ANNEX F

SIMULATION OF AMMONIA BUNKERING RELEASE ON HYPOTHETICAL LOCATION

09/2025

Executive summary

Denmark is a maritime gateway for Scandinavia and Europe, yet there is no established infrastructure or regulatory framework for ammonia bunkering. Green ammonia is emerging as a promising marine fuel, meaning closing all the regulatory gap matters. There is also limited safety research on operational and accidental releases during bunkering in Danish-relevant locations. This study addresses that need by outlining a realistic bunkering set-up and examining potential release impacts. In risk terms the primary hazard of ammonia is toxicity, not flammability, thus public exposure is the key concern.

Dispersion and lethality simulations were performed in Phast to assess accidental releases during ammonia bunkering. A hypothetical Danish site was defined, considering onshore and offshore operations. The analysis focused on ship-to-ship (STS) and terminal/pipeline to ship (PTS) bunkering methods. Twenty scenarios were modelled, considering summer and winter conditions, releases on land and over open water, fully refrigerated and semi refrigerated operating conditions and two release heights.

Across all scenarios, semi refrigerated ammonia releases are vapour dominated and produce large clouds with only small, short-lived pools, while fully refrigerated ammonia releases are pool dominated and leave large, long-lasting pools that sustain evaporation. Dispersion is driven mainly by release height and terrain. Higher release points and open water both increase the vapour footprint for semi refrigerated ammonia and fully refrigerated ammonia, with the strongest effect on semi refrigerated ammonia. Lethality patterns are controlled mainly by storage condition and season. Semi refrigerated ammonia gives longer lethal distances than fully refrigerated ammonia for the same scenario, while summer generally gives longer lethal distances than winter because clouds linger and doses accumulate more near the source.

Near the port, lethal contours for fully refrigerated ammonia stay within the port area for the conditions analysed, while offshore releases of semi refrigerated ammonia and fully refrigerated ammonia over open water keep most of the lethal impact at sea. As a result, fully refrigerated ammonia remains the safer and more realistic bunkering mode for the Port of Rønne, and placing higher risk configurations offshore further reduces offsite toxic risk.

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Prepared by: Juan Carlos Lopez Santiago (DBI)
Reviewed by: Blanca Andres Valiente (DBI)
Approved by: Leonard Sang Tuei (DBI)

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1. ABBREVIATIONS

Abbreviation	Explanation
ABS	American Bureau of Shipping
AEGL	Acute Exposure Guideline Level
AiP	Approval in Principle
DMI	Danmarks Meteorologiske Institut
DNV	Det Norske Veritas
DTL	Dangerous Toxic Load
ESD	Emergency shutdown
HSE	Health and Safety Executive
IGC Code	International Code for the Construction and Equipment of Ships Carrying Liquefied Gases in Bulk
IMO Type C	Pressure vessel type for liquefied gas cargo
LNG	Liquefied Natural Gas
NFPA	National Fire Protection Association
NIOSH	National Institute for Occupational Safety and Health
PEL	Permissible exposure limit
Phast	Process Hazard Analysis Software Tool
PTS	Terminal or pipeline to ship
SLOD	Significant Likelihood of Death
SLOT	Specified Level of Toxicity
STEL	Short term exposure limit
STS	Ship to ship
TTS	Truck to ship
TWA	Time weighted average

2. DEFINITIONS

Term	Definition
AEGL levels	Public protection guideline concentrations for acute releases. AEGL 1 is notable discomfort. AEGL 2 is serious but reversible effects. AEGL 3 is life threatening effects or death. Defined for 10 min through 8 h exposures.
Pasquill stability class	Atmospheric stability category used to represent turbulence and mixing which affects dispersion.

3. INTRODUCTION

Denmark's geographical location positions the country as a gateway for maritime trade and transportation, supporting the seamless movement of goods and passengers between Scandinavia and the rest of Europe. This role is reinforced by the country's strong presence in the global shipping and logistics industry.

As the transition toward sustainable energy sources gains momentum, green ammonia is increasingly recognized as a promising alternative to conventional marine fuels. Despite its potential, Denmark currently has no established infrastructure or regulatory framework to support ammonia bunkering, which presents a significant barrier to its adoption.

In parallel, there is a notable lack of safety research concerning both operational and accidental releases of ammonia during the bunkering process, particularly in locations relevant to Denmark's maritime sector.

This study seeks to contribute to that effort by offering a timely and relevant report for the maritime community. It outlines a hypothetical ammonia bunkering process and examines the potential impacts of ammonia release through a series of representative scenarios.

4. METHODOLOGY

No port in Europe has commenced ammonia bunkering operations, however several have begun preparing safe handling regulations of the fuel as part of a broader shift toward alternative maritime energy solutions. The primary objective of this work is to conduct simulations using Phast software[1] to assess the consequences of accidental ammonia releases during different bunkering operations. A key focus is on evaluating the far-field dispersion of ammonia in order to determine potential impacts on the population living in the surroundings of the plant and port area.

For the purpose of this study, it was decided to base the simulations on a port where ammonia bunkering could hypothetically take place within Denmark.

For the simulations, parameters like weather, the different ammonia bunkering methods, operating conditions during bunkering operations will be considered. The effect on people will be assessed based on toxicological exposure and health impacts of ammonia.

4.1. Phast software

Phast (Process Hazard Analysis Software Tool) is a widely used consequence analysis software developed to model the effects of accidental releases of hazardous materials. The software is developed by Det Norske Veritas (DNV). Phast enables the simulation of scenarios such as toxic dispersion, fires, and explosions, providing insights into potential impacts on people, assets, and the environment. Due to its structured approach and industry acceptance, Phast is a common tool for quantitative risk assessments in the process and energy sectors. [1]

For the current simulations, the version Phast 9.11.124.0 (12-Jul-2025) will be used.

4.1.1. Limitations of Phast software

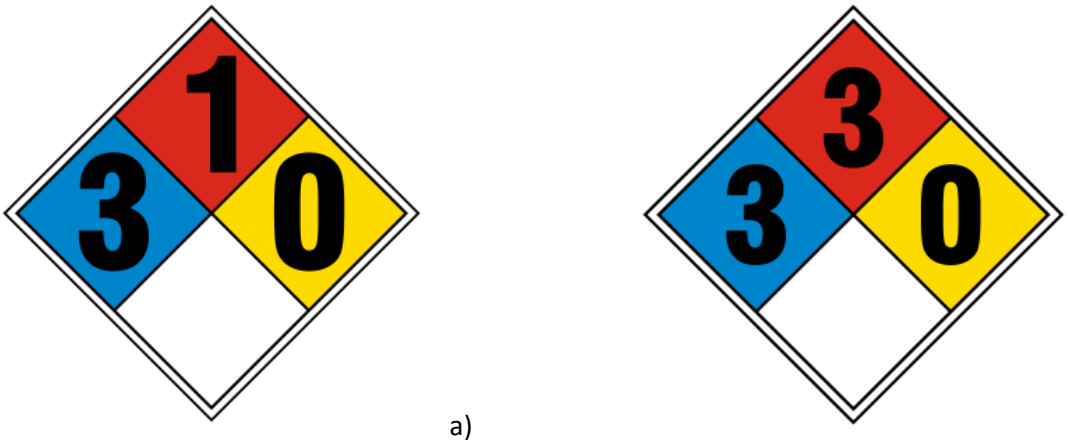
Despite its broad applicability, Phast has several limitations that must be acknowledged:

- It is based on empirical modelling, which introduces simplifications.
- It uses a simplified two-dimensional (2D) model approach, which may reduce accuracy in complex environments.
- It is not well-suited for small-scale geometries, where detailed structural influences are important.
- It does not account for the location of ventilation routes or the presence of suppression systems in nearby buildings.
- Dispersion modelling in confined spaces is limited and may not capture localized effects accurately.
- It does not consider the domino effect, i.e., the impact of one system failure on other interconnected systems.
- Phast displays the maximum dispersion footprint as the envelope of every location reached by the cloud at any time during the simulation, drawn as one continuous contour. It does not necessarily show vapour cloud that may have occurred at any specific time.
- In the far field this can imply a steady presence where the real cloud is thin, intermittent, and strongly affected by wind and changing weather, resulting in vapour clouds with irregular shape.

4.2. Properties of ammonia

At standard temperature and pressure conditions, ammonia is colourless toxic gas with a strong odour. Unlike conventional fuels, where the main concerns are fire and explosion hazards, the primary risk with ammonia is its toxicity.

Ammonia in its gas form is flammable, however because of its high autoignition temperature of 651°C and high flammability limits, the ignition of ammonia is challenging. For this reason, Ammonia gas is not classified as a highly flammable substance due to its high ignition temperature. NFPA 704 [2] gives a rating of 1 in open locations, and 3 only for a confined location.



a) b)

Figure 1: NFPA 704 Anhydrous Ammonia Hazard Diamond. Red colour: Fire hazard. Blue: Health hazard. Yellow: Instability hazard. White: Specific hazard. (a) Open Locations (b) Confined Location [2]

Ammonia is lighter than air, which means it tends to rise and disperse once released into the atmosphere. When ammonia is released into humid air, its rapid evapouration cools the surrounding atmosphere, causing moisture in the air to condense and form a visible white cloud. This visible cloud is composed of both condensed water droplets and ammonia vapour, but it does not mark the true limits of the hazard. Depending on weather and dispersion conditions, ammonia can spread well beyond the visible plume, and harmful concentrations may still be present outside the apparent boundary. [3]

When in contact with water, ammonia is highly soluble, although its solubility decreases as the temperature rises. At 0 °C, it dissolves in water up to 47 % by weight, at 20 °C, this drops to 34 % [4]. When ammonia comes into contact with water, it dissolves rapidly in a strongly exothermic reaction, releasing a significant amount of heat. This heat may cause the solution to boil and vapourise [5].

Table 1. Physical, chemical and flammability and explosive properties of ammonia [4,6–8]

Property	Value
CAS number	7664-41-7
Molecular formula	NH_3
Molecular weight	17.03 g/mol
Boiling point at 1 atm	-33.34 °C
Freezing point at 1 atm	-78 °C
Lower flammability limit	15.2 %
Upper flammability limit	27.4 %
Auto ignition Temperature	651 °C
SLOD DTL	1.03×10^9
Gas properties	
Density at -33.34 °C and 1 atm	0.88 kg/m^3
Density at 25 °C and 1 atm	0.77 kg/m^3
Relative density at 25 °C and 1 atm	0.77
Liquid properties	
Density at -33.34°C at 1 atm	682 kg/m^3

Density at -4°C at 5 bar	633.1 kg/m³
Specific gravity -33.34 °C and 1 atm	0.69
Solubility in water at 0 °C	47 % w/w
Solubility in water at 15 °C	38 % w/w
Solubility in water at 20 °C	34 % w/w

4.2.1. Toxicology exposure and health impacts

Ammonia gas is a hazardous chemical, and human exposure must remain within legal limits, which can differ slightly between countries. These regulations are typically defined based on both the concentration of ammonia in the air and the length of exposure.

From a toxicology point of view, long-term exposure to low levels of ammonia (below 400 ppm) is not linked to chronic health effects. In contrast, high-level releases (above 2000 ppm) can lead to severe acute health consequences. [9]

Table 2 provides guidance on recommended exposure levels, these values are provided for situational awareness and do not replace regulatory limits.

Table 2. Exposure guidance [9]

Ammonia concentration in air (by volume)	Effects
20-50 ppm	Readily detectable odour
50-100 ppm	No impairment of health from prolonged exposure
400-700 ppm	Severe irritation of the eyes, ears, nose, and throat. No lasting effect on short exposure, aggravation of existing respiratory problems could occur
2000-3000 ppm	Dangerous, more than 30 minutes of exposure may be fatal
5000-10000 ppm	Serious oedema, strangulation, asphyxia, rapidly fatal

While the previous table summarises health effects by concentration, the exposure of ammonia to the workers during normal daily operations at their workplace relies on regulatory occupational exposure limits set by national authorities. These include an 8-hour time-weighted average (TWA), which caps the average exposure across a shift, and a 15-minute short-term exposure limit (STEL), which limits brief peaks during tasks. Together, TWA and STEL provide the framework for managing ammonia exposure during normal operations.

Table 3. Guidelines and regulatory limits for ammonia exposure [10]

Authorities or Organisations	STEL 15 mins	TWA 8 hours
California Cal/OSHA Permissible Exposure Limits (PELS) from 29 CFR 1910.1000	35 ppm	25 ppm
EU Indicative Exposure Limit Values in Directives 91/322/EEC, 2000/39/EC, 2006/15/EC, 2009/161/EU (12 2009)	50 ppm	20 ppm
UK Health and Safety Executive (HSE) EH40/2005 Workplace exposure limits	35 ppm	25 ppm
National Institute for Occupational Safety and Health (NIOSH)	35 ppm	25 ppm

In contrast to the TWA a STEL values, the Acute Exposure Guideline Levels (AEGLs), established by the U.S. National Advisory Committee for Acute Exposure to Hazardous Substances, are meant for emergency response. AEGLs define threshold concentrations for airborne chemicals based on both exposure duration and the severity of potential health effects. Unlike workplace limits, AEGLs apply to the general population and are used to assess the risks during accidental chemical releases.

AEGLs are divided into three levels, each corresponding to increasing severity of health effects. AEGL-1 represents the concentration above which individuals may begin to experience mild, temporary symptoms such as irritation or discomfort. AEGL-2 corresponds to concentrations that could lead to more serious, but non-lethal and reversible health effects. AEGL-3 defines the concentration at which life-threatening effects or death may occur. Each level is defined for five specific exposure durations, ranging from 10 minutes to 8 hours, reflecting the importance of both time and concentration in assessing toxic risks.

Table 4. AEGLs for emergency response [10]

Guidelines	10 min	30 min	1 h	4 h	8 h
AEGL-1	30 ppm	30 ppm	30 ppm	30 ppm	30 ppm
AEGL-2	220 ppm	220 ppm	160 ppm	110 ppm	110 ppm
AEGL-3	2700 ppm	1600 ppm	1100 ppm	550 ppm	390 ppm

For the current simulations, the ammonia vapour cloud will be assessed using AEGL-2 and AEGL-3 concentration levels, evaluated at a height of 1.5 m for dispersion over land. The analysis will consider AEGL-2 and AEGL-3 values for exposure durations of 10 minutes.

4.3. Hypothetical bunkering location

In Europe, while no port has yet commenced ammonia bunkering operations, several have begun preparing to handle the fuel as part of a broader shift toward alternative maritime energy solutions.

For the purpose of this study, it was decided to base the simulations on a port where ammonia bunkering could hypothetically take place. To establish a representative scenario for the simulations, contact was made with the Port of Rønne. Strategically located in the island of Bornholm in the central Baltic Sea, Rønne is the easternmost major port in Denmark. It serves as a key maritime hub, supporting a wide range of operations including ferry services, cruise tourism, bulk cargo handling, and offshore wind logistics.

The map below shows the location of all the ports within Denmark part of Danske Havn, indicating Port of Rønne's position within the national port network.

