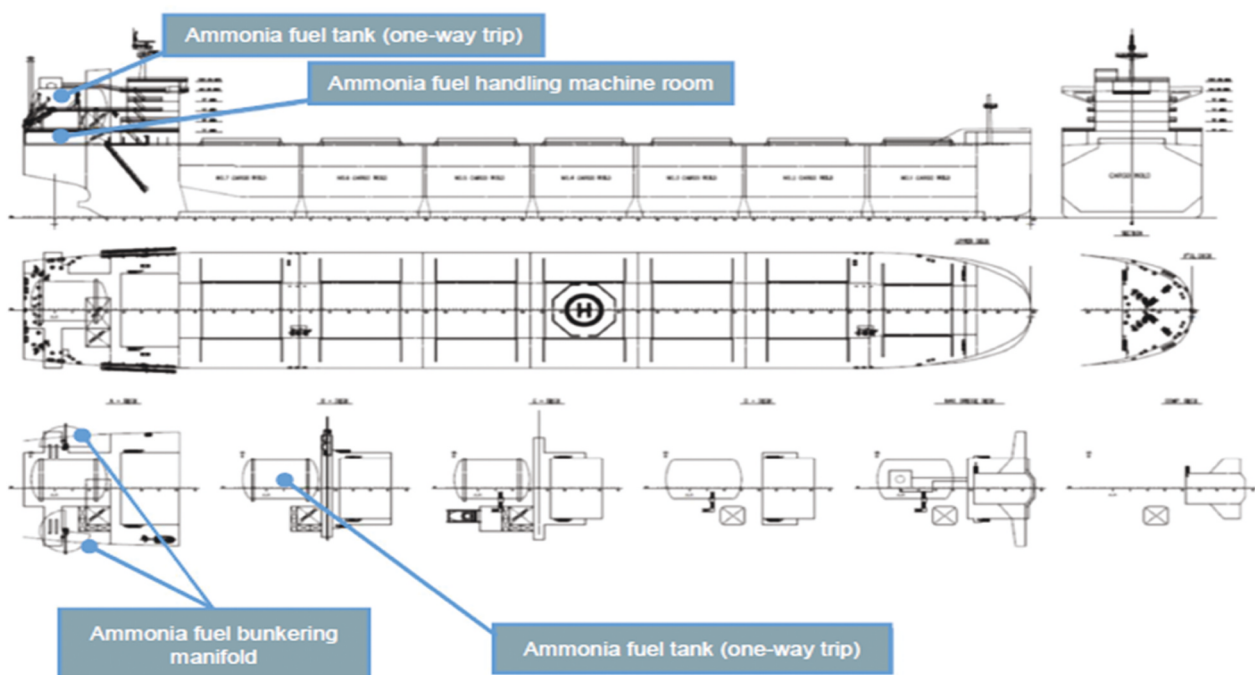


Figure 2. General arrangement of the ammonia-fuelled 80,000 DWT bulk carrier.

that only ICE (using ammonia and hydrogen mixture) and SOFC are the most practical options. ICE are considered a better option than fuel cell because of the high power density, load response, robustness, and lower cost. Current developments in the field include projects like “ShipFC” which is funded by EU and is considering converting an offshore vessel with a 2 MW SOFC which will enable the vessel to sail solely on ammonia for up to 30,000 hours annually. Ammonia alone cannot be combusted in ICE due to its high auto ignition temperature and low flame speed and therefore requires a pilot fuel to assist its burning. In the industry, Wartsila Marine Power has performed combustion tests on an ammonia dual fuelled four stroke ICE last year (Wartsila 2020) and MAN Energy Solutions is targeting 2024 to deliver a new dual fuelled two stroke engines (MAN Energy Solutions, n.d.). The two stroke engine belong the LGI family which are also used for LNG and LPG fuelled engines. These engines are well-proven on the market with tens of thousands of operative hours on alternative fuels, therefore providing a reliable and well-known solution. MAN Energy Solutions has also launched a project named “AmmoniaMot” with partners from industry and research institutes to produce a medium speed four stroke dual fuel engine capable of running of diesel and ammonia. (MAN Energy Solutions 2021)

The combustion of ammonia is free from carbon and SO_x emissions, but other pollutants like NO_x, N₂O and possible slip of ammonia from funnel will be produced. Thus, a post treatment to reduce the combustion by-products will be needed. SCR technology is already mature and is extensively used on vessels. In case of ammonia fuelled engine, ammonia itself can be used as reducing agent in conjunction with oxidation catalysts. This will reduce the need of storing and handling specific chemical onboard and reduce the relative cost of installation and operation. According to Haldor Topsoe, catalysts for the combined removal of NO_x and N₂O from exhaust gasses are commercially available. The cost of the SCR system and the resulting exhaust levels NO_x and N₂O is similar to what is achieved with SCR for conventional fuels.

Fuel systems

Using ammonia as fuel will require changes in the engine room. While many equipment's required for HFO treatment and the SO_x abatement system will no longer be required, new system like LFSS and SCR post treatment (for NO_x abatement) will be added. The LFSS provides ammonia to the engine at required conditions. To minimise the risk of ammonia leak in engine room, the system can either be installed on deck or in a separate ventilated room and connected to engine through a double piping. Installation in engine room is possible as well by making the compartment air lock to prevent any diffusion of ammonia.

For engines that require ammonia at low pressure, the system can be developed similar to the LNG supply system. For engines that will require ammonia at high pressure and in liquid state, the solution in use for LPG and LGIP can be easily adapted with some modification. TCS and FPRs are presently used in LNG or LPG fuelled vessels and are designed according to the IGF and IGC code. These act as a secondary barrier to any leakage where double pipe protection is not practical to arrange. Automatic isolation valves and emergency ventilation shutdown system will be needed to tackle any ammonia leakages.

Regulatory requirements

While the technological requirements for adopting ammonia will be vital, development of a regulatory regime will also play a major in the fuel transition. IMO, through the International Convention for the SOLAS, regulates the use of fuel on international shipping fleet. The SOLAS convention was updated in 2015 to allow use of low flashpoint fuels and requires ships to comply with the IGF code. However, the IGF code up till now has not specifically come up with design requirements to ammonia fuelled ship. For any new ship which is propelled by ammonia fuel, an alternative design approach will be adopted which should demonstrate the risk-based analysis equivalent to the basic functional requirement of the IGF code. International Code for the safe carriage by sea in bulk of liquified gases (IGC code) is another international standard related to transportation of liquified gases. The standards do not permit the use of cargo identified as toxic product as fuel, ammonia is this case. However, requirements of IGC code can provide guidance in designing the storage system for ammonia.

Classification societies provide a faster way to develop rules than IMO. The alternative design approach adopted by classification societies can then be accepted by IMO and even be included in international regulations. With the growing pressure on GHG emissions and stricter regulations on the shipping industry, many classification societies and big industry stakeholders have already started designing and developing rules for an ammonia fuelled vessel. For example, ABS has released a whitepaper on ammonia as marine fuel (ABS 2020), which discusses aspects related to safety, regulatory compliance, design considerations and ongoing research. Another paper released this year (ABS 2021) brings out how different stake holders should consider entire value chain and not just combustion cycle, while considering a shift in marine fuel. Ammonia is said to be the most important fuel in this transition. DNV GL examines what it would take to be adopt ammonia at scale as a maritime fuel in its report (DNV GL 2020). It suggests that ammonia is more favourable than hydrogen and can be a suitable option for future

use in cargo-carrying ships with modified internal combustion engines and low-pressure fuel tanks. The report concludes that not only ammonia's toxicity and corrosiveness is of paramount importance and will require appropriate safety barriers, but also factors like production scalability and methods, cost of green ammonia and handling ammonia spillage are areas of importance. DNV GL also published a safety handbook for design consideration of ammonia fuelled ships (DNV GL 2021). This is seen as an important contribution to the industry and provides a practical guidance on how the most important safety barriers associated with ammonia can be solved. Korean Register published a report (Korean Register 2021) that investigates the characteristics of ammonia and compares it with other next-generation fuels. The report also examines the development status of ammonia fuel cells and internal combustion engines, giving an in depth analysis of key international requirements such as the IGC Code and IGF Code, which will influence further rule development. Haldor Topsøe and Alfa Laval have published a report (Alfa Laval & Haldor Topsoe 2020), which provides a comprehensive and up-to-date overview of the applicability, production, scalability, cost, and sustainability of ammonia as a marine fuel. The report concludes that ammonia is an attractive and low risk choice in the transition phase and as a long-term solution. Other reports have also been published by leading industry experts on the same grounds. However, each of these reports have suggested that the most critical area of concern which needs to be addressed is the risk of ammonia's toxicity to human and environmental safety. It is on the basis of these reports that this paper has tried to explore and investigate the effect of ammonia gas leak dispersion at the most risk prone area of a future ammonia fuelled ship, the engine room.