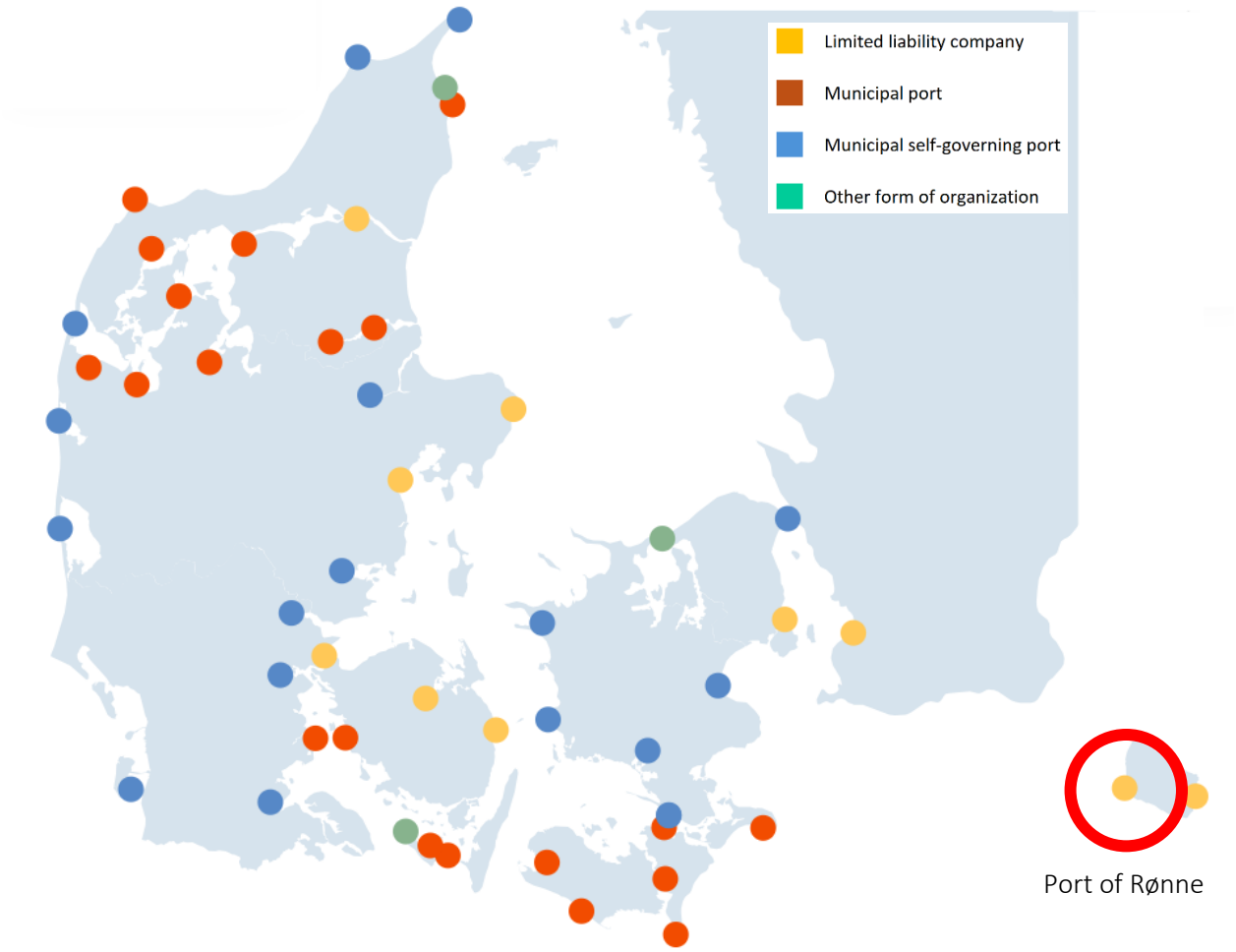


Figure 2. Locations of ports in Denmark with the Port of Rønne marked [11]

During the exchange with port representatives, the area adjacent to quay 33 has been identified as a potential site for terminal/pipeline-to-ship ammonia bunkering operations. Although these locations are not currently used for such activities, they were selected as plausible sites based on existing infrastructure, accessibility, and operational relevance. The quay in question measures 275 meters in length and has a water depth of 11 meters, which would be a limiting factor of the capacity of the bunker vessel that it could accommodate. The pipe rack from the storage tank to the port is usually routed to prioritize safety and accessibility rather than following a straight path, the longest axis of the area, which is under 500 m, will be taken as the pipe rack length.

The potential for ship-to-ship ammonia bunkering operations was also identified along quays 33, as well as along quay 34 and 35, which together have a combined length of 600 m and a water depth of 11 m, and at the planned quay in the north-western part of the port.

It is important to note that these areas are entirely hypothetical and defined solely for simulation purposes.

Figure 3. Port of Rønne and hypothetical area for ammonia bunkering operations

For offshore ship-to-ship bunkering operations, it is assumed that they would occur at a minimum distance of 2 nautical miles (approximately 3.7 km) from the port. However, under normal operating conditions, such activities may be conducted in deeper offshore waters, depending on navigational and safety requirements.

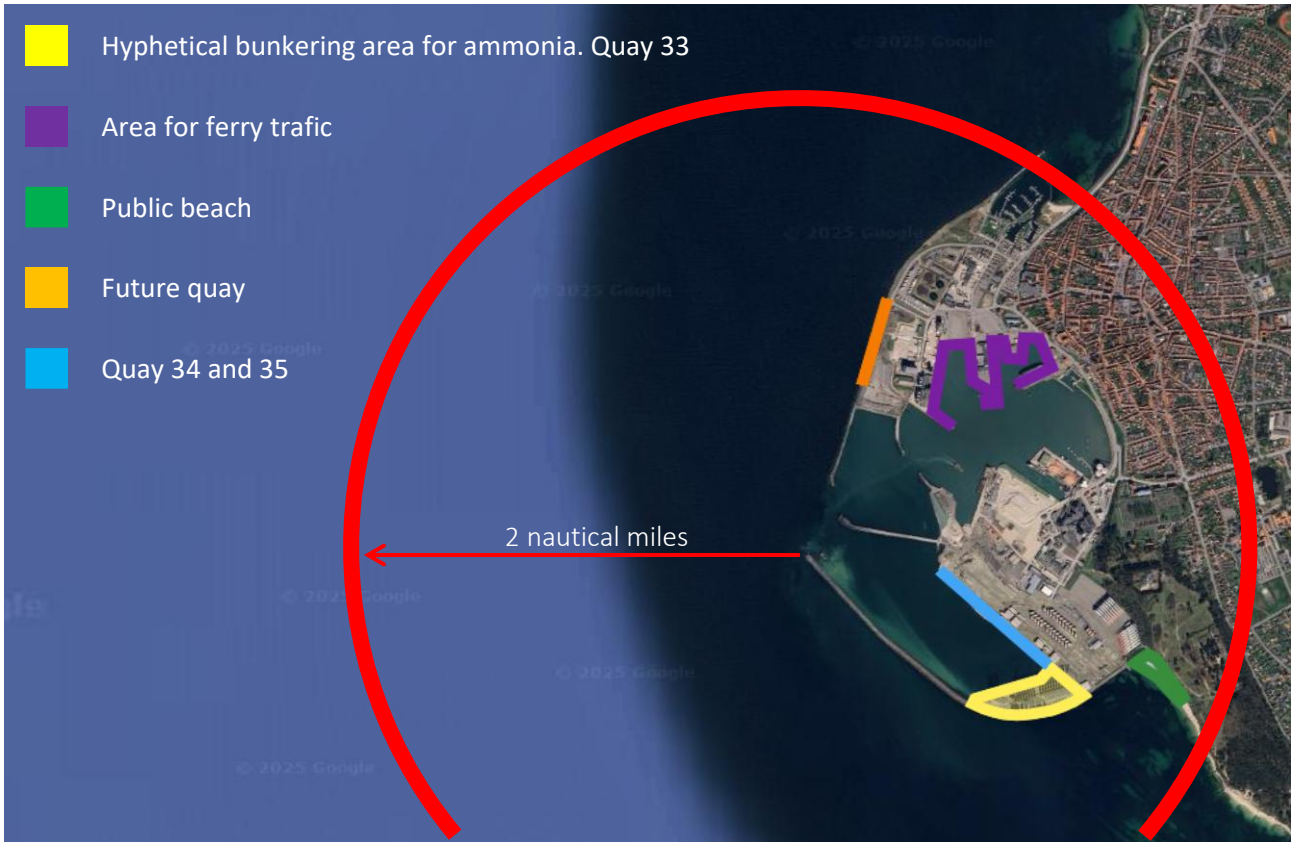


Figure 4. Port of Rønne and hypothetical area for ammonia bunkering operations. 2 nautical miles marked.

4.4. Ammonia bunkering operation

The design of the ammonia bunkering considers that ammonia behaves as a saturated liquid. In contrast to fuels, ammonia cannot remain in liquid form without either being pressurized or cooled, making its handling and storage more complex.

There are four bunkering ammonia bunkering modes:

- ship-to-ship (STS)
- terminal/pipeline-to-ship (PTS)
- truck-to-ship (TTS)
- cassette bunkering

STS, PTS and TTS are considered conventional bunkering methods. Cassette bunkering refers to a method of transferring fuel using pre-filled fuel modules or containers, often called cassettes. These cassettes are swapped in and out of vessels rather than transferring fuel via traditional pipelines or hoses. However, for the current simulation, cassette bunkering is not considered.

In dialogue with the Port of Rønne, it was confirmed that conventional bunkering methods are the most relevant for their operations, with particular emphasis on ship-to-ship (STS) and terminal/pipeline-to-ship

(PTS) methods. Consequently, the study will concentrate on the following scenarios:

- ship-to-ship (STS)
- terminal/pipeline-to-ship (PTS)

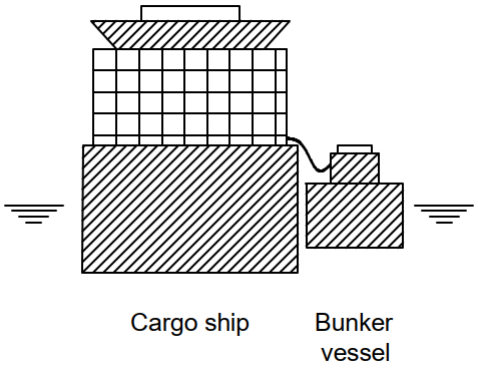


Figure 5. ship-to-ship (STS) bunkering method

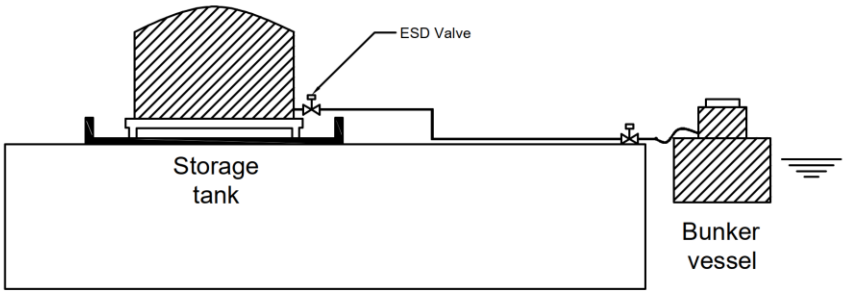


Figure 6. Terminal/pipeline-to-ship (PTS) bunkering methods

4.5. Hypothetical bunkering vessel, cargo ship and storage tank

For the simulations, it is necessary to define the dimensions and heights of the bunker supply and receiving vessel for each bunkering operation:

- The bunker vessel
- the receiving container ship
- the storage tank for ammonia

For the ship-to-ship (STS) ammonia bunkering operation, the simulations require estimates of the vertical geometry of both vessels, specifically the manifold/connection height above the waterline for the bunker vessel and for the receiving container ship. For the terminal/pipeline-to-ship (PTS) ammonia bunkering operation, the simulations require the receiving bunker's manifold height above the waterline and the capacity of the storage tank.

Although there are currently no ammonia bunkering vessels in operation, several designs are under development in response to growing interest in ammonia as a clean marine fuel.

In recent years, the maritime industry has been developing new technologies in response to environmental regulations and market demands. However, for technologies based on novel concepts, it is essential to ensure they meet safety standards equivalent to international conventions and classification rules.

To verify this, classification societies conduct safety inspections. These inspections typically occur once the product design is complete. However, if major issues are identified at that stage, it can significantly delay the development of the vessel. To avoid this, classification societies offer an early-stage design review service to identify and resolve potential problems in advance known as Approval in Principle (AiP). This scheme assesses whether a concept is technically feasible based on classification rules.

While AiP does not grant final approval, it helps clarify regulatory expectations and design requirements early in the process, making final plan approval more efficient. [17]

Several companies have already received AiPs for ammonia bunkering vessel designs. These preliminary designs provide insight into what the final vessels may look like and suggest that operational models could be ready soon.

Several ammonia bunkering vessel designs have already received Approval in Principle from major classification societies:

1. Lloyd's Register has granted AiP for a 10,000 m³ ammonia bunkering vessel developed by Hyundai Mipo Dockyard. The design features two cylindrical Type C tanks, a reliquefication system, and a marine loading arm.

2. Seatrium, an engineering firm, has received AiP from the American Bureau of Shipping (ABS) for its SMDT 25000VX-NH3, a 25,000 m³ ammonia bunker vessel. The vessel has a deadweight tonnage of 19,500 metric tons and uses IMO Type C containment systems for safe storage and handling of ammonia.

3. Korean Register (KR) has awarded an AiP to HD Hyundai Mipo (HD HMD) for its 23,000m3 Ammonia Bunkering Vessel

It is notable that most proposed ammonia bunkering vessel designs incorporate IMO Type C tanks. As detailed specifications for these ammonia vessels are not yet publicly available, a practical approach is to refer to existing bunker vessels for other fuels that use similar tank types. In this context, LNG bunker vessels serve as a useful reference.

The table below presents selected LNG bunker vessels equipped with two bilobed IMO Type C tanks. Based on this data, it can be observed that an LNG bunker vessel with a cargo capacity of 5,800 m³ has a draft suitable for the hypothetical ammonia bunkering location at the Port of Rønne of 11 m. Therefore, the freeboard dimension of 4.3 m of such a vessel will be used in the simulation.

Table 5. Dimensions of some presentative bunker vessels [10]

Bunker vessel name	Cargo tank capacity (m3)	Length	Depth	Draft	Freeboard
LNG Bunker vessel, Coral Fraseri [18]	10000	137.1	11.5	8.3	3.2

LNG Bunker vessel, Coralius [19]	5800 (2550+3250 m3)	99.6	10	5.7	4.3

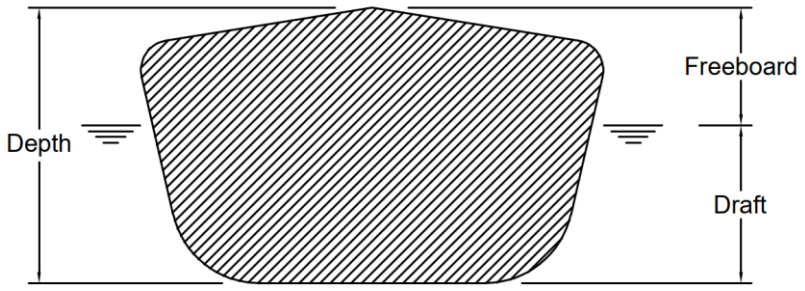


Figure 7. Ship dimensions and terminology

In the simulations, only the largest bilobed IMO Type C tank, with a total capacity of 3250 m³, is considered. In line with common industry practice, the maximum working volume is taken as 90 % of this capacity, corresponding to 2,925 m³. Geometrically, the tank has an approximate length of 68 m. Since the bilobed configuration cannot be directly represented in the model, it is approximated as a single cylindrical tank with a diameter of 7.8 m.

For the simulation, it will be assumed the usage of a storage tank with a total capacity of 10,000 m³. In industry practice, the working (usable) capacity of large above-ground storage tanks is often taken as about 85 % of the gross capacity to allow for vapour space. Based on this value, the effective storage volume is taken as 8,500 m³. Similarly, the tank geometry is assumed to be cylindrical, with a diameter of 35 m and a corresponding height of approximately 10.4 m.

For the present simulations, it was decided to consider for the cargo ship the same freeboard as for the bunker vessel to be able to compare directly the results from the simulations. However, additional simulations will be included considering a higher deck.

Table 6 includes the dimensions of selected Maersk container ships used as a basis for this scenario. For the current simulation, a Triple E class (first generation) container ship has been selected, as it features one of the tallest freeboards among Maersk vessels, measuring 15.8 metres. Because its draft, this container ship would only be involved in ship-to-ship bunkering offshore.

Table 6. Dimensions of some presentative container ships operated by Maersk [10]

Class	Length	Depth	Draft	Freeboard
Triple E class (first generation) [12]	399.2	30.3	14.5	15.8
Triple E class (second generation) [13]	399.2	30.3	16	14.3
E class [14]	397.7	30.2	17.5	12.7
Edinburgh class [15,16]	366.5	29.9	15.5	14.4

It is important to note that the current simulation does not account for leakage at ground level. As reported in [20] and [21] , the height of the release is one of the main factors influencing ammonia concentrations in the far field (around 200 m from the source). Higher release points tend to result in higher concentrations at this distance. In contrast, the release height has little to no impact on concentrations in the near field.

4.6. Weather parameters

Weather data used in this analysis was obtained from the Danmarks Meteorologiske Institut (DMI). The nearest weather station to Rønne port is located at Bornholm Airport, approximately 4 km to the southeast. This station, identified by ID 06190, provides a range of meteorological data, from which hourly records were selected for the period spanning July 1st, 2020, to July 1st, 2025.

Solar radiation data and soil temperature at a depth of 10 cm was not available in the weather station located in Bornholm Airport. For this reason, the data from the Nexø Vest was used. This weather station is located 25.87 km from Rønne port to the east. This station, identified by ID 06197, also provides a range of meteorological data, from which hourly records were selected for the period spanning July 1st, 2020, to July 1st, 2025.

As previously discussed, the main objective is to assess the far-field dispersion of ammonia. For this type of simulation, wind speed and the Pasquill stability class are the most influential parameters [22,23]. Over the 5-year period considered, August exhibited the lowest average wind speed, while January had the highest. Because these months represent the most extreme conditions of wind speed, all the other parameters will be referenced to these two months over the 5-year span.

In August, the difference between the highest and lowest temperatures during the day and night is minimal. Therefore, the higher value of 18.85 °C will be used. Similarly, for January, the lowest temperature of 2.72°C will be used.

Solar radiation was averaged using only daytime values, excluding all 0 kW/m² readings that occur at night. The data shows that August has higher solar radiation and longer daylight hours, while January has both lower radiation and shorter days. Because of this, the average of the daytime solar radiation will be used for August, while a value of 0 kW/m² will be used for January. Based on that, the Pasquill stability class is set using daytime conditions for August and nighttime conditions for January, as outlined in [24].

Table 7. Input weather parameters

Parameters	Summer	Winter
Month	August	January
Wind speed	4.15 m/s	6.53 m/s
Relative humidity	78.61 %	86.55 %
Highest ambient temperature	18.85 °C	3.22 °C
Lowest ambient temperature	17.9 °C	2.72 °C
Surface temperature	18.48 °C	3.32 °C
Wind direction	179°, from South to North	214°, from Southwest to Northeast
Solar radiation (During daytime)	291.46 W/m^2	53.38 W/m^2
Daytime (Duration)	5 AM – 9 PM (16 hours)	8 AM – 4 PM (8 hours)
Period of time	Day	Night
Pasquill stability class [24]	C	D

4.7. Operating conditions

Liquid ammonia can be stored under three different conditions:

- Fully refrigerated ammonia
- Semi-refrigerated ammonia
- Non-refrigerated ammonia (Pressurized)

Each of these storage types operates within a specific temperature and pressure range:

Table 8. Storage operating conditions for ammonia [10]

Storage condition	Operating temperature	Operating pressure
Fully refrigerated	-33.34 °C	1 bar
Semi-refrigerated	-10 °C to 4 °C	3 bar to 5 bar
Non-refrigerated (Pressurized)	19 °C to 37 °C	8 bar to 14 bar

For the purposes of this report, two representative storage conditions have been selected for the simulations: fully refrigerated and semi-refrigerated.

The semi-refrigerated scenario will use an operating condition of 4°C and 5 bar, while the fully refrigerated scenario will be based on -33.34°C and 1 bar. These conditions were chosen to reflect the most relevant release scenarios in the context of ammonia bunkering and transfer operations.

The non-refrigerated (pressurized) condition is not considered in this analysis, as the maritime industry is moving toward liquefied ammonia storage and bunkering for practical, safety, and efficiency reasons. Moreover, according to [10], the limited capacity of non-refrigerated pressurized tanks makes them unsuitable for the large bunker volumes required by ocean-going vessels.

In the fertilizer industry, the ammonia transfer process has been carried out for decades worldwide. Transfers from a fully refrigerated tank to fully refrigerated tank, are usually carried out at a transfer rate of 250 to 750 tonne/hr [25]. These flow rates will be considered for the simulations.

For the simulation of semi-refrigerated transfer, the assumed conditions of 4°C at 5 bar correspond to a liquid density of 633.1 kg/m³. Considering the mass flow rate of 750 tonne/hr, it is estimated a volumetric flow rate of 1184.74 m³/h. For the fully refrigerated scenario, a liquid density of 682 kg/m³ at -33.34°C and 1 atmosphere is used. A transfer mass flow rate of 750 tonne/hr is assumed, which results in a volumetric flow rate of approximately 1099.7 m³/h.

Table 9. Mass flow rate and volumetric flow rate of operating conditions

Storage condition	Operating temperature	Operating pressure	Mass flow rate	Volumetric flow rate
Fully refrigerated	-33.34 °C	1 bar	750 t/h	1099.7 m³/h
Semi-refrigerated	4 °C	5 bar	750 t/h	1184.65 m³/h

4.8. Transfer assemblies

To safely and efficiently transfer fuel or other liquid cargo during bunkering operations, ports and vessels rely on specialized equipment designed to handle a variety of operational and safety requirements. The choice of transfer system depends on factors such as the size of the port, the frequency of operations, the type of fuel, and the level of precision and safety needed. Two main types of transfer assemblies are commonly:

- hose assemblies
- marine loading arms.

A marine loading arm is a more advanced and fixed solution for fuel transfer, typically used in large-scale or high-frequency bunkering operations. These systems consist of rigid piping sections that form an articulated arm, mounted on a pedestal or base. The arm is capable of controlled movement, allowing precise alignment with the vessel's manifold. It provides a secure and stable connection, enhances operator safety, and can accommodate different vessel sizes and manifold heights. These loading arms are often permanently installed at dedicated bunkering stations or on specialized bunker barges.

A hose assembly is the conventional method for transferring bunker fuels. It consists of flexible hoses equipped with end fittings and connection couplings on both ends. Typically, two hoses are used, one for liquid and one for vapour return. According to [10], leaks, ruptures, and accidental pull-away incidents involving connecting hoses are considered among the most likely causes of loss of containment during ammonia bunkering operations.

After speaking with the Port of Rønne, they supported that for a port of their size and operational scale, hose assemblies are the preferred method for fuel transfer due to their practicality and suitability. Based on this, only hose assemblies will be considered in the simulation. Since this method involves flexible hoses, any potential leak will be assumed to originate from a hose positioned on the deck of the bunker vessel.

Guidelines for STS hoses [26] indicate that a single hose section is usually no longer than 12 metres. These sections are often joined in sets of two or three to form hose strings, with typical total lengths of 27.3 metres (three 9.1 m sections) or 24 metres (two 12 m sections). However, the overall length can vary based on factors such as the STS operation site, the type of vessels involved, and the manufacturer's design. For this simulation, a length of 27.3 meters will be considered for the hose assembly.

4.9. Release duration

When an ammonia release occurs due to a leakage from a pipeline, the substance will continue to flow through the pipeline until the Emergency Shutdown (ESD) system is activated. To stop the release, the ESD system must close the isolation valves and shut down the loading pumps. Once this action is completed, only the liquid remaining in the pipeline is expected to be discharged.

According to Section 18.10.2.1.3 of the International Gas Code (IGC), any ESD valve in a liquid piping system must close fully within 30 second [27]. In addition to this closing time, the activation time of the ESD system must also be considered. Activation can be initiated through three different sources:

- Gas detectors in the area

- Manual pull stations operated by personnel in the vicinity
- Instrumentation within the system that would detect the pressure loss or lower flow i.e. pressure transmitter or flow meters.

Since the location of these devices and the corresponding activation time depend on the specific plant design, it is assumed that activation would take approximately 30 seconds.

As a reference, a person is expected to reach a manual pull station located within 36 m within 30 seconds, assuming an average walking speed of 1.2 m/s[28]. In contrast, [29] recommends that for undefined routes, the maximum travel distance to a manual call point should not exceed 30 m.

Consequently, the total time from the onset of the ammonia release to the closure of the pipeline transporting ammonia is estimated to be about 1 minute.

For the terminal/pipeline-to-ship (PTS) bunkering operation, it will be assumed that the ESD valve is located in the outlet of the storage tank, upstream in the pipeline to the bunker vessel, as shown in Figure 6.

4.10. Lethality calculation

Dangerous Toxic Load (DTL) describes the combined effect of airborne concentration and exposure duration that produces a specified level of toxicity in the general population. The Health and Safety Executive (hse) from the UK defines two reference levels: Specified Level of Toxicity (SLOT) and Significant Likelihood of Death (SLOD). For the current simulations, SLOD will be considered [8]. SLOD corresponds to conditions that would cause about 50% mortality in an exposed population. Because directly relevant human data are scarce. For ammonia, the SLOD DTL is 1.03 x 10^9 (ppm^n.min) [8].

Because directly relevant human data are scarce, these reference loads are derived mainly from single short term animal inhalation studies and then mapped to human impact using transparent rules. This may cause some uncertainty, but it can provide a consistent basis for consequence calculations and for comparing scenarios [30].

Phast implements toxicity using a probit model that links toxic load to expected lethality.

The probit number is calculated using the following equation [31]:

$$Pr = A + B \cdot ln(Dose_{threshold})$$

Equation 1. Probit number

Phast considers the concentration is roughly constant over the exposure. For this assumption, the Dose threshold is given by:

$$Dose_{threshold} = C_{ref}^{N_{threshold}} \cdot t_{ref}$$

Where:

- A is -16.21 ppm for ammonia, according to Phast.
- B is 1 for ammonia, according to Phast.
- $Dose_{threshold}$ is the standardised toxic concentration delivered at a location.

- $N_{threshold}$ is the toxic load component. For ammonia, $N_{threshold}$=2, according to Phast.
- t_{ref} is the exposure time in minutes.

Considering the probit numbers, the following equation is used to calculate the lethality fraction within a range from 0% to 100%. As shown in Figure 8, ahigher Probit number means higher lethality.

$$P_{Death} = \frac{1}{2}\left\{1 + \text{erf}\left[\frac{(\text{Pr} - 5)}{\sqrt{2}}\right]\right\}$$

Equation 2. Probability of death in then calculated from Probit number

If the computed toxic load ($Dose_{threshold}$) equals the SLOD DTL for ammonia, then Pr will be close to 5 and the expected lethality will be close to 50%. Loads above the SLOD DTL push Pr above 5 and increase the predicted lethality, while loads below the SLOD DTL do the opposite

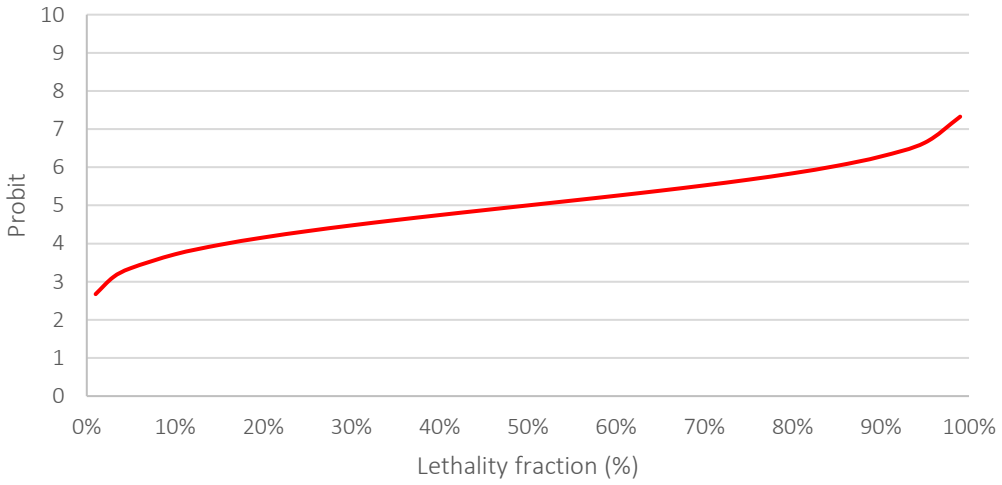


Figure 8. Lethality fraction for different Probit numbers.

5. DESCRIPTION OF SCENARIOS

For the present simulation campaign, two ammonia bunkering methods are assessed in order to capture the range of transfer methods and locations that may be relevant to the port: Ship-to-ship (STS) and Terminal/pipeline-to-ship (PTS).

Table 10. Characteristics of ammonia bunkering methods

Ammonia bunkering method	Ship-to-ship (STS)	Terminal/pipeline-to-ship (PTS)
Bunker supply	Bunker vessel	Storage tank
Receiving vessel	Container ship	Bunker vessel
Shore tank capacity	-	10000 m^3
Working bunker vessel capacity	2925 m^3	-
Connection	8” hose 27.3 m	8” pipeline 500 m

		8” hose 27.3 m
Orifice size	8”	8”
Release direction	Horizontal	Horizontal
High release elevation	4.3	4.3
Low release elevation	0	0
Phast scenario	Pressure vessel – Short pipe release	Long pipeline – Location specific breach

For the ship-to-ship (STS) ammonia bunkering method, four locations will be considered:

1. Alongside the future quay
2. Alongside Quay 34 and 35
3. Alongside Quay 33
4. 2 nautical miles to the west of the port of Rønne.

For terminal/pipeline-to-ship (PTS), only one location is considered:

1. Alongside Quay 33

It is important to outline that for the ship-to-ship (STS) ammonia bunkering method, the offshore scenario located 2 nautical miles west of the Port of Rønne is modelled as open water, whereas the other 3 locations alongside a Quay are modelled as Land.

For both ammonia bunkering methods, two weather parameters are considered: Summer and Winter. Similarly, two operating conditions are considered: fully refrigerated and semi-refrigerated, following the mass flow rate and volumetric flow rate stated in Table 9.

A summary of the scenarios to be simulated are the following:

Table 11. Scenarios considered for simulations. In total, 20 scenarios will be simulated, grouped into 5 different scenarios.

Scenario ID	Ammonia bunkering method	Location	Weather	Operating conditions
Scenario 1				
Scenario 1.1	Ship-to-ship (STS)	Alongside the future quay	Summer	Fully refrigerated
Scenario 1.2	Ship-to-ship (STS)	Alongside the future quay	Summer	Semi-refrigerated
Scenario 1.3	Ship-to-ship (STS)	Alongside the future quay	Winter	Fully refrigerated
Scenario 1.5	Ship-to-ship (STS)	Alongside the future quay	Winter	Semi-refrigerated
Scenario 2				
Scenario 2.1	Ship-to-ship (STS)	Alongside Quay 34 and 35	Summer	Fully refrigerated
Scenario 2.2	Ship-to-ship (STS)	Alongside Quay 34 and 35	Summer	Semi-refrigerated
Scenario 2.3	Ship-to-ship (STS)	Alongside Quay 34 and 35	Winter	Fully refrigerated
Scenario 2.4	Ship-to-ship (STS)	Alongside Quay 34 and 35	Winter	Semi-refrigerated
Scenario 3				
Scenario 3.1	Ship-to-ship (STS)	Alongside Quay 33	Summer	Fully refrigerated
Scenario 3.2	Ship-to-ship (STS)	Alongside Quay 33	Summer	Semi-refrigerated
Scenario 3.3	Ship-to-ship (STS)	Alongside Quay 33	Winter	Fully refrigerated
Scenario 3.4	Ship-to-ship (STS)	Alongside Quay 33	Winter	Semi-refrigerated
Scenario 4				
Scenario 4.1	Ship-to-ship (STS)	2 nautical miles to the west of the port	Summer	Fully refrigerated
Scenario 4.2	Ship-to-ship (STS)	2 nautical miles to the west of the port	Summer	Semi-refrigerated
Scenario 4.3	Ship-to-ship (STS)	2 nautical miles to the west of the port	Winter	Fully refrigerated
Scenario 4.4	Ship-to-ship (STS)	2 nautical miles to the west of the port	Winter	Semi-refrigerated
Scenario 5				
Scenario 5.1	Terminal/pipeline-to-ship (PTS)	Alongside Quay 33	Summer	Fully refrigerated
Scenario 5.2	Terminal/pipeline-to-ship (PTS)	Alongside Quay 33	Summer	Semi-refrigerated
Scenario 5.3	Terminal/pipeline-to-ship (PTS)	Alongside Quay 33	Winter	Fully refrigerated
Scenario 5.4	Terminal/pipeline-to-ship (PTS)	Alongside Quay 33	Winter	Semi-refrigerated

6. SIMULATION RESULTS

As noted earlier, the primary safety concern for ammonia in these scenarios is toxic exposure to people in the surrounding area. Toxic impact is governed by two coupled factors, namely concentration and duration of exposure.

The consequence analysis presents ammonia vapour cloud to characterize toxic effects from the release. All footprints were evaluated at a height of 1.5 m above ground. Concentration maps are shown for the 10 minute AEGL-2 and AEGL-3 thresholds of 220 ppm and 2700 ppm.

The TNO Purple Book [31] states that the averaging time for toxic substances should be comparable to the expected exposure time. Following this guidance, the averaging time in these simulations is set at 10 minutes. As explained in the Purple Book, this value is arbitrarily selected to fall between the conditions of a short release, with an exposure time of 30 to 60 seconds, and a long release, with an exposure time of approximately 30 minutes.

Phast estimates lethality using a probit approach. For a given toxic dose it calculates a probit value using internal parameters for ammonia and converts this to a probability of death on a continuous scale from 0 to 100%. Lethality contours are reported for probabilities of 3%, 10%, 50% and 99%, which are then used to derive downwind distances and footprint maps.

6.1. Scenario 1, 2, 3 – Release on land, STS

The following section is applicable for scenarios 1, 2 and 3 (see Table 11):

- Scenario 1: Ship-to-ship (STS) ammonia bunkering method alongside the future quay
- Scenario 2: Ship-to-ship (STS) ammonia bunkering method alongside Quay 34 and 35
- Scenario 3: Ship-to-ship (STS) ammonia bunkering method alongside Quay 33

For all these scenarios, it is considered that the dispersion phenomena occur on land.

6.1.1. Released mass. Release elevation of 4.3 m

The total mass released reflects the discharge of the pipe inventory after the ESD valve closes at one minute. Because the discharge is governed by internal process conditions, the total mass is the same in summer and winter.

Table 12 shows that, for the release of semi refrigerated ammonia, most of the mass is released in the form of a vapour cloud, fully refrigerated ammonia is released mostly as liquid that forms a pool. This difference is mainly due to the storage conditions. Semi refrigerated ammonia is stored at higher pressure and temperature, so when it is suddenly depressurised to atmospheric pressure almost all of the liquid flashes to vapour, with only a small portion raining out and forming a pool. In contrast, fully refrigerated ammonia is stored close to atmospheric pressure and near its atmospheric boiling point, so only a small fraction can flash to vapour on release and most of the inventory spills as cold liquid, which collects on the ground as a pool and then gradually evapourates.

For fully refrigerated ammonia, winter produces a slightly larger initial vapour cloud and a correspondingly smaller pool compared with summer. This is mainly due to the higher wind speed and denser, colder air in winter, which together reduce the amount of ammonia vapour that slumps towards the ground, so a slightly larger fraction of the release remains in the initial vapour cloud rather than forming a pool on the ground.