Past research

There have been studies that bring out ammonia's suitability as a marine fuel, only a few reports have quantified its toxicity risk onboard a marine vessel. Technical publications based on life cycle assessment, power generation capability, technological and regulatory requirements, risk assessments of ammonia exposure to human and environment, and system design for safety related to ammonia storage, handling, and consumption are used by the author to gain an in-depth knowledge on the topic.

To understand the nature of ammonia gas dispersion and to model an as close as to a real ammonia leak in a ship's engine room, gas dispersion studies related to ammonia have been looked into. Since ammonia

fuelled vessel are still into design phase, studies related to ammonia leaks in other industries proved effective. There are mainly four different approaches to study gas dispersion:

- (a) Full-scale test
- (b) Model (hydraulic or aerualic) test
- (c) Use of empirical and mathematical code
- (d) Numerical modelling and CFD simulation

Different studies have been carried out for studying ammonia dispersion using the above mentioned techniques. Table 2 brings out some major work that have been closely studied for understanding gas dispersion modelling. It is seen that CFD simulation provides an advantage over all other techniques as it does not require complex experimental procedures, is relatively cheaper than setting up experiment, provides a large number of cases to modelled and has a rapid nature of study.

Most of the studies referred to were related to large area dispersion and involved large quantity of leaks. It was necessary to understand how ammonia gas dispersion would behave in an enclosed space with forced ventilation. A gas dispersion model pertaining to natural gas leak in an engine room is studied for understanding gas behaviour in an enclosed space (JianLi, Rui, and Konovessis 2016). The study showed as to how gas dispersion depends on leakage rate, position and direction of release, temperature gradient, ventilation and the machinery equipment located in the engine room. Another study (Pomonis 2021) brought out the behaviour of ammonia gas dispersion in a ships engine room. The report brings out toxicity analysis of ammonia gas and overall fire behaviour if the gas leak lead to a fire incident. The report also compares the fire caused by ammonia fuel to that caused by diesel and LNG. However, the simulation carried out is based on the FDS model which is good for studying fire propagation but not very effective for studying gas dispersion and factors like leakage quantity, temperature gradient, and ventilation have not been coupled with the ammonia gas dispersion.

Ammonia being a gas at atmospheric conditions and highly toxic can be lethal to humans and the environment if not contained within the safe exposure levels. Several accidents around the world which are related to fertilizer, refrigeration and chemical industry have shown how fatal ammonia can be. Since there is no global database for statistical analysis of ammonia release accidents, examples can be found from news media and governmental database. Looking into these incidents it becomes imperative to closely study the crew and environmental safety before ammonia is used as a fuel on ships. The study thus tries to get an



Table 2. Ammonia gas dispersion studies referred to for paper.

References	Aim/ Methodology adopted	Main Outcome	Learnings	Shortcomings
(Bouet, Duplantier, and Salvi 2005)	Ammonia large scale atmospheric dispersion experiments in industrial configurations/ Physical test model	The objectives of the experiment was to measure anhydrous ammonia concentrations in a range of few meters to 2 km from the release, in order to generate data to be used to improve 2-phase discharge and dispersion modelling. Fifteen trials were carried out with various release configurations corresponding to industrial situations (impinging jets on the ground and on a wall at various distances, release through a flange without seal).	Important takeaways from this report is that the ammonia cloud can behaves like a heavy gas and no elevation of the cloud may occur. The temperature in the ammonia jet can fall below -70°C. Solid obstacles (wall or ground) located at a few meters from the discharge point, have a considerable effect on the concentration values. Liquid ammonia pool formed after impact with an obstacle does not evaporate quickly.	Physical modelling carried out in open area. Result would differ when same kind of test would be carried out in an indoor environment.
(Quest Consultants Inc 2009)	Risk analysis of motor gasoline, LPG, and anhydrous ammonia as an automotive fuel/ Quantitative Risk Analysis & Numerical modelling of gas leak	Quantification of risk in two different scenarios posed by exposure of ammonia to the public near a roadway where leak would occur from a tanker and a fuelling station.	Consequence analysis was performed by using numerical modelling of the gas cloud and a graph was generated between mortality and concentration of ammonia.	The modelling carried out is for an open area with specific whether conditions set to achieve results. This method would prove inadequate for studying an internal gas dispersion in enclosed space.
(INERIS 2005)	Large scale atmospheric dispersion test for ammonia leak/ Full scale test and numerical modelling	A number of physical tests were conducted to improve knowledge on atmospheric gas dispersion of ammonia. The result demonstrate that integral type of dispersion model (Numerical modelling) only gave correct levels of ammonia concentration leeward from a free release. Plume dispersion modelling is not suitable for ammonia gas dispersion as it does not account in for obstacles in vicinity of release.	Large scale ammonia dispersion can be modelled using numerical modelling. Physical tests give the best results in accessing gas dispersions but are costly and take more configuration to achieve correct results.	Numerical modelling are unsuitable for enclosed spaces such as an engine room.
(Orozco et al. 2019)	Assessment of an ammonia incident in the industrial area of Matanzas/ ALOHA software	The study describes and quantifies the effect of virtual ammonia release accidents from a tank in the industrial area of Matanzas on the population and the environment using Atmospheric Transport and Dispersion model. Results estimated number of casualties using the different scenarios and predicted that toxic vapour cloud would have the highest casualties.	A similar approach can be used to estimate number of casualties around an ammonia fuelled vessel when at a port and there is a leakage from the vessel. However, this approach would deem unfit for an enclosed space such as engine room.	Only outdoor gas dispersion can be modelled using this model.
(Tan et al. 2017)	Experimental and numerical study of ammonia leakage and dispersion in a food factory/ Wind tunnel test and CFD modelling	A small-scale wind tunnel study is carried out to depict the nature of gas dispersion and is coupled with changing wind conditions, source height and release rate. The result is then compared with a simulation work on the CFD software.	The study gives shows that CFD simulation can give convincing results of when compared to the experiment values. The change in source conditions and environmental conditions have a great impact on the toxicity analysis of ammonia.	Results compared are for CFD simulation carried out on a full scale model and wind tunnel test on a scaled down model. Although the result are convincing, the CFD model should also be done for a small scale model to get exact results.
(Mastellone, Ponte, and Arena 2003)	Design of mitigation systems for indoor and outdoor ammonia releases/ BREEZE Accidental Release Modelling Software	A specific model was developed to estimate the time concentration of ammonia profile after a release inside an enclosure. The concentration when isolation valve is closed manually reaches more than 8500 mg/m ³ in 600 s compared to 2500 mg/m ³ when the valve is automatically shut.	The time duration of leakage has a great impact on concentration of ammonia gas that accumulates in an indoor environment.	The modelling carried out in indoor environment did not consider obstacles and ventilation of the room.
(JianLi, Rui, and Konovessis 2016)	CFD analysis of natural gas dispersion in engine room space based on multi-factor coupling/ ANSYS CFD software	Gas dispersion in an enclosed space depends on multiple factors like obstacle placement, temperature gradient of walls and obstacle, ventilation and direction of leak. Vortex and jet formation are seen in the simulation that can be effective in determining the location of gas detectors.	CFD is seen as an effective method for simulating gas dispersion in an enclosed space with forced ventilation. Heat dissipation from machinery can be coupled with gas dispersion to get a more real scenario.	The engine room modelled was for a small vessel. Size of engine room would also effect the gas dispersion. Natural gas dispersion is used which will has a different buoyancy characteristic.
(Pomonis 2021)	Engine room fire safety evaluation of ammonia as marine fuel/ PYROSIM FDS software	Flammability and toxicity risk of ammonia leak is studied and compared to diesel and LNG. The simulation result showed that ammonia poses more risk due to toxicity and less risk of fire.	Ammonia gas dispersion can be undertaken in an engine room model, coupling it with different leak scenarios and configuration. Results can also be compared with other gaseous fuels like LNG and LPG.	The software used is reliable for simulating fire propagation and insufficient to get accurate results for gas dispersion. Ventilation and temperature gradient due to machinery operation have not been considered.

answer to the effect of ammonia gas dispersion in an engine room of a ship and quantify the exposure limits and levels. Ammonia is no doubt harmful for human health, but what would be the concentration and exposure time if an accidental leak occurs onboard is what the paper presents.

Research AIM and contribution

The problem that this paper will address is a derivative of the necessity to take a decision about the future, today. It seeks to address the question that each stakeholder in the maritime industry has about ammonia's potential as a marine fuel, *How safe is it to use ammonia as a fuel onboard vessel?*

The problem had to be addressed by identifying the best way to evaluate toxic effects of ammonia gas dispersion in an enclosed space on a vessel and the most efficient method that could answer the problem statement was to undertake a CFD simulation for a case specific vessel. The simulations will be coupled with factors like location of ammonia leak, ventilation of the engine room, machinery placement and heat flux generated by engine operation. This approach will be an effective method in analysing toxicity effect of ammonia on personnel working in the vicinity and give an estimate of time required for evacuation and remedial action to bring down concentration to minimal. The result will be used to recommend methods for increasing the safety for ship's crew and environment from such an incident. The topic is novel and will contribute to the industry in a better understanding of the risk involved in operating an ammonia fuelled vessel.