For semi refrigerated ammonia in summer, the release is entirely an immediate vapour cloud with no pool. In winter, a small pool of 466.50 kg appears, which is much smaller than the initial pool formed in fully refrigerated ammonia releases. As mentioned previously, when semi refrigerated ammonia is released it is mostly vapour, and the seasonal difference comes from how much of that two phase jet rains out and forms a liquid pool caused by the weather conditions.

After one hour the remaining pool mass is consistently higher for fully refrigerated ammonia than for semi refrigerated ammonia, for which case the residual liquid is negligible or zero.

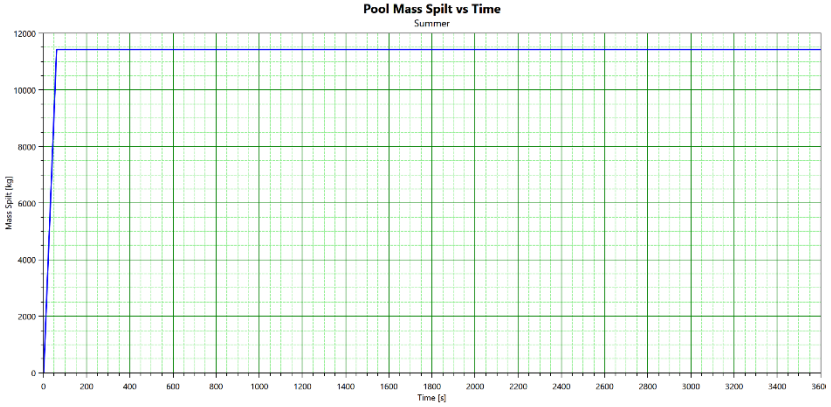
Table 12. Mass balance for scenarios 1, 2 and 3. Release elevation of 4.3 m

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Total mass released (kg)	13103.10	13059.83	13103.10	13059.83
Mass released as vapour cloud (kg)	1676.73	13059.83	1818.70	12593.33
Total mass released as a liquid pool (kg)	11426.37	0.00	11284.40	466.50
Mass vapourized from the pool (kg)	10555.03	0.00	10497.17	442.37
Mass remaining in pool after 1 h (kg)	871.34	0.00	787.23	24.13

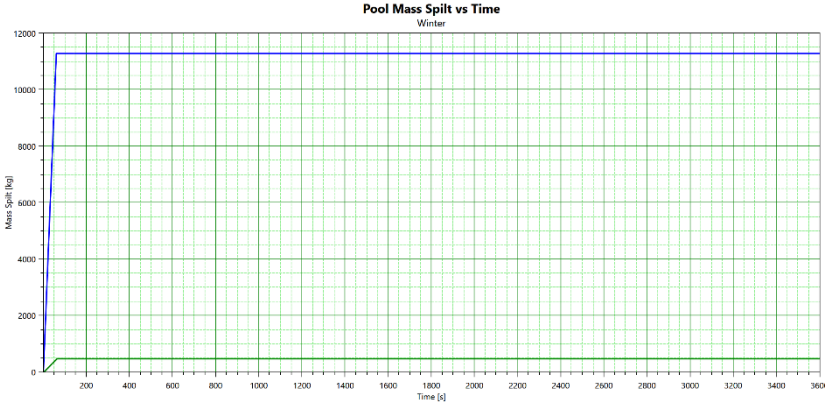
Legend:

Fully refrigerated

Semi refrigerated



a)



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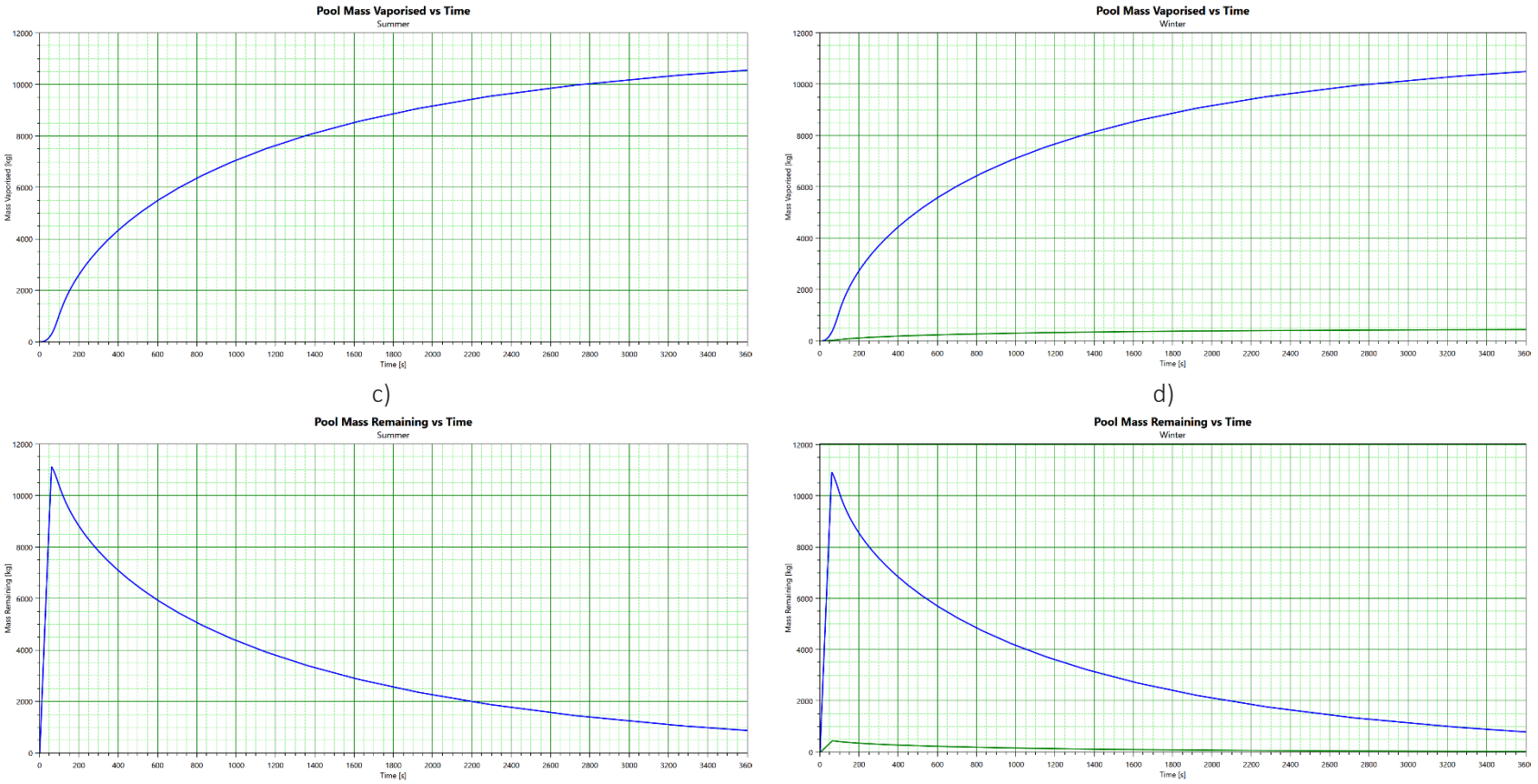


Figure 9. Ammonia pool mass split for scenario 1, 2 and 3. a) Pool mass split vs time during summer b) Pool mass split vs time during winter c) Pool mass vapourized vs time during summer d) Pool mass vapourized vs time during winter e) Pool mass remaining vs time during summer f) Pool mass remaining vs time during winter.

6.1.1.1. Released mass. Release elevation of 15.8 m

As in Table 12, Table 13 describes how the released inventory is split between vapour cloud and liquid pool, but considering a release height of 15.8 m. The table shows that for semi refrigerated ammonia, the initial release appears entirely as a vapour cloud, whereas fully refrigerated ammonia is still released mostly as liquid that forms a pool on the ground.

For fully refrigerated ammonia the mass released as vapour cloud is higher in winter than in summer. In addition, the higher release point increases the initial vapour cloud for both seasons. The greater height gives the jet more time to flash, entrain air and break up into finer droplets

before it can reach the ground, so a larger proportion of the released ammonia remains airborne in the initial cloud and a smaller proportion rains out to form the pool.

For semi refrigerated ammonia, with the release taking place at 15.8 m, the two phase jet of vapour and droplets remains fully airborne and no rainout is predicted, so no liquid pool forms on the ground. Compared with the release at 4.3 m, the increased height means that, in winter as well, the complete release is now represented as a vapour cloud.

Table 13. Mass balance for scenario 1, 2 and 3. Release elevation of 15.8 m

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Total mass released (kg)	13103.10	13059.83	13103.10	13059.83
Mass released as vapour cloud (kg)	3420.24	13059.83	4030.67	13059.83
Total mass released as a liquid pool (kg)	9682.86	0.00	9072.43	0.00
Mass vapourized from the pool (kg)	8935.34	0.00	8436.53	0.00
Mass remaining in pool after 1 h (kg)	747.51	0.00	635.90	0.00

6.1.2. Dispersion. Release elevation of 4.3 m

Table 14 presents dispersion footprints at times chosen to approximate 2, 5, 10, 30 and 60 minutes, since Phast does not use uniform time steps.

For both concentrations and seasons, the vapour cloud from semi refrigerated ammonia extends farther at early times but then dissipates quickly, whereas the cloud from fully refrigerated ammonia is shorter initially but persists longer and is still present after about 30 minutes. This behaviour reflects the different release mechanisms. Semi refrigerated ammonia is almost entirely released as vapour, meaning the initial vapour cloud is longer but the cloud soon dilutes below the concentration thresholds. Fully refrigerated ammonia, by contrast, produces a smaller vapour fraction at release and leaves a substantial liquid pool on the ground that continues to evapourate over time. As a result, the cloud is more limited in extent at the beginning but is maintained by ongoing pool evapouration and therefore remains detectable for much longer.

Seasonal effects are strongest at early times and depend on the concentration threshold. At both 220 ppm and 2700 ppm, winter footprints are a few hundred metres longer than summer footprints at about 2 and 5 minutes for both operating modes. This is mainly because higher wind speeds and denser colder air in winter carry the cloud more rapidly downwind while limiting vertical dispersion in the initial phase, so the cloud stays above the thresholds over a longer distance close to the source.

At 220 ppm this relationship reverses by about 10 minutes, when the summer cloud stays and becomes longer for most cases, whereas at 2700 ppm winter is longer only at about 2 minutes and from about 5 minutes onward summer generally extends farther, with a small exception around

10 minutes for the semi refrigerated case. For semi refrigerated ammonia at 220 ppm this means that the winter cloud not only reaches farther at early times, but in this case also remains above the threshold for longer than in summer.

Figure 12 a) and b) and Figure 11 a) and b) show that in Phast the reported dispersion distance is the farthest reach of any part of the cloud at the stated concentration, regardless of whether that portion of the cloud remains connected to the source. If a detached cloud travels downwind, the reported distance reflects that farther cloud.

Table 14. Dispersion footprint for scenario 1, 2 and 3 at 4.3 m height

	Time (s)	Summer		Time (s)	Winter	
		Fully refrigerated	Semi refrigerated		Fully refrigerated	Semi refrigerated
Dispersion footprint at 220 ppm (m)	106	468.08	779.60	105	706.80	962.28
	316	812.43	1693.36	313	713.05	2420.64
	596	391.50	0	590	403.17	210.28
	1788	207.13	0	1804	177.59	148.99
	3505	0	0	3468	0	0
Dispersion footprint at 2700 ppm (m)	106	318.98	679.30	105	378.70	778.01
	316	135.91	0	313	112.13	0
	596	116.40	0	590	89.46	0
	1788	46.62	0	1804	0	0
	3505	0	0	3468	0	0

Legend:

Fully refrigerated @ 2700 ppm

Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm

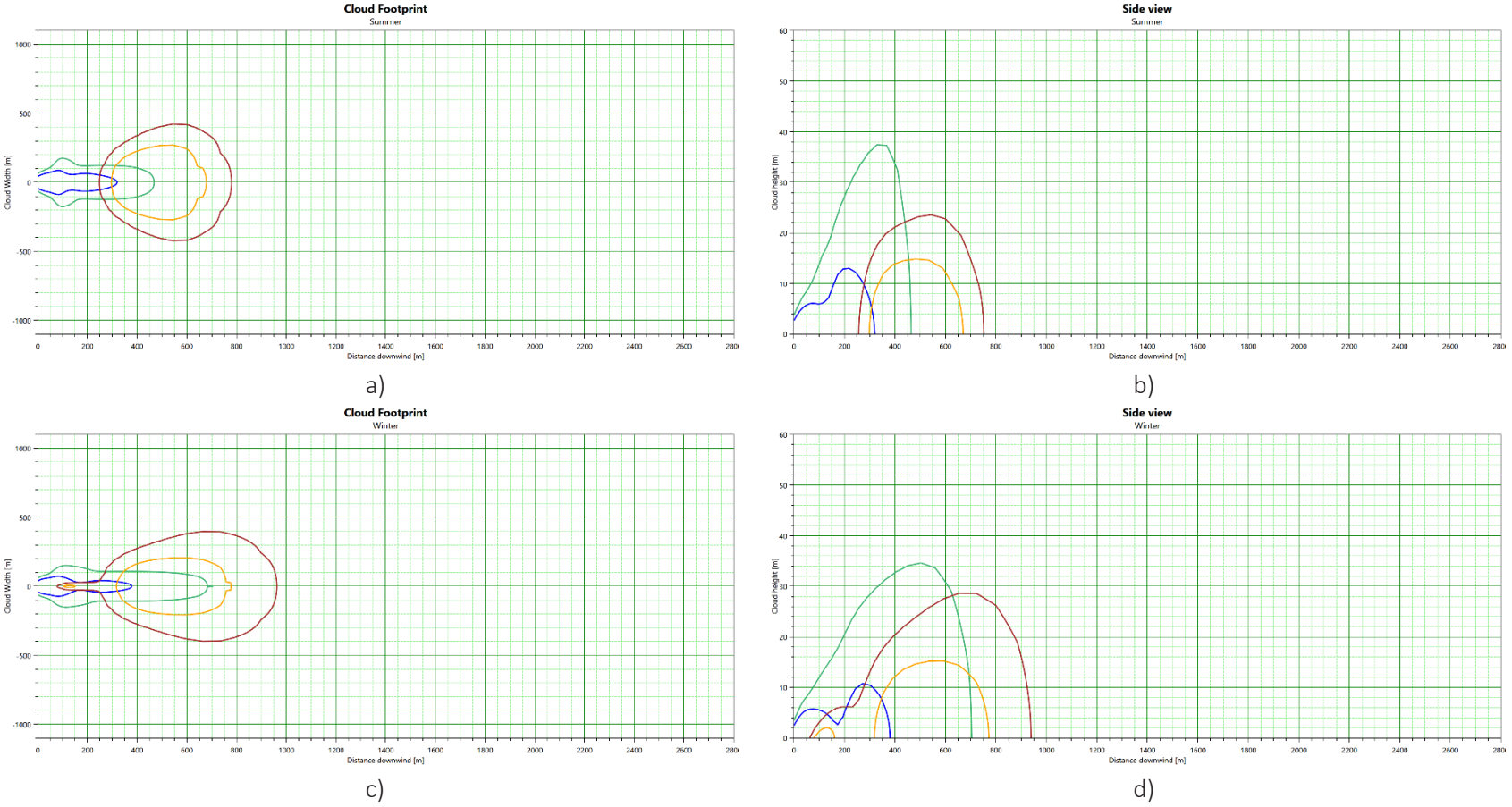


Figure 10. Cloud footprints for scenario 1, 2 and 3. a) Dispersion footprint during summer, time step=106 seconds, b) Dispersion sideview during summer, time step=106 seconds, c) Dispersion footprint during winter, time step=105 seconds, d) Dispersion sideview during winter, time step=105 seconds.

Legend:

Fully refrigerated @ 2700 ppm

Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm

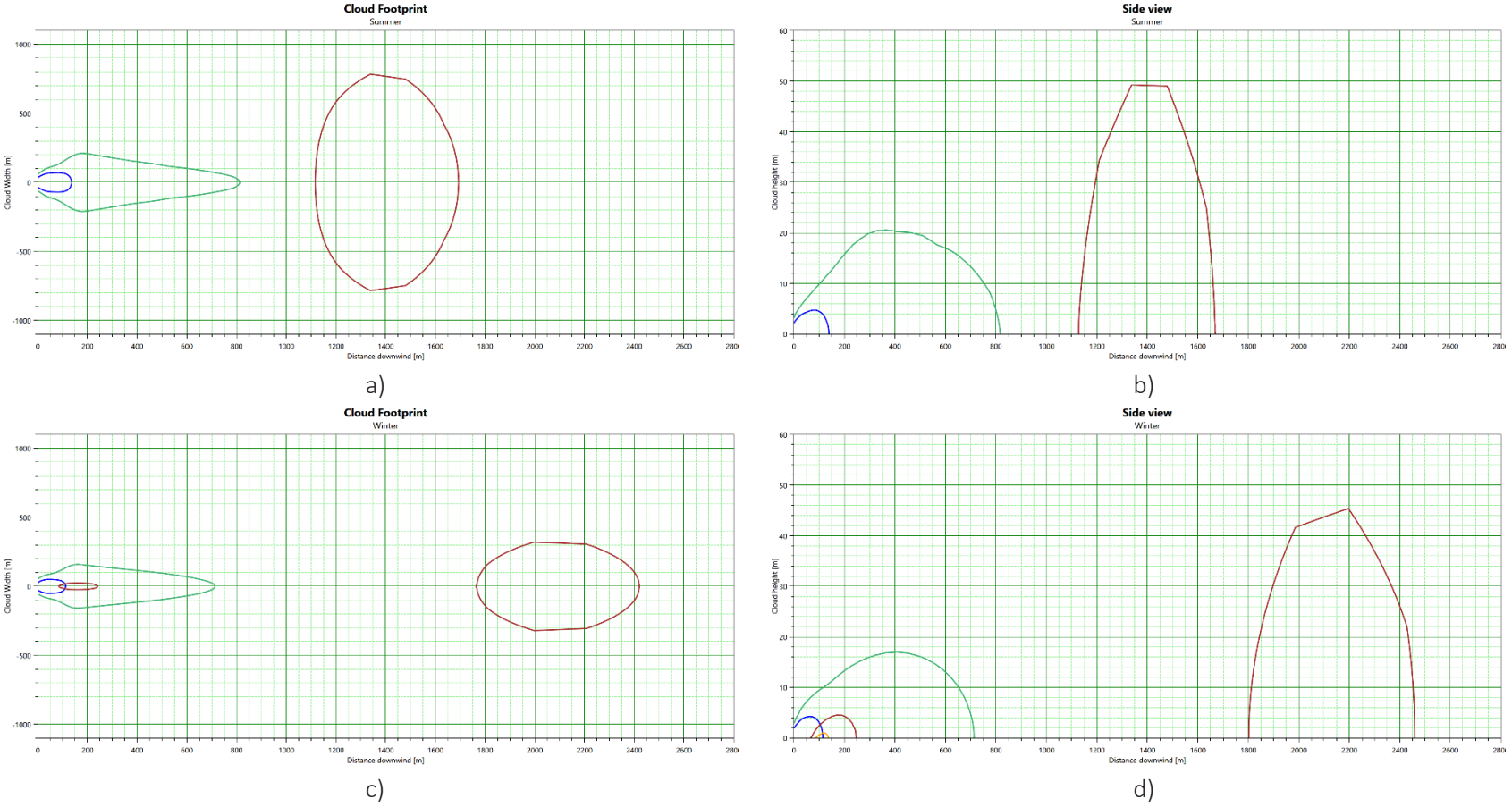


Figure 11. Cloud footprints for scenario 1, 2 and 3. a) Dispersion footprint during summer, time step=316 seconds, b) Dispersion sideview during summer, time step=316 seconds, c) Dispersion footprint during winter, time step=313 seconds, d) Dispersion sideview during winter, time step=313 seconds.

Legend:

Fully refrigerated @ 2700 ppm

Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm

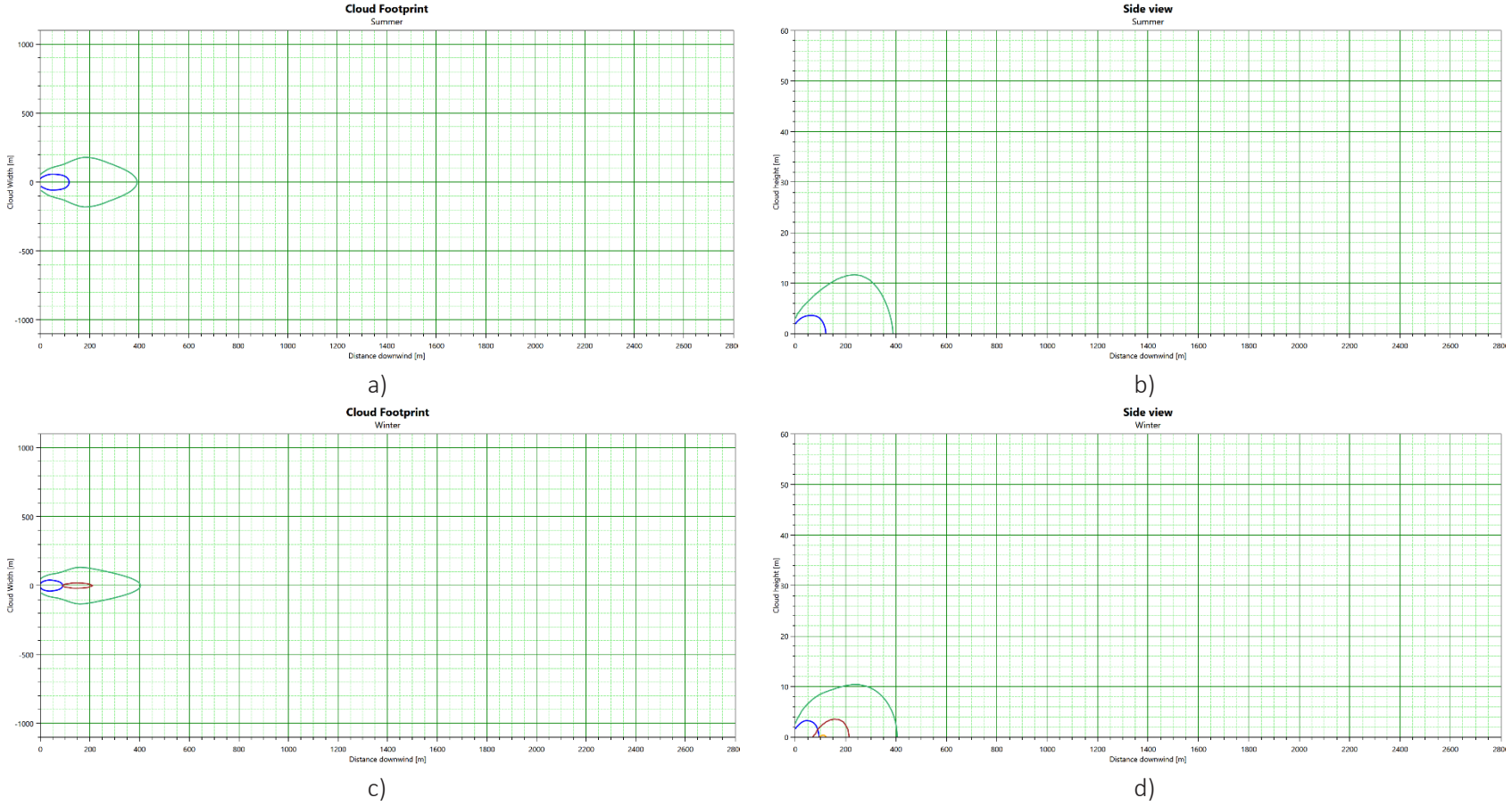


Figure 12. Cloud footprints for scenario 1, 2 and 3. a) Dispersion footprint during summer, time step=596 seconds, b) Dispersion sideview during summer, time step=596 seconds, c) Dispersion footprint during winter, time step=590 seconds, d) Dispersion sideview during winter, time step=590 seconds.

Legend:

Fully refrigerated @ 2700 ppm

Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm

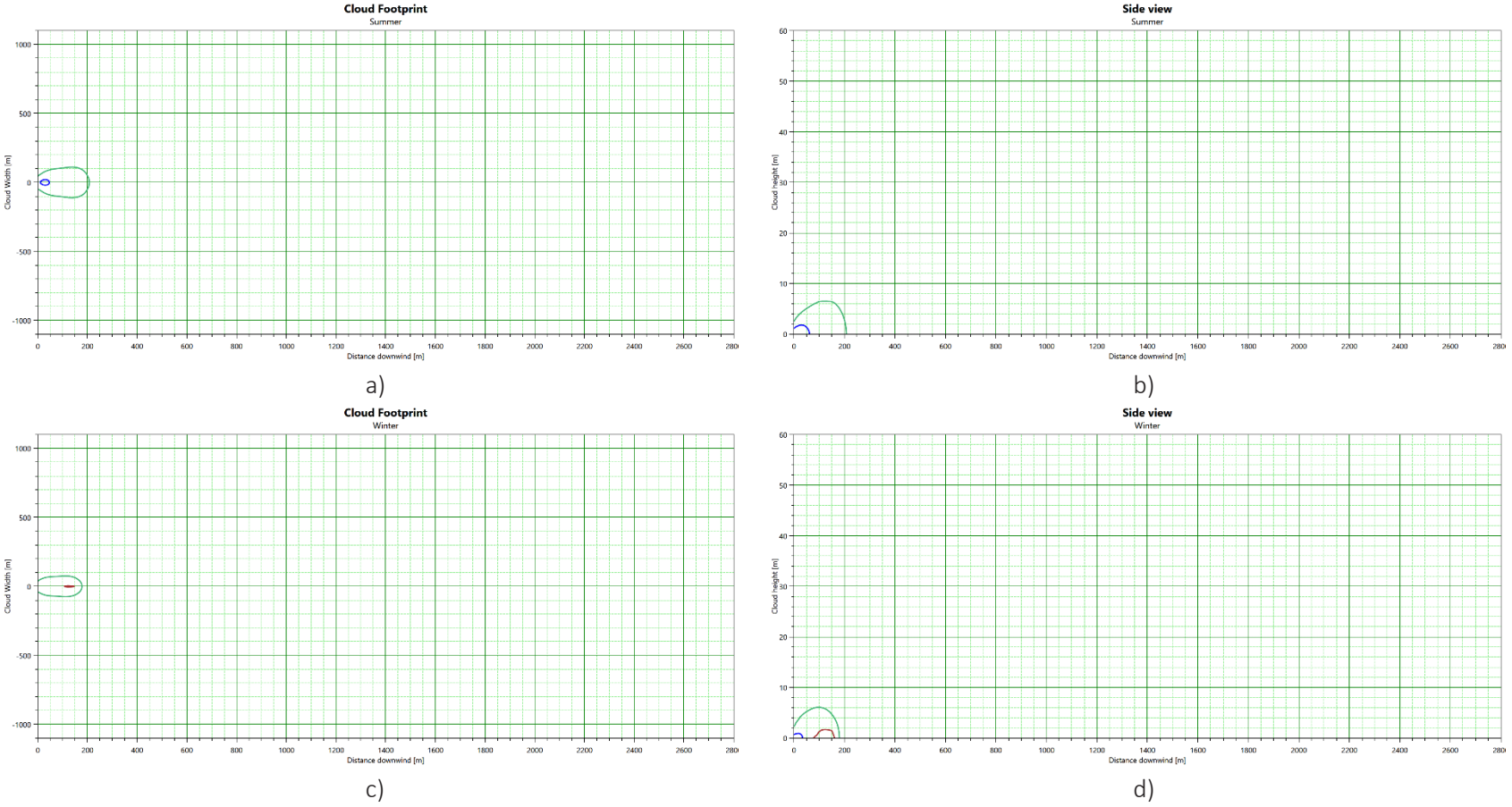


Figure 13. Cloud footprints for scenario 1, 2 and 3. a) Dispersion footprint during summer, time step=1788 seconds, b) Dispersion sideview during summer, time step=1788 seconds, c) Dispersion footprint during winter, time step=1804 seconds, d) Dispersion sideview during winter, time step=1804 seconds.

6.1.2.1. Dispersion at 15.8 m height

Table 15 shows dispersion footprints for scenarios 1, 2 and 3 with the same operating conditions as in Table 14, except the release elevation is set to 15.8 m. As previously discussed, these results are included to provide insight into outcomes when the release occurs at 15.8 m, which corresponds to the height of a large cargo ship.

The main change introduced by the higher release elevation of 15.8 m is the more airborne behaviour of the cloud, especially for semi refrigerated ammonia. Because the release starts higher, the vapour and droplets have more time to entrain air before they reach the ground, so the early footprints at 220 ppm and 2700 ppm become longer, particularly in winter. Releases of fully refrigerated ammonia still retain clouds with high concentrations for longer times, but the contrast in early footprint length between semi refrigerated and fully refrigerated ammonia is now more pronounced.

The time evolution of the footprints remains the same as for the lower release height. At 220 ppm the clouds grow from the first to the second time point and then contract until they disappear, while at 2700 ppm they are largest at the first time and then steadily decrease. What changes with the higher source elevation is that semi refrigerated ammonia, especially in winter, can maintain a measurable 220 ppm footprint at later times while still producing long footprints at the beginning of the event.

Table 15. Dispersion footprint for scenario 1, 2 and 3 at 15.8 m height

	Time (s)	Summer		Time (s)	Winter	
		Fully refrigerated	Semi refrigerated		Fully refrigerated	Semi refrigerated
Dispersion footprint at 220 ppm (m)	105	480.98	833.90	105	723.52	1030.49
	316	1331.84	1833.23	313	641	2525.87
	597	376.74	0	590	383.39	0
	1789	207.90	0	1805	182.79	0
	3507	0	0	3471	0	0
Dispersion footprint at 2700 ppm (m)	105	382.71	729.01	105	433.73	828.57
	316	139.91	0	313	120.68	0
	597	118.75	0	590	96.17	0
	1789	51.64	0	1805	0	0
	3507	0	0	3471	0	0

6.1.3. Maximum dispersion footprint. Release elevation of 4.3 m

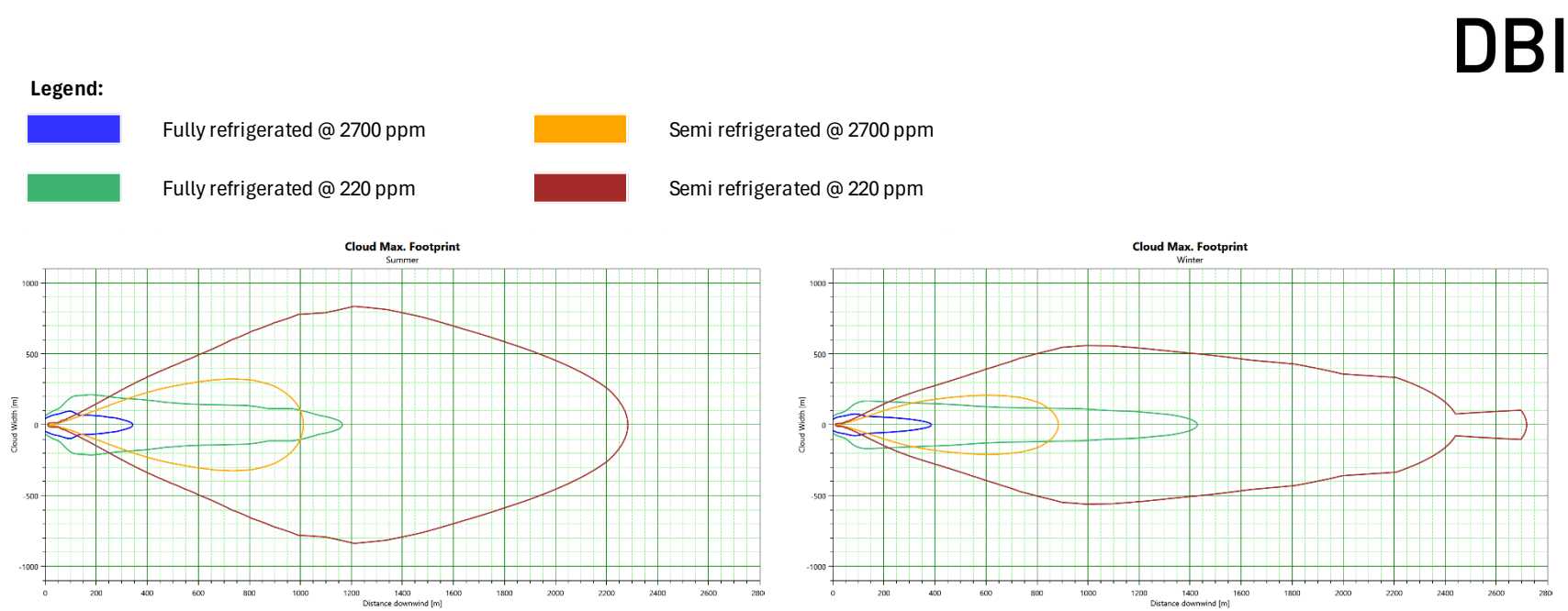
It is important to outline that the "Maximum dispersion footprint" in Phast shows the envelope of all locations reached by the vapour cloud at any time during the simulated release and dispersion. It is drawn as a single continuous contour that combines all these positions and therefore does not necessarily correspond to the shape of the vapour cloud at any particular moment in time.

Semi refrigerated ammonia produces the longest maximum dispersion footprints at both concentration levels and in both seasons.

Seasonal effects are also evident. At 220 ppm, winter footprints are longer than summer footprints for both operating modes. At 2700 ppm, winter slightly increases the footprint for fully refrigerated ammonia, while for semi refrigerated ammonia the maximum footprint is somewhat shorter in winter than in summer.

Table 16. Maximum dispersion footprint for scenarios 1, 2 and 3. Release elevation of 4.3 m

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Maximum dispersion footprint at 220 ppm (m)	1202.85	2345.72	1494.94	2786.51
Maximum dispersion footprint at 2700 ppm (m)	345.72	1023.30	388.58	896.15



a) b)

Figure 14. a) Maximum dispersion footprint for scenario 1, 2 and 3 during summer b) Maximum dispersion footprint for scenario 1, 2 and 3 during winter.