Methodology adopted

In order to access the successful outcome of the paper, a clear methodology needed to be followed. Figure 3 illustrates the sequential order of how the paper was planned and executed.

Step 1: Modelling of engine room

The process of simulating ammonia leak in an engine room would be most beneficial if an in-service ammonia fuelled ship is taken as case vessel. However, there is no such vessel in operation at this stage. The LNG carriers were the first of the marine vessels to be propelled by dual fuel LNG engines. This gave the industry a practical experience and confidence in using LNG as fuel. Similarly, it is anticipated that ammonia fuel will first embed its way in ammonia carriers. These carriers are similar to LPG and LNG carriers except that the cryogenic storage temperatures for ammonia is much higher than LNG. Therefore, it was apt to use data of an LNG or LPG

vessel for the modelling of engine room and simulation setup. The vessel selected is a 114,277 GWT LNG tanker which is built by Hyundai Heavy Industries at Ulsan Shipyard in 2010. It is assumed that vessel with similar architecture would be fuelled by ammonia in future. The main characteristics of the ship are shown in Table 3 for reference.

The IGF Code classifies gas fuelled vessel's machinery spaces in two categories: gas safe and emergency shutdown (ESD) protected spaces. The major difference between the two is that a single point of failure cannot result in a gas release in gas safe machinery spaces, while this may occur in ESD-protected spaces. The case vessel selected has an inherent gas safe engine room. This type of configuration requires an independently ventilated compartment which houses the gas fuel preparation equipment and safety isolation valves. Two Gas Unit Valve (GUV) room adjacent to engine room are used for this purpose in the selected vessel and are isolated from all other compartments on the ship. Gaseous fuel is pumped to the engine through a double walled piping where the area between the piping is monitored by gas detectors and is separately ventilated. An ESD protected machinery space is isolated by gas tight and separately ventilated compartments. Emergency shutdown is activated if any gas leak is detected in the compartment. The fuel preparation and isolation valves are thus catered in the machinery space itself. Fuel pipelines may not be double piped in such a configuration of engine room. It is opined that either of these configurations may get adopted with some modification for the future ammonia fuelled ships too. Since the risk for an ESD protected space is higher, the engine room of case vessel was modified to depict an ESD protected space. It is assumed that the leakage simulated will occur from a single walled pipeline.

The general arrangement drawings of the case vessel were used to identify key parameters and dimensions. The engine room of the case vessel consist of two decks and houses mainly the diesel generators which power the propulsive motor on the deck below. The overall dimensions of the engine room is 30 m × 33 m × 11 m (L × B × H). The fresh air supply in the engine room is provided by four supply fans through ventilation ducts which have a volume flow rate of 2650 m³/min. The ventilation ducts have 60 openings in total which are angled at 45° towards the diesel engines. Exhaust ventilation is carried out by two exhaust fans which suck air at a flow rate of 2400 m³/min and are located symmetrically above the diesel engines. The ducts have been modelled as close to their original locations and dimensions using technical drawings and equipment manuals. SolidWorks which is a computer aided design programme published by Dassault Systems is used to model the engine room. Due to the complexity of the engine room machinery and piping system, only the major equipment have been

included in the model. This simpler approach has been utilised to shorten the simulation run times. This method is also in line with studies that have been carried out on a similar basis. Figure 4 shows the modelled engine room in an isometric view with all the major equipment and ventilation ducts.

To analyse gas concentrations, 10 measuring points are selected in the model to record the mass fraction of ammonia dispersion (in ppm) for the three leakage scenarios. The location of these measuring points are shown in Table 4. It is assumed that the measuring points are location of gas detectors and alarm will be triggered at set point during the simulation. As shown in Table 5, there are two different safety alarms set in an ammonia gas detector. The STEL value of ammonia gas is around 35 ppm as accepted in the industry work safety standards. Therefore, 35 ppm is taken to be the first alarm. Ammonia has a very high LEL of 15% or 1,50,000 ppm. To simply say, it takes a high concentration of ammonia and a strong energy source to make ammonia ignite. According to HSE (HSE 2004) guidelines, the flammable gas detectors should be set at 10% of LEL. Thus, the second alarming limit that the ammonia gas detector should use is 15,000 ppm. Since the response time of alarm equipment needs to be considered, which would be at least 30–60 s, the simulation is carried out for 150 s. In order to improve the detection accuracy, any leakage should be detected by at least two detectors.

CFD software selection and validation

The most critical step in getting successful results was to identify a suitable software that could handle gas dispersion studies. While there have been many models to simulate hazardous gas dispersions, these are only suitable for open air environment and are simplifications of conservation equations of mass,

momentum and energy. CFD analysis are now being used extensively for more complex environments like buildings, manufacturing plants, enclosed spaces, etc., which consider the impact on dispersion due to barriers, ventilation and temperature gradients. The author opined that Flow Simulation package, which is an add-on to the SolidWorks, is apt for the paper requirements. Flow Simulation is a finite-volume based CFD programme that models fluid flow using the Navier–Stokes equations. Since the CAD model is native to the programme, it can easily identify solid edges or boundaries of the solid model and can then refine the mesh more accurately. The meshing of the model is integrated with the simulation module and gets automatically refined and modified with any change in the geometry. Also, simulation setup for internal flow analysis is easy and ammonia is a pre-defined species in the module.

There are not many studies on gas dispersion that have been carried out using Flow Simulation module of Solidworks. Therefore, it was necessary to check the software’s capability in simulating a gas dispersion. A CFD simulation carried out by Wei Tan et al. (2020) was selected to check the appropriateness of the Flow Simulation software. In the article (Tan et al. 2020) published, the author has used ANSYS to simulate a large scale ammonia leak in a food factory located in Tianjin, China. The study was chosen because the details of model and simulation setup are provided in detail. A model similar to one made in the report was created using SolidWorks which was used to carry out a simulation similar to that presented in the report. The results of the simulation were convincing and near to results provided in the article. The results have been compared in Table 4. This activity provided a strong validation for the Flow Simulation software’s aptness in simulating an ammonia gas dispersion study.

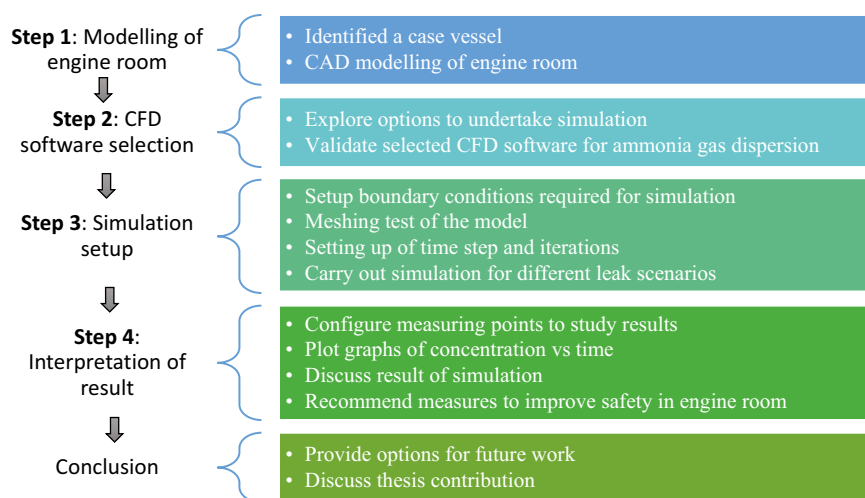


Figure 3. Strategy adopted for research paper.

Table 3. Key characteristics of the case vessel.

Feature	Details
Ship name	LNG Abdelkader
Type of ship	Segregated Ballast LNG carrier
Classification	Bureau Veritas
Length overall	298 m
Length between perpendiculars	285 m
Breadth moulded	46 m
Depth moulded	26.8 m
Draft design	11.9 m
Diesel generator engine	Wartsila 12V50DF x 2 (11,400 kW), 9L50DF x 2 (8550 kW)
Gas oil tank capacity	112 tons/139.7 m ³

Simulation setup

Boundary conditions

There are four types of boundary conditions used in the simulation: volume flow rates of inlet air ducts and exhaust opening, thermal condition for side walls (denoting bulkhead) and engine surface, and mass flow of ammonia gas release. The following values have been designated in the simulation to these boundary conditions:-

(a) Each one of the four supply fans provide an air volume of 2650 m³/min to four long inlet air ducts. Each inlet air duct have 15 openings. It is assumed that each of the openings provide equal volume of air in the engine room with a fully developed flow. Thus, volume flow rate of each inlet duct is calculated to be 2.95 m³/s. The size of each duct is same as that provided in the technical drawing.

(b) Two exhaust trunkings de-ventilate engine room using exhaust fans of capacity 2400 m³/min. Thus the volume flow rates of the exhaust openings is calculated to be 40m³/s each. Opening dimension have been taken from technical drawing.

(c) The side walls which represent the bulk heads are assumed to be at a temperature of 28°C. The engines surface thermals are taken from the technical manual

which state that the average surface temperature when engine is operating is approximately 95°C at 80% load.

(d) API states that a typical gas release is said to be small for gas pipes below 6.35 mm and medium for 6.35–50.8 mm (API 2008). Thus the hydraulic surface diameter of ammonia leakage is assumed to happen at 50 mm. The release rate of ammonia gas leak is computed using the equation below, which is based on discharge of gases and vapours at sonic velocity through an orifice. The ammonia is taken to be released at a pressure of 15 bar, temperature of 35°C and mass concentration of one. These are the standard conditions ammonia is stored in a high pressure storage tank. It is assumed that ammonia's injection pressure which is around 800 bar is achieved only after supply reaches to engine. Thus, the leakage rate is calculated to be 0.144 kg/s.

$$W_n = \frac{0.9 \times \pi \times d_n^2 \times P_s}{1000 \times 4} \sqrt{\left(\frac{k \times MW}{R \times T_s}\right) \left(\frac{2}{k+1}\right)^{\frac{k+1}{k-1}}}$$

Where W_n is the theoretical release rate associated with the n th release hole size in kg/s, d_n is the specific release hole diameter, which is 50 mm, P_s is the normal operating pressure which is

1500 kPa, k is the release fluid ideal gas specific heat capacity ratio which is 1.32 for ammonia, MW is the release fluid molecular weight, which is 0.017 kg/mol for ammonia, R is the universal gas constant, 8314 J/(mol K), and T_s is the storage or normal operating temperature (308.15 K).

Leakage scenarios

The air inside the engine room is taken to be at a temperature of 35°C and with a relative humidity of 50%. As the failure probability of joints is higher than pipe wall, it is assumed that leakage happens

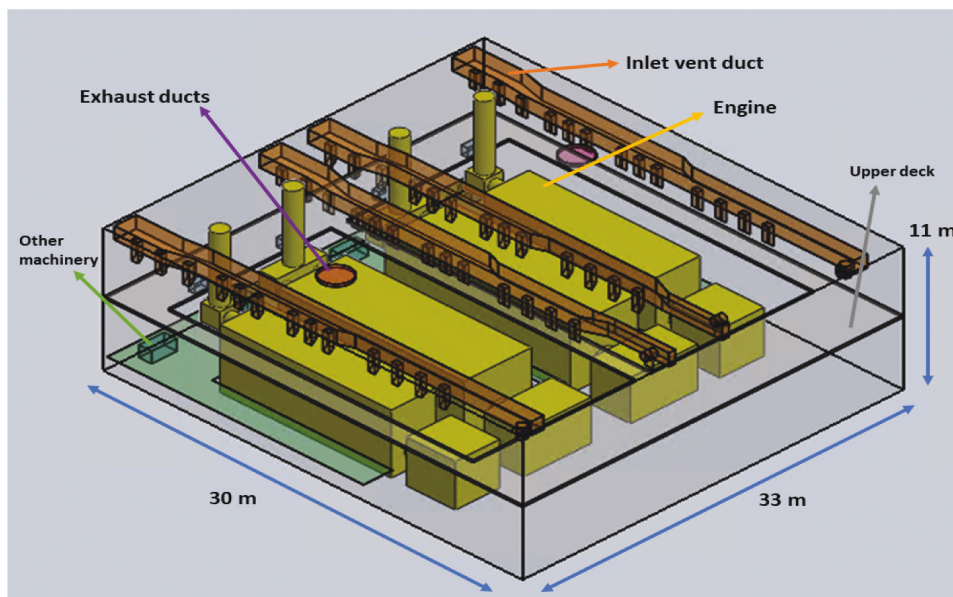


Figure 4. CAD model of engine room.

Table 4. CFD software validation.

Results produced from ANSYS (Tan et al. 2020)

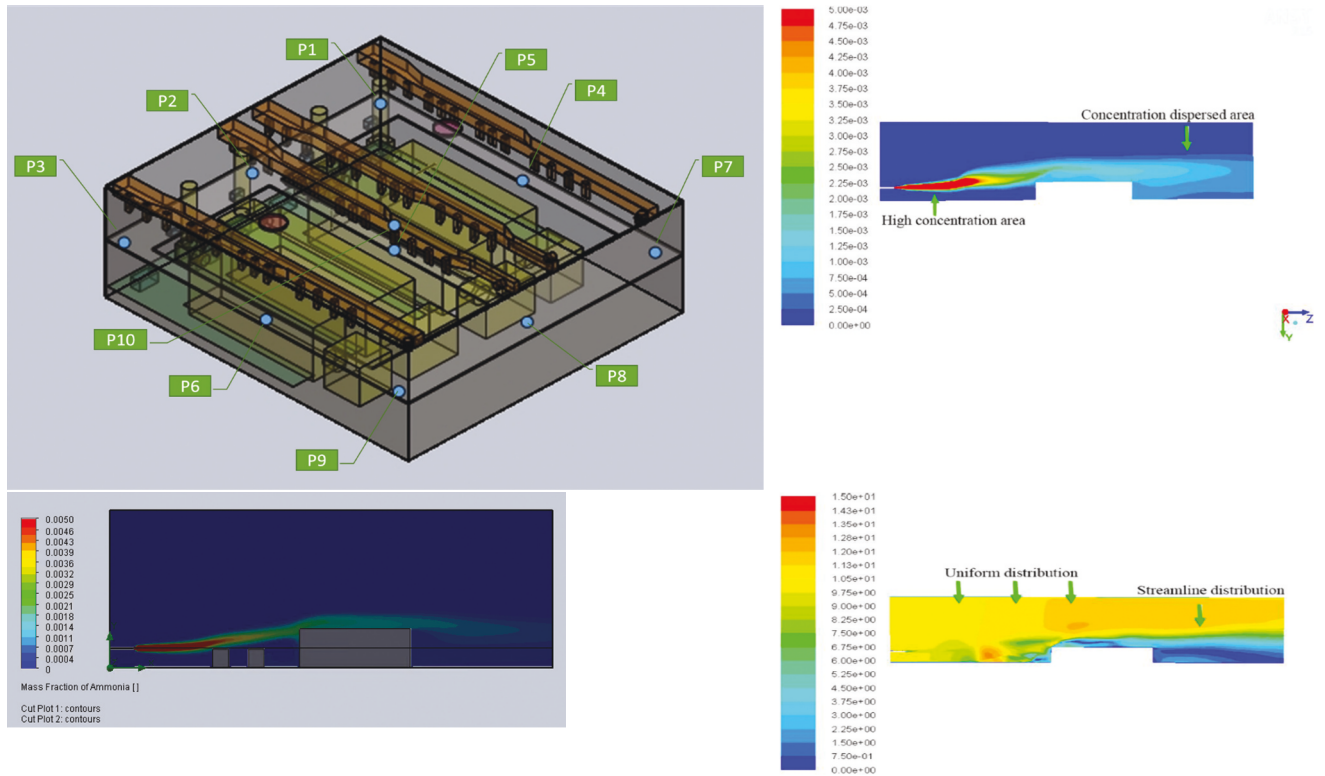
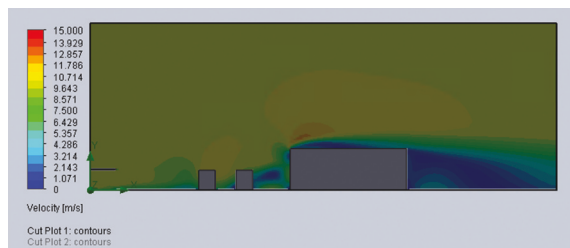


Table 5. Location of measuring points defined.

Measuring point	X co-ordinate (m)	Y co-ordinate (m)	Z co-ordinate (m)
P1	1	5	1
P2	1	5	15
P3	1	5	29
P4	16.5	5	1
P5	16.5	5	15
P6	16.5	5	29
P7	31	5	1
P8	31	5	15
P9	31	5	29
P10	16.5	10.5	15



from butt joints. Three different scenarios are considered on port side of the model behind the engine area, as fuel lines are concentrated in this region. The leakage scenario, termed as L1, L2 and L3 hereon, depict gas leakage in the transverse, vertical and longitudinal directions respectively. All leakages are taken to be at different heights as per the fuel pipe routing. The simulations are time dependent and carried out for a physical time duration of 150 s with time step of 1 s which was manually adjusted to decrease the computational time.