6.1.3.1. Maximum dispersion footprint. Release elevation of 15.8 m

Comparing Table 16 against Table 17 shows that increasing the release height to 15.8 m increases the maximum dispersion footprint for every combination of operating mode, season and concentration. The higher elevation enhances the long range reach of the cloud, particularly for semi refrigerated ammonia in summer, while preserving the overall ordering and seasonal trends observed at the lower release height.

Table 17. Maximum dispersion footprint for scenarios 1, 2 and 3. Release elevation of 15.8 m

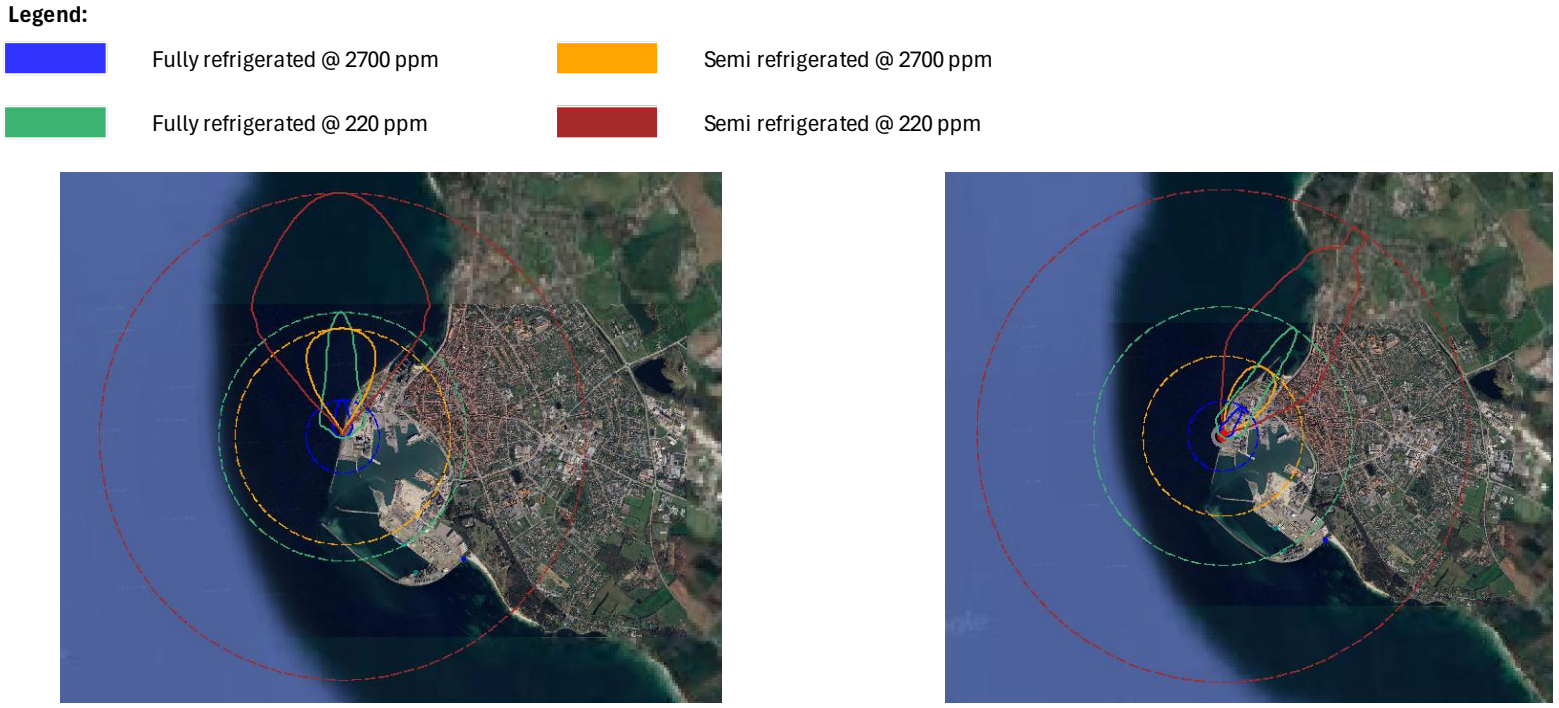
	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Maximum dispersion footprint at 220 ppm (m)	1432.74	2716.14	1796.45	2813.93
Maximum dispersion footprint at 2700 ppm (m)	422.48	1179.47	439.54	955.79

6.1.4. Maximum dispersion footprint at site

The maximum dispersion footprint plots are imposed over a real scale map of the region surrounding the port of Rønne.

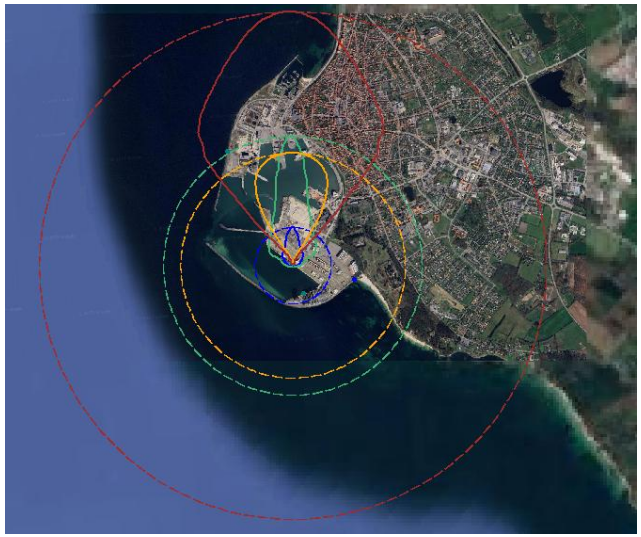
It is important to outline again that the "Maximum dispersion footprint" in Phast represents the envelope of all locations reached by the vapour cloud at any time during the simulated release and dispersion. It is drawn as a single continuous contour that merges all these positions and therefore does not correspond to the shape of the vapour cloud at any specific moment. Any point inside a contour is a location that could experience that concentration at some time during the event, but not necessarily all at once or for the same duration.

If the wind direction differs from the prevailing direction used in the main scenarios, it is assumed that the wind speed does not exceed the value applied for that prevailing direction. In practice this means that, for other wind directions, the dispersion footprint of the vapour cloud is expected to be shorter. The concentric circles shown around the source are included only as distance guides. They do not indicate simultaneous exposure or any particular exposure duration.

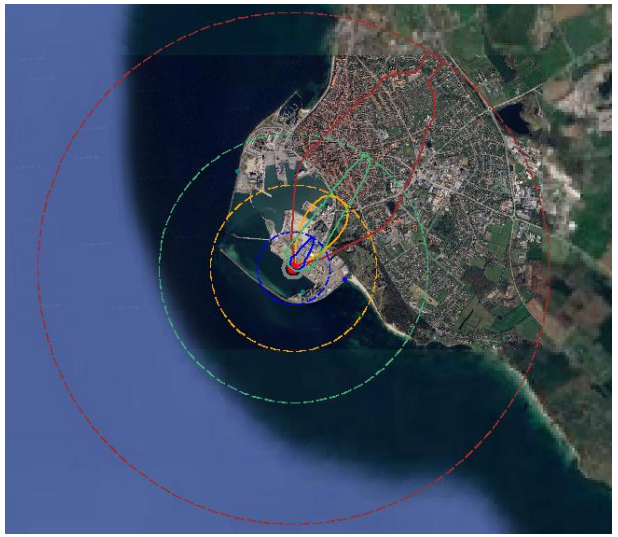


a) b)

Figure 15. a) Maximum dispersion footprint for scenario 1.1 and 1.2 in summer b) Maximum dispersion footprint for scenario 1.3 and 1.4 in winter

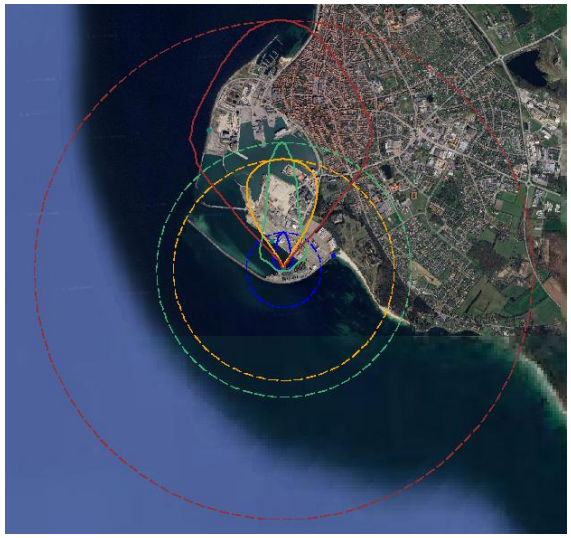


a)



b)

Figure 16. a) Maximum dispersion footprint for scenario 2.1 and 2.2 in summer b) Maximum dispersion footprint for scenario 2.3 and 2.4 in winter



a)

b)

Figure 17. a) Maximum dispersion footprint for scenario 3.1 and 3.2 in summer b) Maximum dispersion footprint for scenario 3.3 and 3.4 in winter

6.1.5. Lethality. Release elevation of 4.3 m

From Table 18, the distances increase as the lethality fraction decreases. For every scenario, the 99 percent lethality zone is closest to the source, the 50 percent zone is farther, then 10 percent, and finally the 3 percent lethality contour is the most distant.

Semi refrigerated ammonia releases always produce longer lethal ranges than fully refrigerated ammonia releases at the same lethality level and in the same season. The difference becomes much more marked at low lethality levels. At 3% lethality in summer, semi refrigerated ammonia reaches 575.29 m compared with 150.54 m for fully refrigerated. In winter the 3% distances are 474.25 m for semi refrigerated and 136.24 m for fully refrigerated. This reflects the fact that semi refrigerated ammonia is almost entirely released as vapour, so the toxic cloud carries a significant dose much farther downwind.

Summer always gives longer lethal distances than winter for a given product and lethality fraction. This indicates that, although winter can give longer instantaneous footprints at early times, the stronger winter winds also dilute the cloud more quickly so the time integrated dose is smaller and the probit based lethal distances are reduced.

Table 18. Distances of lethality fractions for scenarios 1, 2 and 3. Release elevation of 4.3 m

Lethality fraction	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
99%	47.69	65.91	31.42	54.35
50%	106.36	289.60	89.17	262.14
10%	134.88	491.44	118.07	409.04
3%	150.54	575.29	136.24	474.25

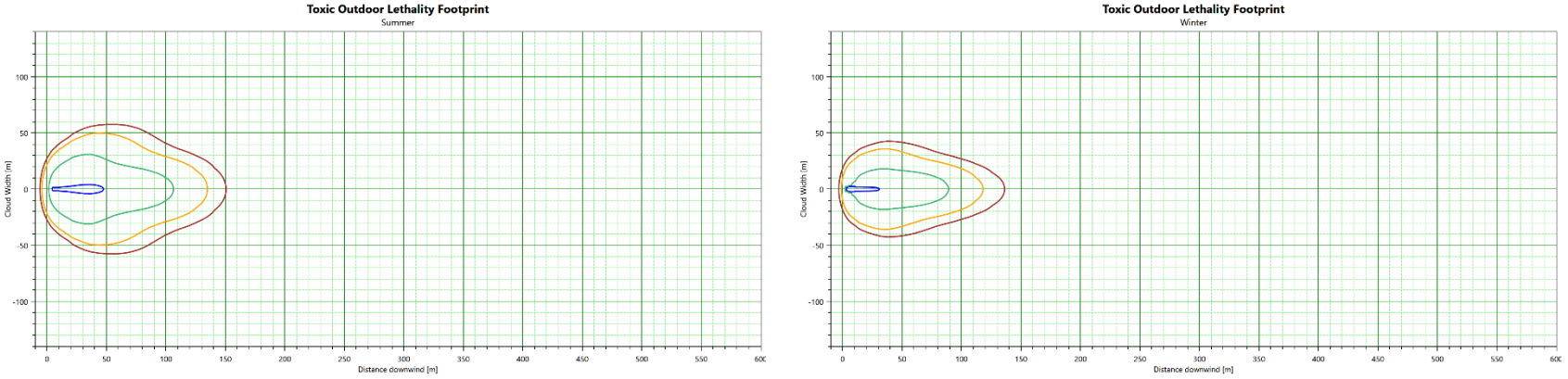
Legend:

Lethality fraction 99%

Lethality fraction 10%

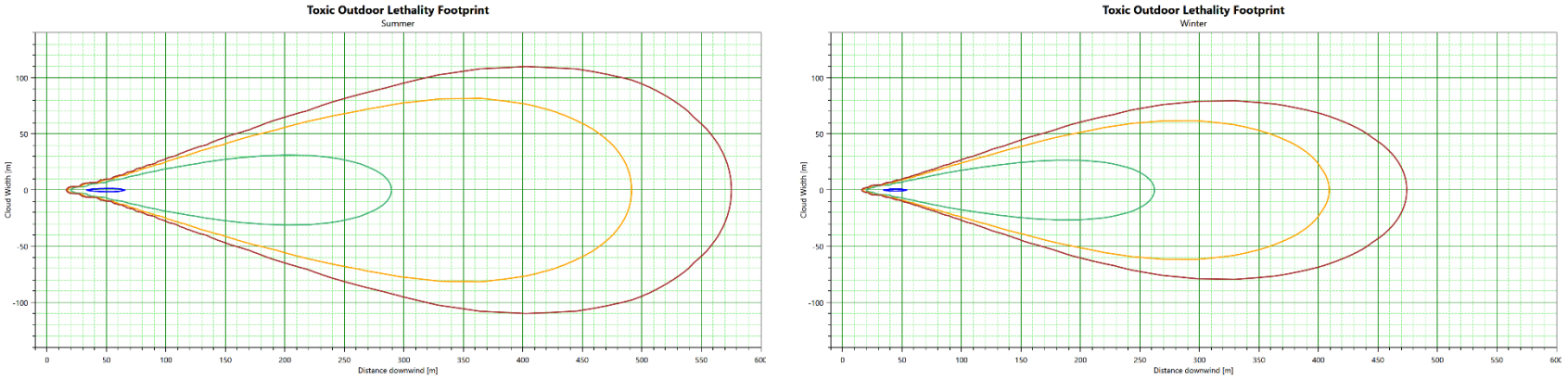
Lethality fraction 50%

Lethality fraction 3%



a) b)

Figure 18. a) Toxic outdoor probit footprint for scenarios 1, 2 and 3 for fully refrigerated ammonia during summer b) Toxic outdoor probit footprint for scenarios 1, 2 and 3 for semi refrigerated ammonia during summer



a) b)

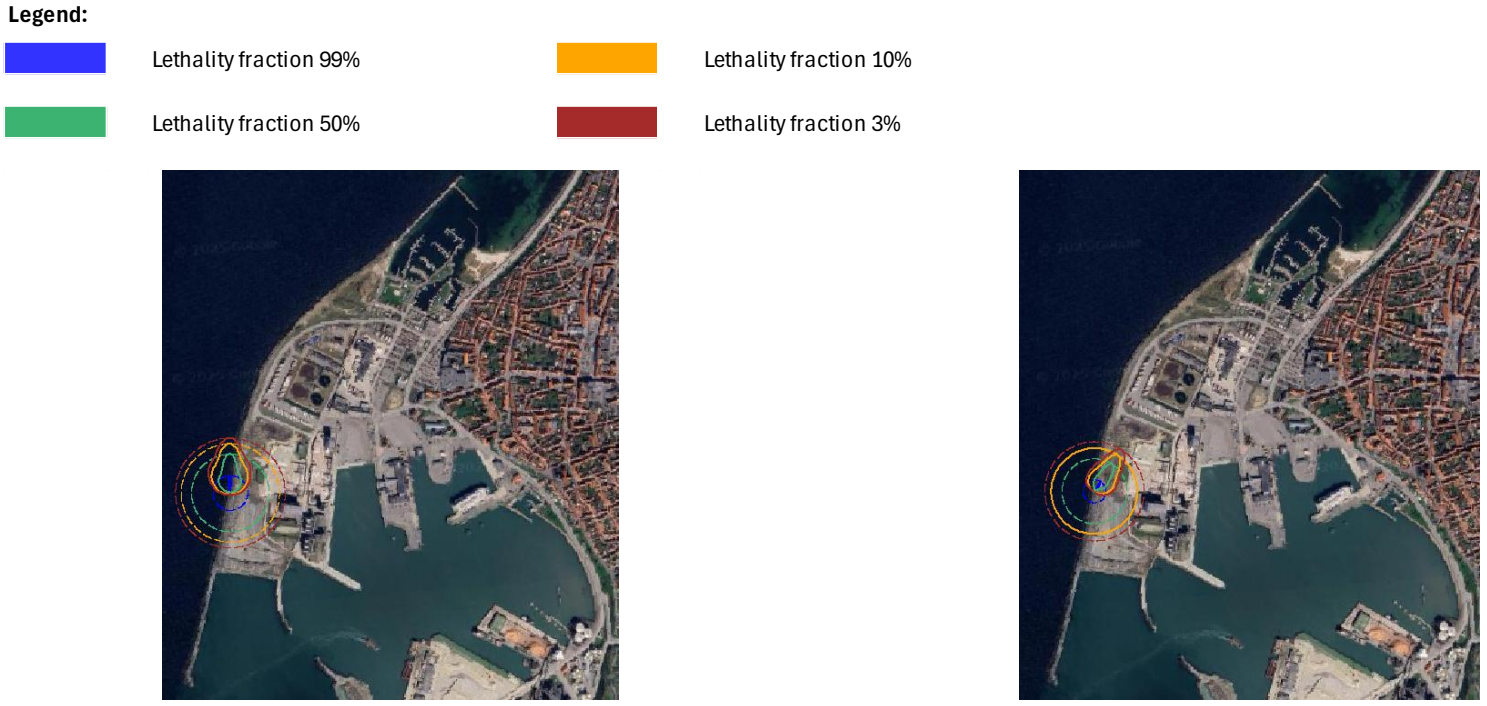
Figure 19. a) Toxic outdoor probit footprint for scenarios 1, 2 and 3 for fully refrigerated ammonia during winter b) Toxic outdoor probit footprint for scenarios 1, 2 and 3 for semi refrigerated ammonia during winter

6.1.6. Lethality at site

Given the results from the previous section, the lethality plots for the geographic location of the Port of Rønne was limited to the fully refrigerated ammonia operation, which is both the safer and the more plausible operating condition.