Meshing test

Flow Simulation module automatically meshes the model into cuboid shaped cells based on the cartesian plane. The density of cubes in the model can then be increased or decreased to get a better mesh. However, it was necessary to generate a mesh that would cater for gas dispersion behaviour at prime locations in the model. This was achieved by a simulation run carried out without any leakage of ammonia for obtaining a steady air flow field and temperature field. The result of the simulation is shown in Figure 5. These figures

illustrate that vortex flows occur under the interaction of walls and machinery equipment, which go against the gas dilution and heat emissions. Intensive flow with relative high velocity is seen near the wall, which is beneficial for gas dilution as the gas pipelines are positioned there. Further, rarefied flow with low velocity on the top between inlets and outlet is seen which may lead to gas concentration near the wall. Due to heat release from machinery equipment, gas buoyancy may get affected and thus area near the engine is also an area of concern.

Dense mesh were manually introduced at these prime locations to get a better result. Figure 6 illustrates the final mesh generated in the model to study the leak scenarios. The model was meshed into 12,46,147 cells, which included 5,97,993 cells consisting of solid surface and the rest fluid domain cells.

Simulation result

Leakage scenario L1

As seen in Figure 7, a jet is immediately caused by the ammonia gas with high velocity. The extent and mixing of the released gas depends only on the properties of the jet as the velocity inside the jet is higher than that of the ambient air. The jet tends to spread sideways and is taken over by passive dispersion deflected under the action of ambient air flow. Deflection and dispersion is also seen in the jet by the engine surface. The gas dispersion area gradually grows up and fills almost half of the engine room in the port side. In the initial stage of leakage (<30 s), gas is locally concentrated near the leakage due to formation of vortex flow. Later, due to the impact of buoyancy and air flow, gas cloud rises gradually and starts to accumulate the ceiling.

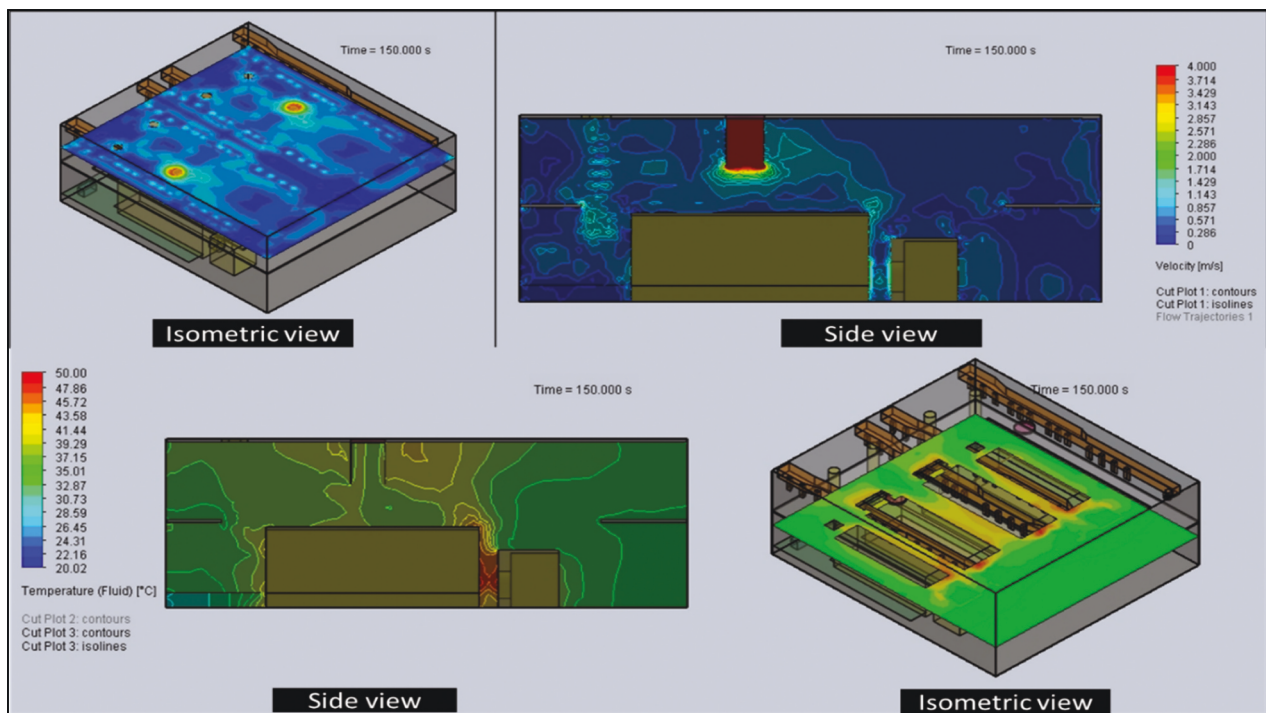


Figure 5. Simulation for evaluating area of critical importance to aid meshing.

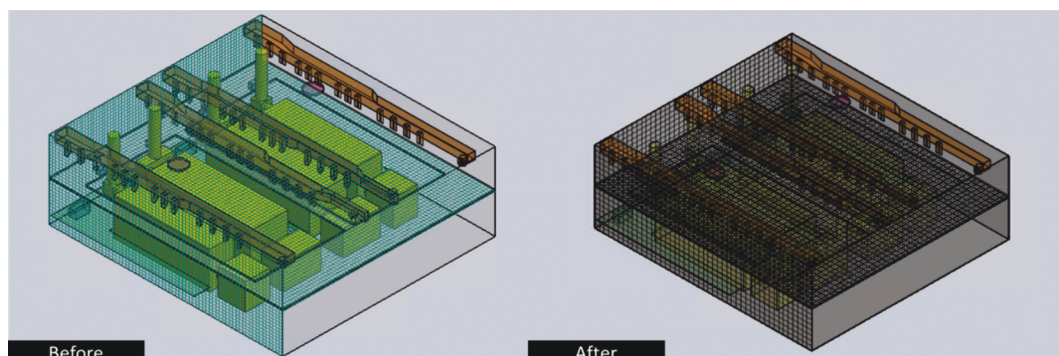


Figure 6. Meshing carried out for better results.

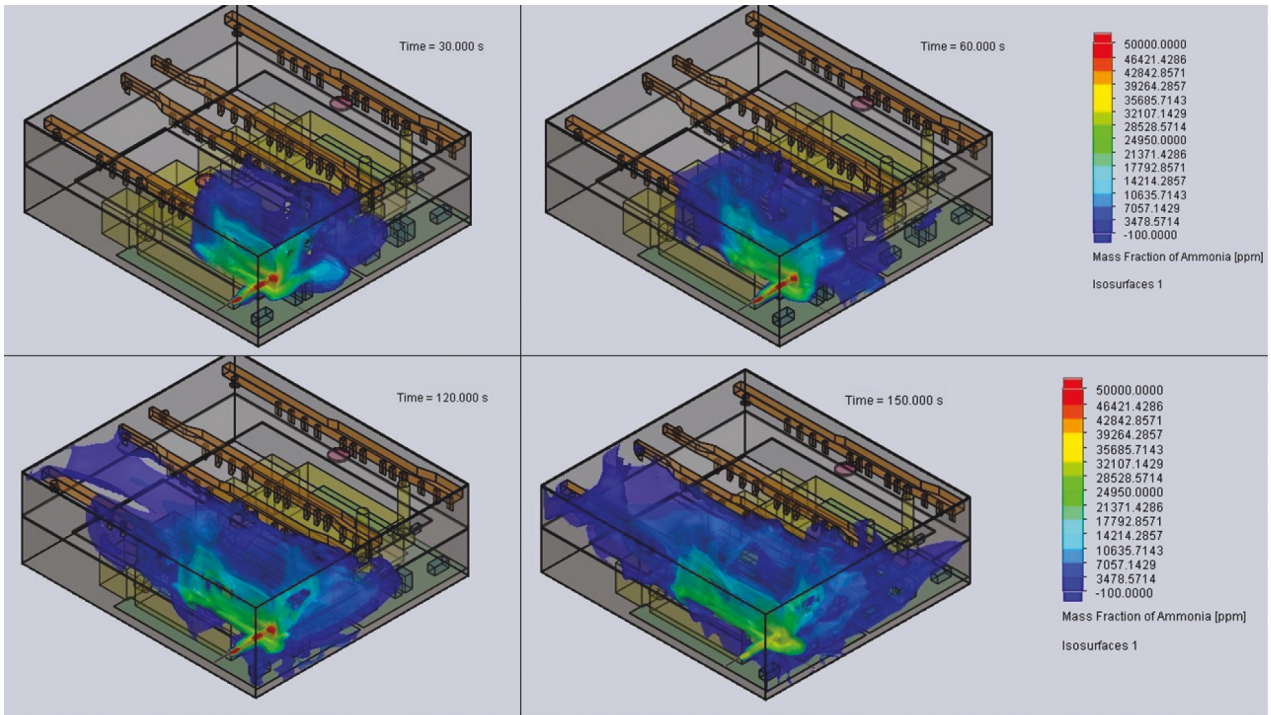


Figure 7. Transverse leakage L1 simulation.

The gas cloud formed above is pumped out of the exhaust outlets. The concentration of ammonia gas kept fluctuating near the jet area once the simulation reached a steady state (120–150 s).

Figure 8 shows the variation of ammonia concentration at measuring points over the time duration of leakage. It is observed, as gas cloud starts dispersing sideways, P4 detects ammonia at a concentration of 5 ppm within a duration of 15

s. Measuring points P5 and P10 would also give an alarm at 47 s and 50 s respectively. The second alarm limit set at 15,000 ppm corresponding to flammability risk is not reached during the entire duration of release. Ammonia concentration will not be sufficient to create a risk of fire in such a leakage scenario. The concentration of ammonia rapidly increases and covers the port side of engine room within 60 s of dispersion. The

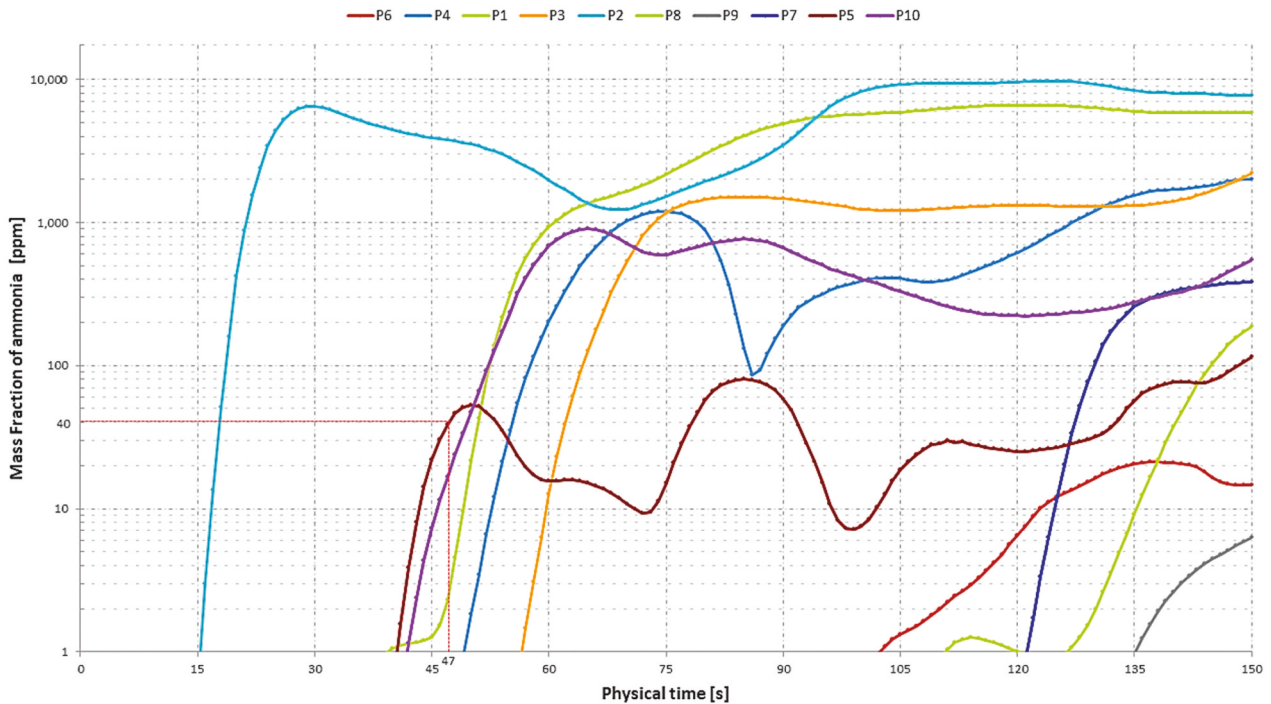


Figure 8. Variation of ammonia concentration for leakage L1.

maximum value reached in the simulation is at measuring point P2, where the concentration reaches almost 10,000 ppm in a duration of two minutes. The most important concern brought out in this scenario is that ammonia concentration near the port engine rises exponential to reach 6000 ppm in an interval of 15 s.

Leakage scenario L2

The simulation (Figure 9) shows that a jet is formed by the gas leakage and releases straight up to the ceiling of engine room. Affected by the eddy current formed by deflection by the ceiling, ammonia gas cloud concentrates near the ceiling and is dispersed in the entire engine room within a short period of time. Further it is seen that the jet being blocked by the ceiling causes a high concentration area just above the leakage which increases the probability of fire and explosion. Gradually the gas spread over the entire engine room and high concentration develops in a two meter radius of the leakage. The radius gradually keeps increasing and the concentration near the source becomes constant after two minutes in simulation.

Ammonia concentration for leakage scenario L2 (vertical) is shown in Figure 10. Four out of 10 measuring points (P2, P10, P5, and P4) detect the concentration of gas within 45 s time frame. The concentration unlike in L1 grows gradually and 1000 ppm is only crossed after 60 s of gas release. It is evident that the concentration does not reach the second alarm limit and thus cause no risk of fire

due. It is also seen that the gas immediately forms a cloud near the top corner of port side and then gradually moves further away from the leakage. A maximum concentration of 4325 ppm is reached within two minutes of simulation at P4.

Leakage Scenario L3

Gas cloud in case of leakage L3 in longitudinal direction are seen to spread over the entire length of the engine room within a small duration of time (<30 s) as seen in Figure 11. Unlike the other two scenarios, the concentration near the source is almost negligible over the first minute. As simulation time increases, gas cloud starts forming around the mid-plane and ceiling of the engine room. Concentration keeps on increasing near the mid-plane and is also seen to cover the area near source due the deflection and dispersion by the inlet air flow (120–150 s).

Figure 12 shows the variation of concentration of ammonia for leakage scenario L3 (longitudinal). As brought out in the graph, two measuring points (P7 and P1) detect a 5 ppm concentration within 30s of leakage. A key finding of this simulation is that the second alarm (set at 1500 ppm) would sound after two minutes into the leakage and thus provides an evidence that the flammability risk related to ammonia cannot be neglected. The concentration of ammonia is more towards the port side of the engine room, however at a distance away from the source initially. Gradually due to dispersion and

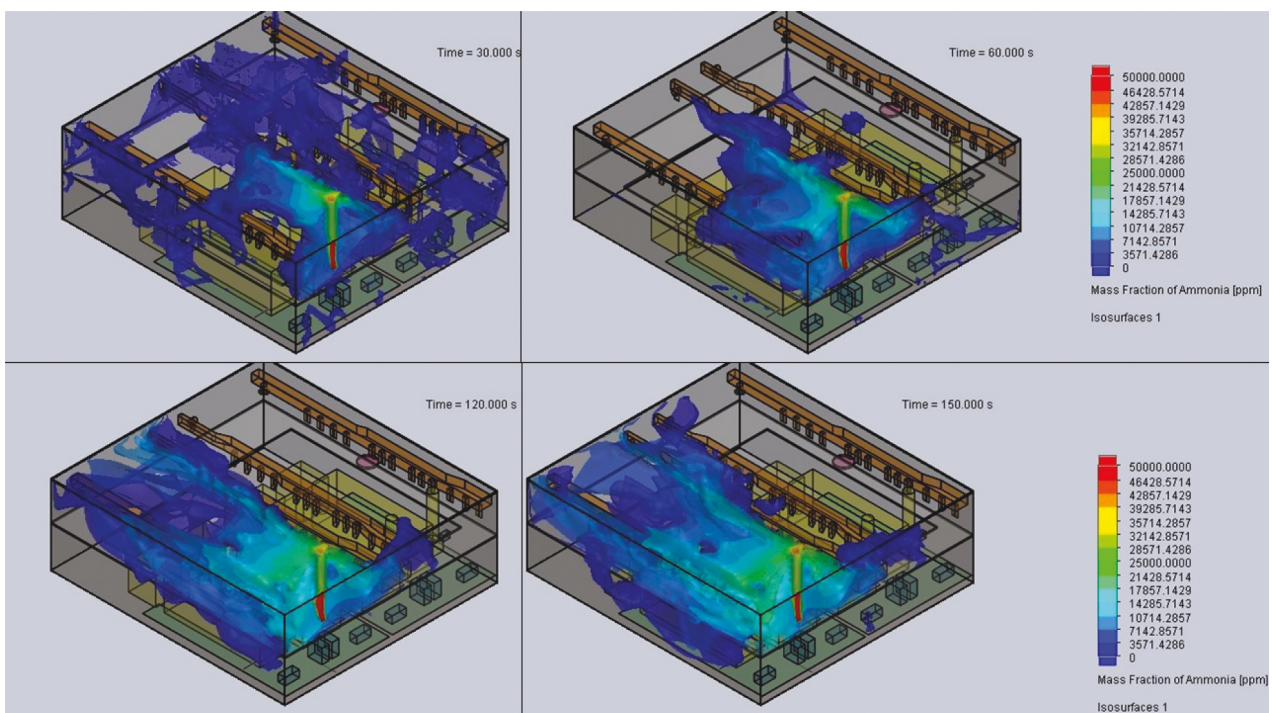


Figure 9. Vertical leak L2 simulation.