In Figure 20, Figure 21 and Figure 22, the fully refrigerated lethality contours remain within the Port of Rønne and do not extend into populated areas.

These results reflect only the lethality analysis calculated using the probit methodology for outdoor dispersion for the specific given conditions stated in this document. They do not account for confinement, terrain channelling, building induced recirculation, or accumulation in enclosed spaces, or other operating or weather conditions.



a) b)

Figure 20. a) Toxic outdoor probit footprint for scenario 1.1: Fully refrigerated ammonia in summer b) Toxic outdoor probit footprint for scenario 1.3: Fully refrigerated ammonia in winter

a)

b)

Figure 21. a) Toxic outdoor probit footprint for scenario 2.1: Fully refrigerated ammonia in b) Toxic outdoor probit footprint for scenario 2.3: Fully refrigerated ammonia in winter

a)

b)

Figure 22. a) Toxic outdoor probit footprint for scenario 3.1: Fully refrigerated ammonia in b) Toxic outdoor probit footprint for scenario 3.3: Fully refrigerated ammonia in winter

6.2. Scenario 4 - Release on water, STS

The following section is applicable for scenario 4:

- Ship-to-ship (STS) ammonia bunkering method at 2 nautical miles to the west of the port of Rønne

The key difference between scenarios 1, 2, and 3 and scenario 4 is that dispersion occurs over open water rather than land.

6.2.1. Released mass. Release elevation at 4.3 m

While comparing Table 12 and Table 19, it is possible to observe the total mass released is identical within each season and storage mode, so the differences come from how the release partitions between the initial vapour cloud and the pool.

For fully refrigerated ammonia, the overall behaviour over water is very similar to the land case. The release still appears mainly as a liquid pool with a smaller initial vapour cloud. Over water, the pool fraction becomes slightly larger and the initial vapour cloud slightly smaller, and the pool evapourates a bit more within the first hour. However, the amount of liquid that remains after one hour is very similar to the land case, so the long lasting liquid inventory is essentially unchanged.

For semi refrigerated ammonia, changing from land to water has a more visible effect. Over land in summer, the release appears entirely as vapour, with no pool. Over water, a small pool now forms, although it almost completely evapourates within the first hour and only a very small residual layer remains. In winter, the pool over water is clearly larger than over land, and the initial vapour cloud is correspondingly smaller, but again most of this pool evapourates during the first hour and only a small amount of liquid is left on the water surface.

Table 19. Mass balance for scenario 4. Release elevation at 4.3 m

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Total mass released (kg)	13103.10	13059.83	13103.10	13059.83
Mass released as vapour cloud (kg)	1573.73	12864.48	1702.17	12427.91
Total mass released as a liquid pool (kg)	11529.37	195.35	11400.93	631.92
Mass vapourized from the pool (kg)	10651.22	183.06	10607.37	598.34
Mass remaining in pool after 1 h (kg)	878.15	12.29	793.56	33.58

6.2.1.1. Released mass. Release elevation at 15.8 m

The overall pattern by storage mode also remains. Fully refrigerated ammonia continues to produce a substantial liquid pool on the water with a smaller initial vapour cloud, whereas semi refrigerated ammonia is dominated by vapour. The seasonal trend for fully refrigerated ammonia is also preserved, since in both height cases winter gives a somewhat larger initial vapour cloud and a correspondingly smaller pool than summer.

What changes with a release height of 15.8 m is the split between cloud and pool, especially for fully refrigerated ammonia. At the higher elevation a much larger fraction of the fully refrigerated release is counted as initial vapour cloud and the pool mass is reduced. The extra height gives the flashing jet more time to entrain air and remain airborne before droplets can fall out onto the water, so less liquid reaches the surface in the near field.

At 15.8 m, in contrast to an elevation of 4.3 m, no pool is predicted at all for semi refrigerated ammonia and the entire release is treated as vapour cloud in both seasons. The higher elevation keeps the two phase jet fully airborne, so droplets do not accumulate on the water surface in sufficient quantity to be represented as a separate pool.

Table 20. Mass balance for scenario 4. Release elevation at 15.8 m

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Total mass released (kg)	13103.10	13059.83	13103.10	13059.83
Mass released as vapour cloud (kg)	3032.83	13059.83	3500.14	13059.83
Total mass released as a liquid pool (kg)	10070.27	0.00	9602.97	0.00
Mass vapourized from the pool (kg)	9290.45	0.00	8927.49	0.00
Mass remaining in pool after 1 h (kg)	779.82	0.00	675.47	0.00

6.2.2. Dispersion. Release elevation at 4.3 m

In Phast, the terrain is defined by the surface type and the surface roughness length. The surface type controls heat and moisture exchange between the surface and the cloud. Surface roughness length sets the intensity of mechanical turbulence that mixes the cloud. Open water has a roughness length of 0.2 mm, which is lower than the roughness length of 18 cm considered for the Land terrain used for scenarios 1, 2 and 3. Over open water the very small roughness weakens mechanical mixing, so dilution is slower, and the cloud can travel farther.

For both fully refrigerated and semi refrigerated ammonia, the overall ordering stays the same as in scenario 1 - 3. Semi refrigerated ammonia releases still give the longest footprints at both 220 ppm and 2700 ppm, and fully refrigerated ammonia releases still show shorter footprints that remain detectable for a longer time. Seasonal behaviour is also broadly consistent. Winter continues to produce longer footprints than summer

at the earliest times for fully refrigerated ammonia at both concentration levels.

The main differences appear in how far and how long the clouds travel once the release is over water. For fully refrigerated ammonia, the 220 ppm and 2700 ppm footprints are noticeably longer over water than over land at the early and intermediate times, in both summer and winter. The cloud is carried farther downwind, although the basic pattern of growing to a maximum distance and then shrinking to a few hundred metres before disappearing is similar in both environments. For semi refrigerated ammonia the contrast is stronger. Over land, the 2700 ppm footprint appears only at the first time step and the 220 ppm footprint disappears or is very short by about 10 minutes. Over water, the semi refrigerated cloud reaches much larger distances at both 220 ppm and 2700 ppm and remains above the thresholds for longer, with footprints of several kilometres around 5 to 10 minutes.

Table 21. Dispersion footprint for scenario 4 at 4.3 m height

	Time (s)	Summer		Time (s)	Winter	
		Fully refrigerated	Semi refrigerated		Fully refrigerated	Semi refrigerated
Dispersion footprint at 220 ppm (m)	106	568.12	896.53	105	732.62	192.17
	316	1337.35	2106.54	313	1903.90	2676.39
	596	649.98	3475.84	590	673.42	3691.43
	1788	323.60	0	1805	300.10	204.35
	3505	0	0	3470	0	0
Dispersion footprint at 2700 ppm (m)	106	500.59	830.60	105	547.22	995.30
	316	163.13	1784.02	313	146.78	2269.01
	596	125.83	0	590	110.69	0
	1788	0	0	1805	0	0
	3505	0	0	3470	0	0

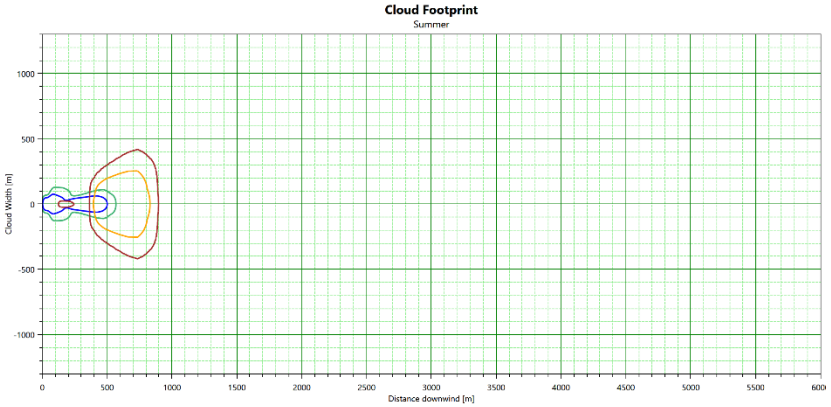
Legend:

Fully refrigerated @ 2700 ppm

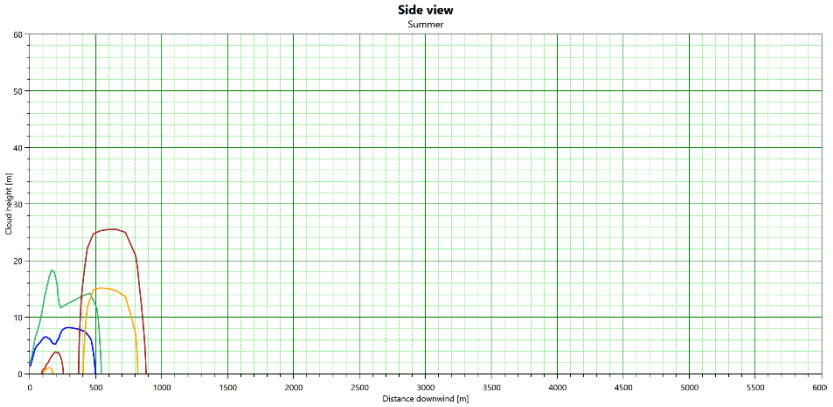
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a)



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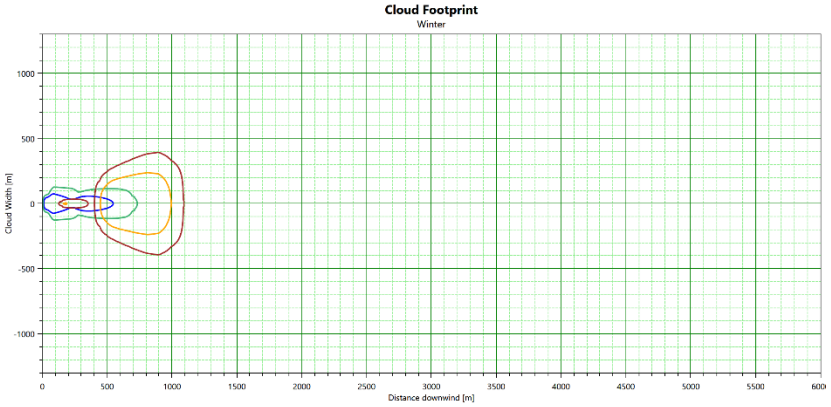
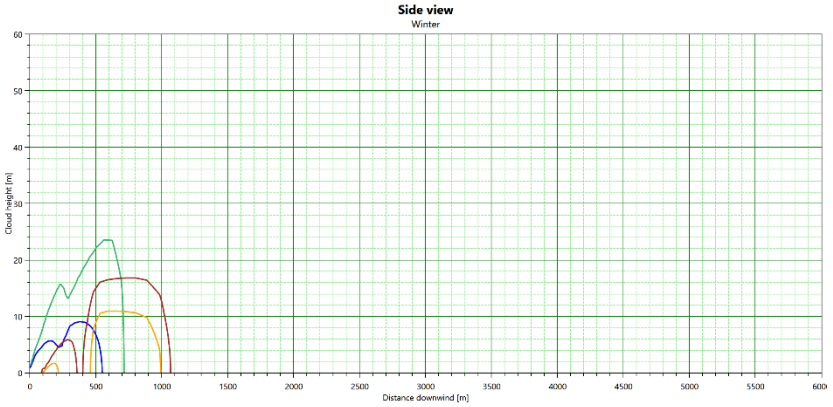


c)



d)

Figure 23. Cloud footprints for scenario 4. a) Dispersion footprint during summer, time step=106 seconds, b) Dispersion sideview during summer, time step=106 seconds, c) Dispersion footprint during winter, time step=105 seconds, d) Dispersion sideview during winter, time step=105 seconds.

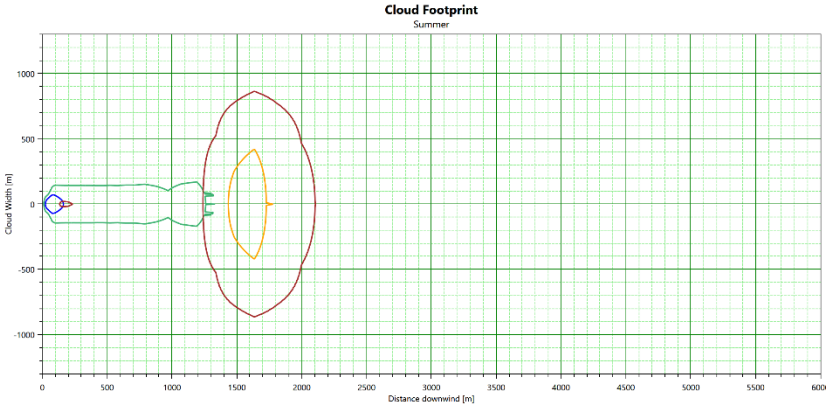
Legend:

Fully refrigerated @ 2700 ppm

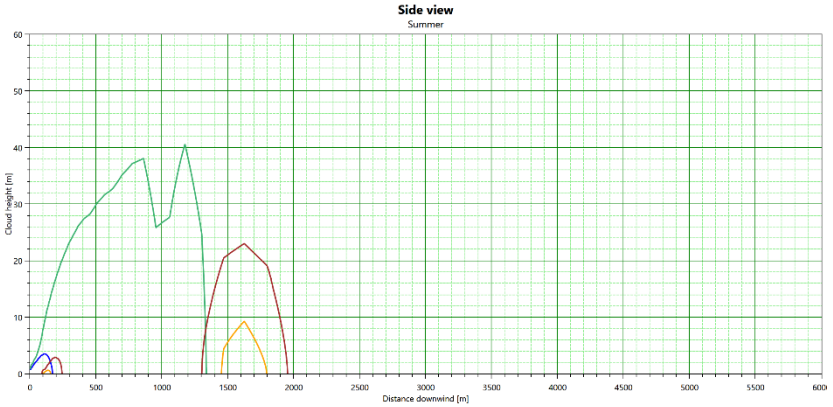
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a)



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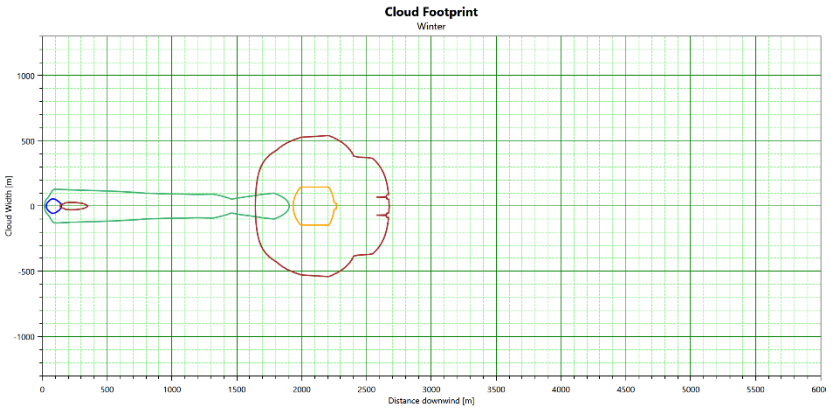
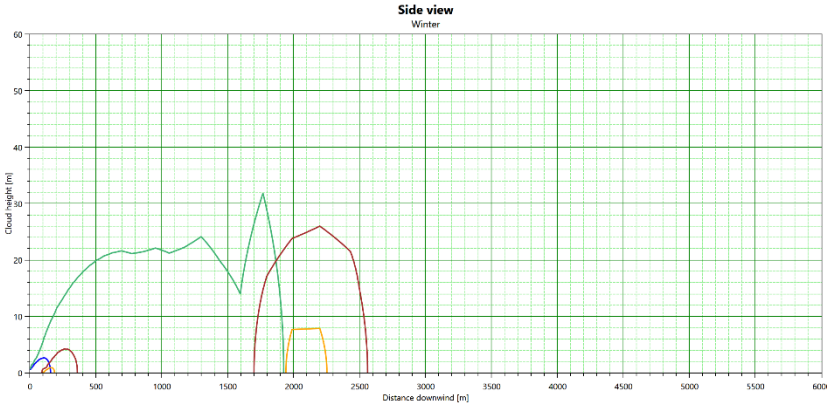


c)



d)

Figure 24. Cloud footprints for scenario 4. a) Dispersion footprint during summer, time step=316 seconds, b) Dispersion sideview during summer, time step=316 seconds, c) Dispersion footprint during winter, time step=313 seconds, d) Dispersion sideview during winter, time step=313 seconds.