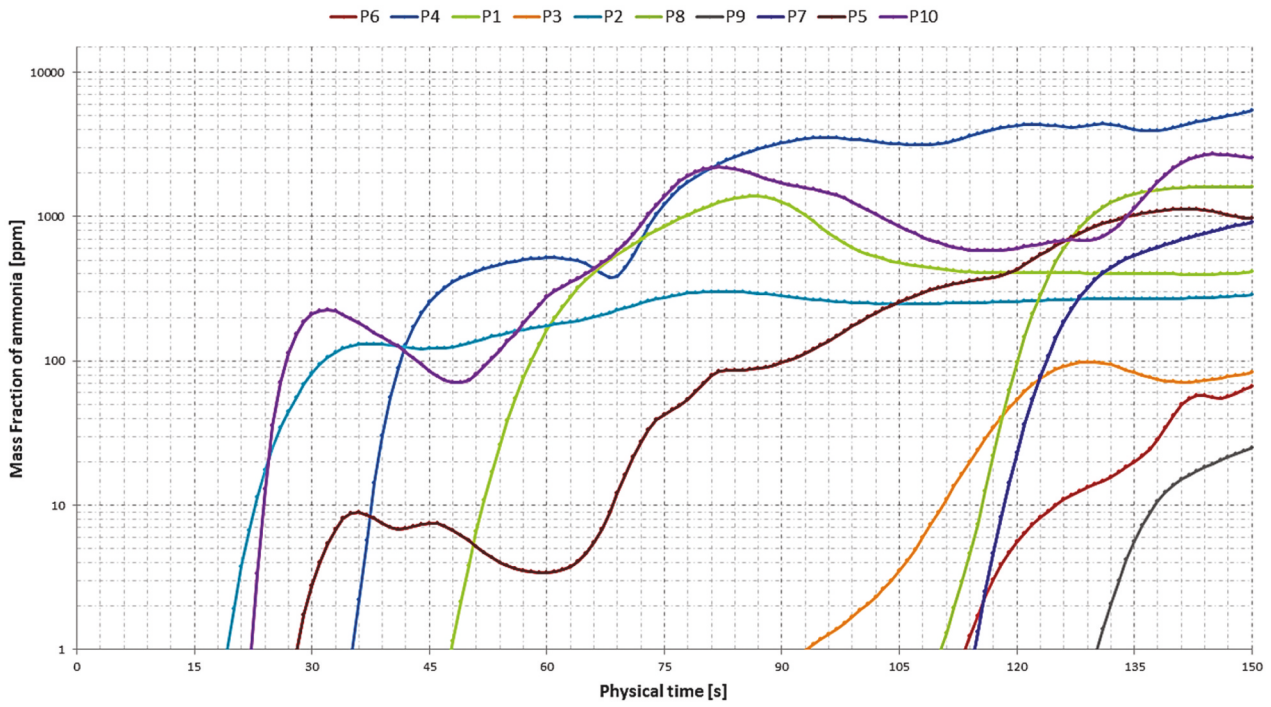


Figure 10. Variation of ammonia concentration for leakage L2.

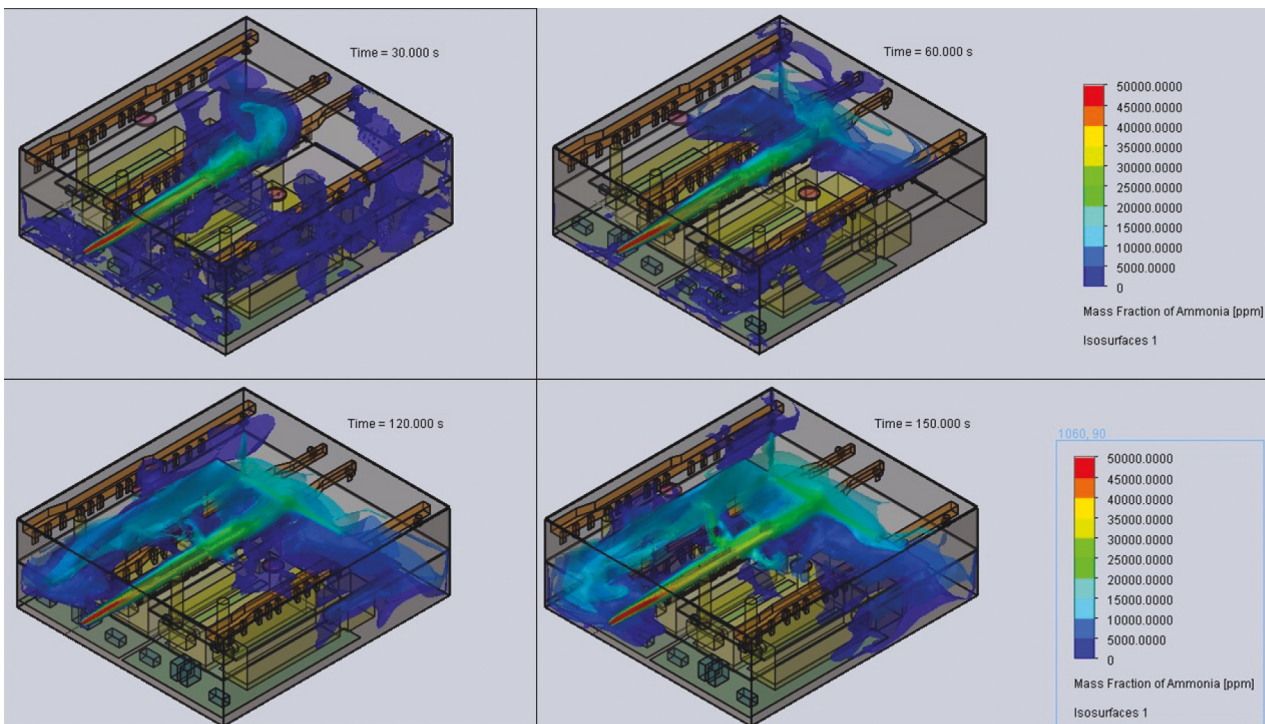


Figure 11. Longitudinal leak L3 simulation.

barriers, the gas cloud starts dispersing at the mid plane of the engine room. The concentration of ammonia is the highest at point P7. Also, the average concentration in this Scenario is higher than the other two scenarios leading to an evidence that longitudinal leak in an engine room would have the highest risk of toxicity.

Post leakage analysis

It was deemed essential to also evaluate whether the ventilation provided in the engine room was sufficient to extracting the ammonia gas after leakage was stopped (See Figure 13). For this purpose, the leak scenario L3 is further continued for a duration of 600 s. It was assumed that the leak would stop within 120 s by initiation of

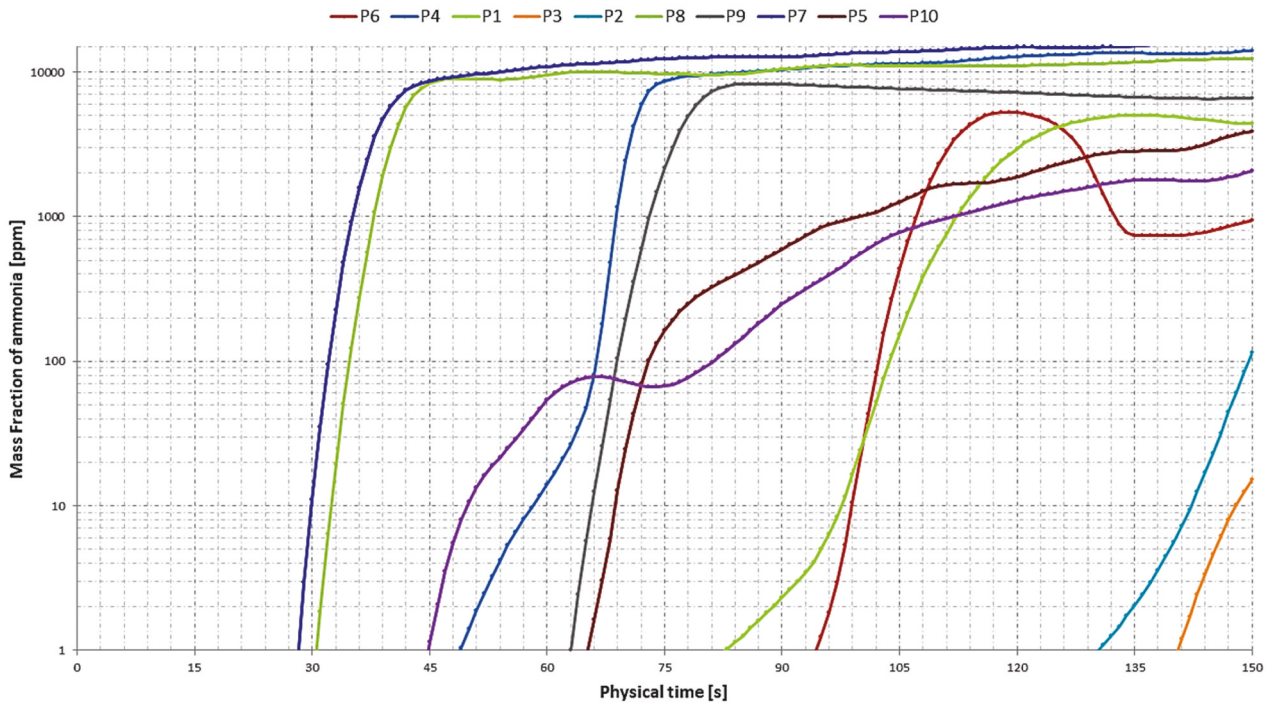


Figure 12. Variation of ammonia concentration for leakage L3.

safety isolation valves in the fuel system. Figure shows that the concentration of ammonia start decreasing after 120 s and attain a constant value between 1000 and 2000 ppm after 500 s. This denotes that the engine room ventilation is not sufficient for extracting ammonia gas from engine room. Therefore, extra ventilation blowers would be required to reduce the concentration of gas further below the permissible limit.

Key findings

An exposure of 5 ppm concentration of ammonia for 5minute duration can be lethal to human respiratory system. For results obtained by CFD simulation, it is

seen that ammonia concentration would reach more than 1000 ppm and in some cases 10,000 ppm within a short duration of time. Assuming that an extra 30–60 s would be required for initiation of safety isolation valves in fuel system, over and above 45 s of detecting ammonia leak, only a short time of evacuation would be available for any personnel inside the engine room. It can also be inferred that a person working on port side of engine room in leakage scenarios L1 and L2 would be at a high risk if evacuation is not carried out within the first two minutes of leakage. Leakage scenario L3 is seen to have the highest risk of toxicity. However, the alarm activation in this scenario would also occur earlier, thus giving more time for

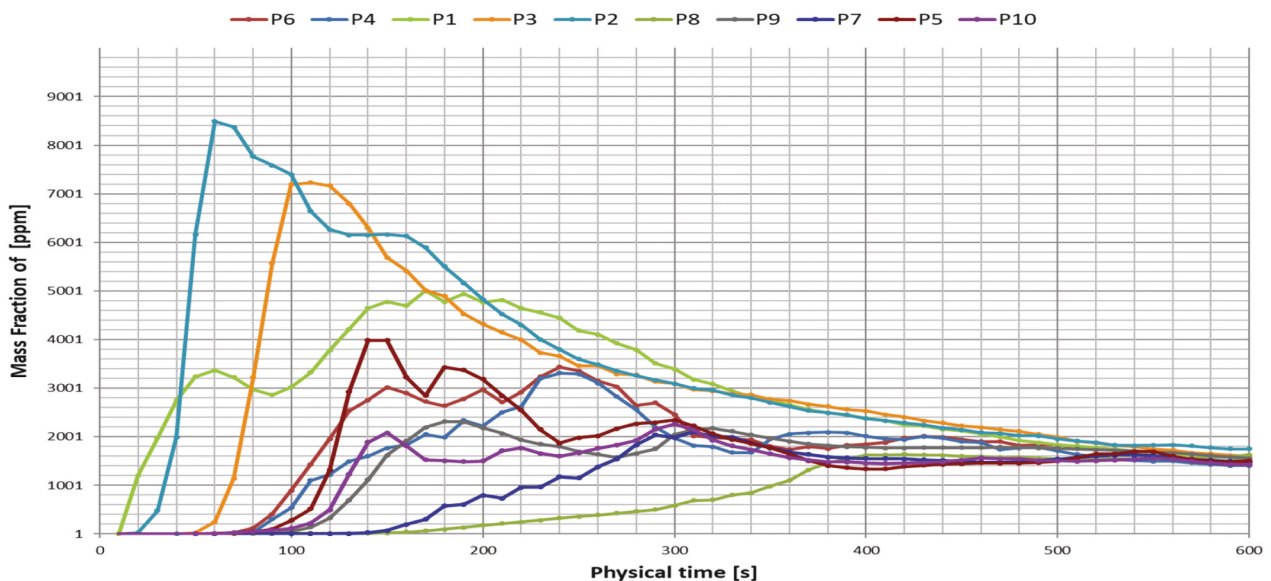


Figure 13. Concentration of ammonia with leakage stopped at 120 s for leakage L3.

reaction. Position of gas detectors at locations of the measuring points is deemed sufficient in detecting and triggering alarms. Although the flammability risk is not seen in the first two scenarios, chances of ammonia fire can develop if leakage are not controlled in timely manner.

Discussion

Recommendation

The simulation carried out using the CFD software has been effective in understanding the problem statement introduced at starting of the paper. It is brought out that ammonia gas dispersion in an enclosed space is effected by placement of barrier, temperature gradients of walls and equipment, leakage location and direction, and ventilation flow rates. The following recommendations are made by author to improve safety in engine room for addressing an incident related to ammonia gas leak:-

- (a) Ventilation requirement for engine rooms of ammonia fuelled vessels would be more as compared to an LNG carrier. This can be met by designing exhaust blowers which operate on two volume flow rates, the higher one initiated when any leakage is detected.
- (b) Scrapping technology would be required before releasing extracted ammonia gas into the atmosphere. The height of release should be kept above the exhaust release of the engines in order to decrease the risk of ammonia exposure to the crew.
- (c) Risk of ammonia fire cannot be neglected and electrical system design inside engine room would require spark proof standards. An effective way to fight ammonia fire would also be required for worst case scenario.
- (d) Special training would be required for the crew to understand the risk involved in ammonia gas leak. The training should also cover first aid required to ammonia exposure and firefighting with ammonia caused fire.
- (e) Safety audits of gas detector system and emergency isolation valves of ammonia fuel lines on a regular basis to improve the dependency on the system.
- (f) Inherent gas safe engine rooms would be more preferred than ESD safety engine rooms in case of ammonia due to the high risks involved.

Paper contribution

The paper has made a worthwhile contribution to the academic research in the area of maritime safety enhancement and ammonia's acceptance as a marine

fuel. The novelty of the research carried out is in its investigation of ammonia's safety characteristics and especially toxicity risk analysis. CFD has been shown to provide a good example for carrying out research on gas dispersion models inside an enclosed space with complex geometry. The results produced can act as an effective base for future researchers to undertake more leakage scenarios and for different engine room configurations. Finally, the paper provides an answer to the question, how safe is ammonia as a marine fuel? It is opined that even though ammonia is toxic and poses fire risk to an extent, its implementation would prove to be a paramount alternative fuel in transition to a decarbonised maritime sector.

Future work

The paper carried out may be observed to be an aid for future researchers. Many factors have been overlooked and assumed. These can be extensively looked upon in the future for improving a better understanding into the topic. An analysis that quantifies the risk with number of injuries or fatalities can provide an in-depth knowledge on ammonia's risk to crew onboard. As the paper has brought out, ventilation requirements of engine room of a future ammonia fuelled vessel would be more than conventional design. This aspect can be studied further to introduce guidelines for designing phase. Study can be undertaken to determine effective ways in controlling ammonia gas dispersions that occur by accidental leaks. CFD simulation can be used to determine time required to evacuate ammonia gas with effective extraction methods. As ammonia's toxicity was studied in the paper, likewise hydrogen gas leak can be modelled to compare risk involved in using either or both these fuels.

Conclusion

Ammonia is seen to be the most convenient marine fuel that can bridge the gap between the short term goals projected by the IMO and fully replacing carbon rich fuels for a sustainable shipping future. It provides the best solution to the problem of storage and distribution related to hydrogen and has a well-established infrastructure in place for a starting point. The ammonia industry has an experience of more than 100 years in handling, storing and distributing ammonia and can guide the future regulatory regime in uptake of ammonia as a marine fuel. The behaviour of a gas release inside an enclosed space is completely different to the known behaviour of the same release occurring outdoors. Given sufficient time, even the smallest of leaks can exceed the LEL (explosive) or TLV (toxic) levels within the entire room volume. CFD is seen to be an effective method in studying an indoor ammonia gas release. This paper applies CFD to

illustrate ammonia gas dispersion resulting from different leak scenarios inside an engine room space with ventilation and machinery. It is seen that the dispersion is affected by the volume of engine room, leakage rate, direction and position of leak, temperature gradient of working machinery and bulk heads, gas pressure and temperature, barriers and ventilation. The results have been promising and coincide with the fact that ammonia poses more of a health hazard than a fire hazard. The study also provides evidence of how CFD can be effective in studying HVAC effectiveness on gas fuelled marine vessels. The paper concludes that ammonia is dangerous and has a high risk in terms of toxicity when applied onboard as a marine fuel, but with good planning and effective safety protocols, ammonia leak can be controlled and personnel evacuated in time before it becomes fatal.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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