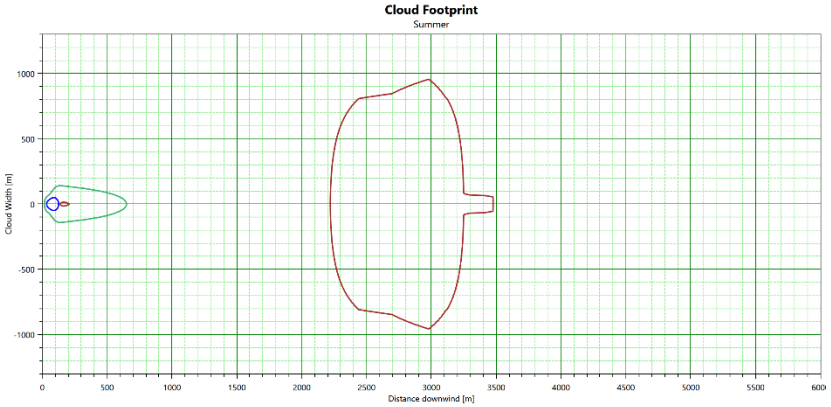
Legend:

Fully refrigerated @ 2700 ppm

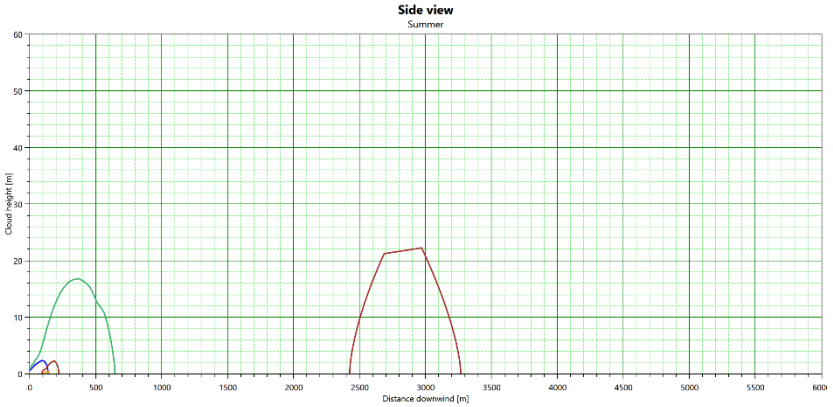
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a)



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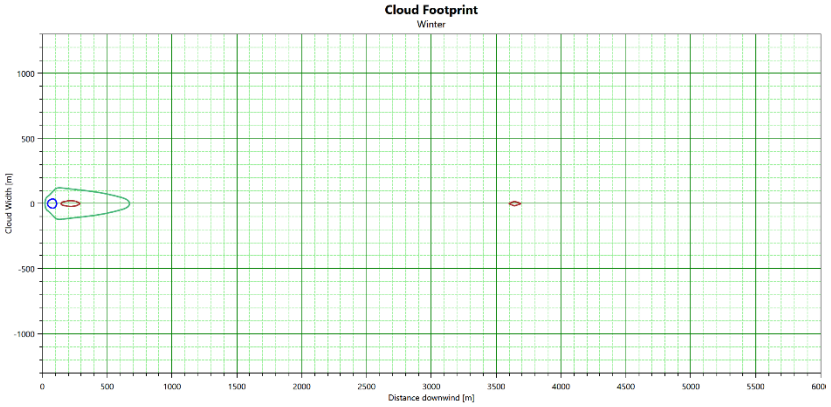
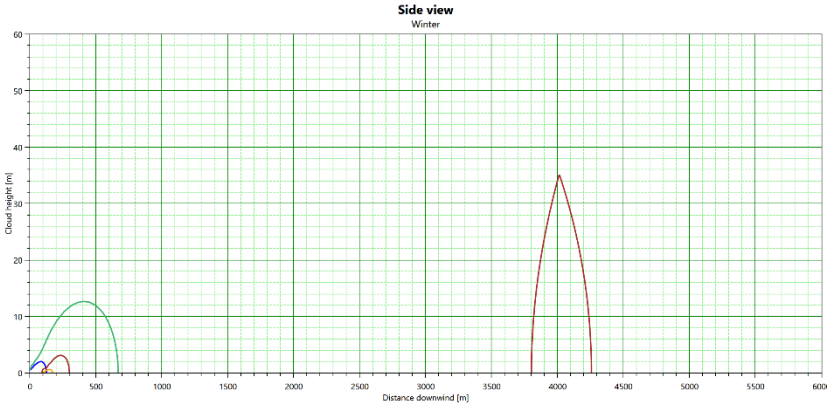


c)



d)

Figure 25. Cloud footprints for scenario 4. a) Dispersion footprint during summer, time step=596 seconds, b) Dispersion sideview during summer, time step=596 seconds, c) Dispersion footprint during winter, time step=590 seconds, d) Dispersion sideview during winter, time step=590 seconds.

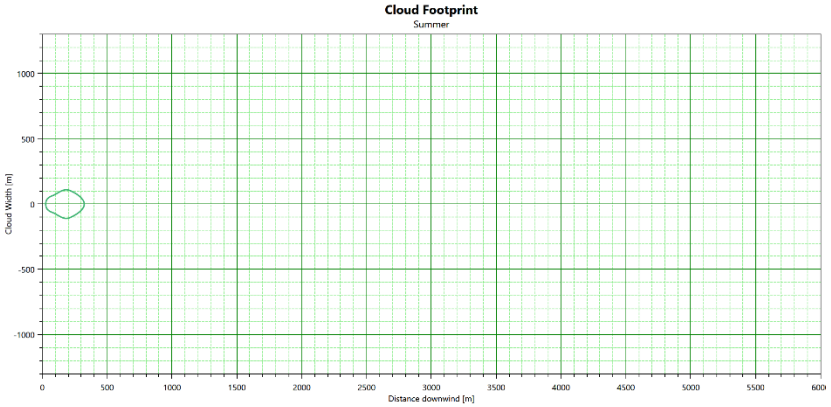
Legend:

Fully refrigerated @ 2700 ppm

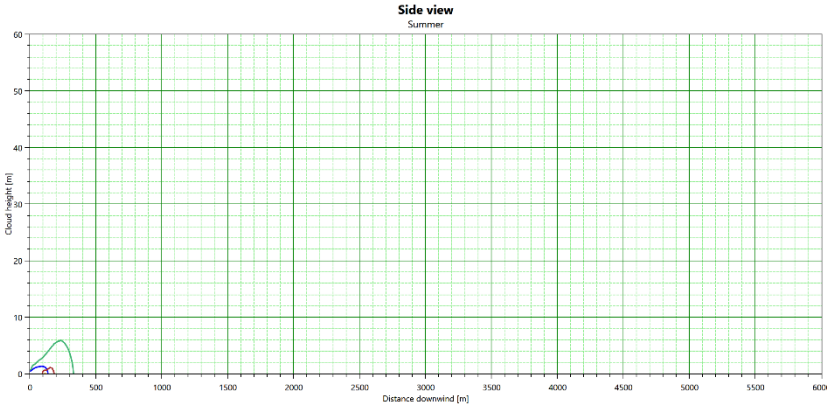
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a)



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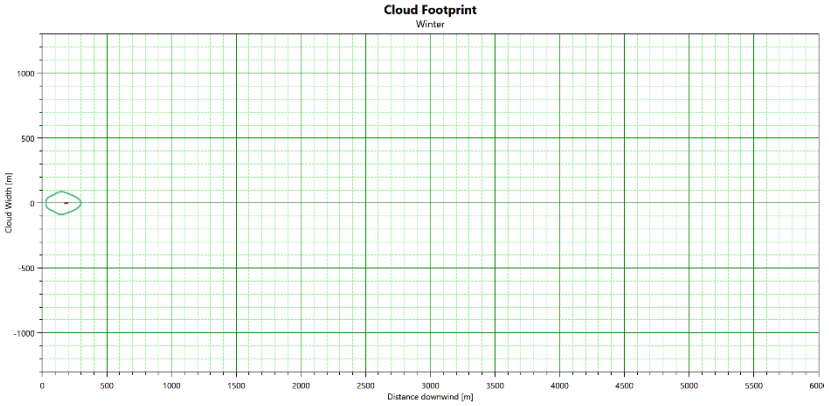

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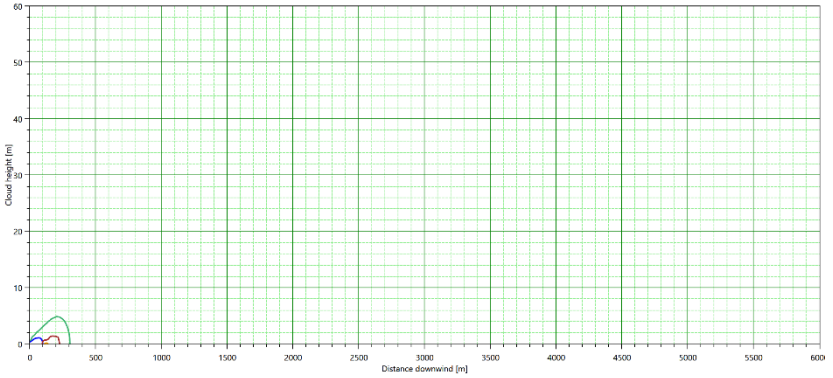


d)

Figure 26. Cloud footprints for scenario 4. a) Dispersion footprint during summer, time step=1788 seconds, b) Dispersion sideview during summer, time step=1788 seconds, c) Dispersion footprint during winter, time step=1805 seconds, d) Dispersion sideview during winter, time step=1805 seconds.

6.2.2.1. Dispersion. Release elevation of 15.8 m

When comparing Table 21 with Table 22, the dispersion behaviour remains the same. Semi refrigerated ammonia still gives longer footprints than fully refrigerated ammonia at both 220 ppm and 2700 ppm. Fully refrigerated releases still show shorter footprints that persist for longer, with a 220 ppm cloud remaining out to about 30 minutes in both summer and winter. The seasonal pattern for fully refrigerated ammonia also remains, winter footprints are longer than summer footprints at the early times for both concentrations.

The main differences are linked to the greater release elevation, which strengthens the downwind reach of the cloud, particularly for semi refrigerated ammonia. For fully refrigerated ammonia, increasing the release height from 4.3 m to 15.8 m noticeably enlarges the early and peak footprints at both 220 ppm and 2700 ppm in summer and winter.

For semi refrigerated ammonia the effect is stronger. At 220 ppm in winter, the first footprint increases from less than 200 m at 4.3 m to more than 1 km at 15.8 m, and the maximum distances around 600 s become several hundred metres longer, approaching 4.5 km. At 2700 ppm the semi refrigerated cloud is also longer at the first two times for the higher release height, although it still disappears by about 10 minutes.

Table 22. Dispersion footprint for scenario 4 at 15.8 m height

	Time (s)	Summer		Time (s)	Winter	
		Fully refrigerated	Semi refrigerated		Fully refrigerated	Semi refrigerated
Dispersion footprint at 220 ppm (m)	106	631.03	894.44	105	788.12	1090.84
	316	1445.91	2039.83	313	2059.06	2672.96
	597	620.73	3504.68	590	638.33	4478.16
	1791	318.51	0	1805	295.77	0
	3511	0	0	3471	0	0
Dispersion footprint at 2700 ppm (m)	106	567.48	832.34	105	691.71	1000.10
	316	167.75	1795.91	313	155.65	2335.92
	597	133.10	0	590	120.22	0
	1791	0	0	1805	0	0
	3511	0	0	3471	0	0

6.2.3. Maximum dispersion footprint at 4.3 m height

Comparing Table 23 with Table 16, for a release height of 4.3 m on land and over water, the overall hierarchy of scenarios remains the same. In

both environments the semi refrigerated release always gives longer maximum footprints than the fully refrigerated release at both 220 ppm and 2700 ppm.

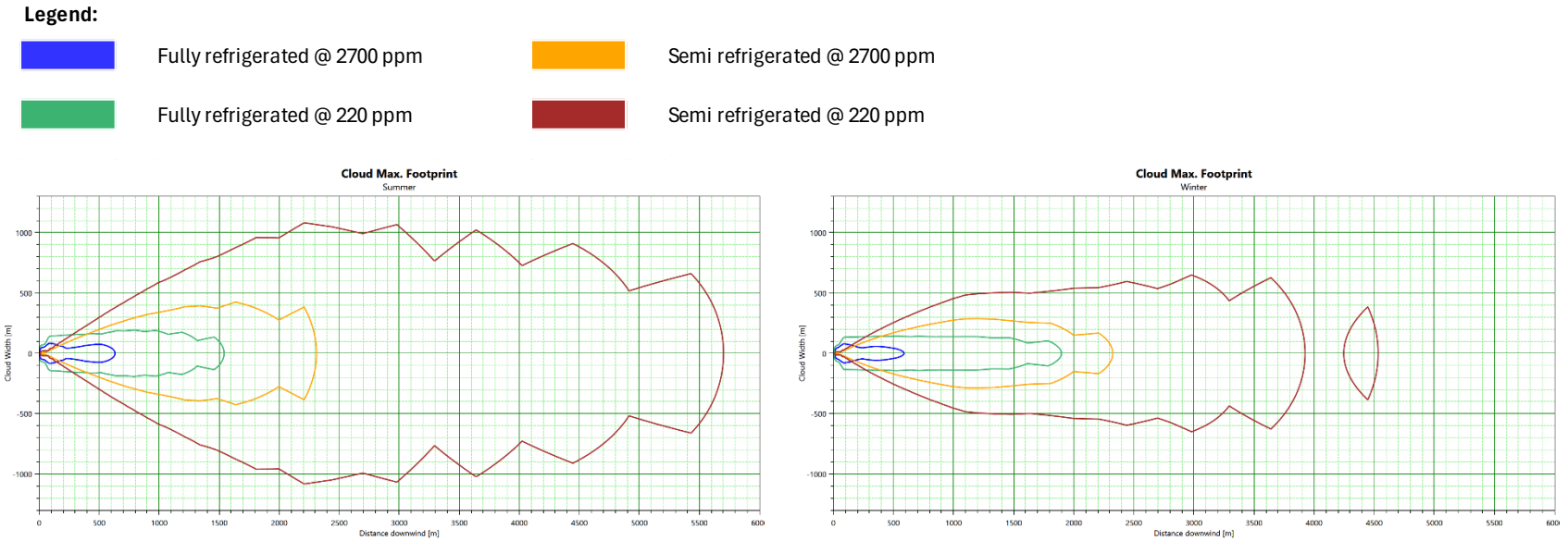
For fully refrigerated ammonia the seasonal pattern is also preserved. At 220 ppm the winter maximum footprint is longer than the summer footprint on both land and water, and at 2700 ppm winter remains similar to or slightly longer than summer.

The main differences arise from the much greater downwind reach over water, particularly for semi refrigerated ammonia. All maximum footprints increase when moving from land to water, but the increase is modest for fully refrigerated releases and very pronounced for semi refrigerated releases. At 220 ppm the semi refrigerated footprint grows from a few kilometres on land to several kilometres over water, and at 2700 ppm it also becomes much longer. The stronger increase in maximum footprint over water, especially for semi refrigerated ammonia, is consistent with how a vapour-dominated cloud interacts with the marine surface. Over water the surface is smoother and more homogeneous than land, so for the same meteorological conditions the cloud experiences less surface roughness, less mechanical turbulence near the ground and a more uniform boundary layer. This combination tends to reduce near-field dilution and allows the cloud to travel farther before it drops below 220 ppm or 2700 ppm. Semi refrigerated ammonia is released almost entirely as vapour, so its behaviour is governed mainly by atmospheric transport and dilution rather than by a sustained pool source. As a result, when the surface is changed to water the semi refrigerated cloud benefits most from this more efficient downwind transport and its maximum footprint increases dramatically, while the fully refrigerated cloud, which is still strongly tied to a local pool source, increases much less.

In addition, the seasonal ordering for semi refrigerated ammonia at 220 ppm reverses between land and water. On land the winter footprint is longer than the summer footprint, whereas over water the summer footprint becomes the longest. This reversal reflects the different balance between transport and dilution over the sea surface: for a vapour-dominated semi refrigerated release, the smoother marine surface and summer conditions favour slower dilution and longer range persistence than in winter, so the cloud maintains 220 ppm over a greater distance in summer. At 2700 ppm the summer semi refrigerated footprint is already slightly longer than winter on land and becomes clearly longer over water for the same reason.

Table 23. Maximum dispersion footprint for scenario 4 at 4.3 m height

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Maximum dispersion footprint at 220 ppm (m)	1708.76	6370.36	2103.07	4988.44
Maximum dispersion footprint at 2700 ppm (m)	639.97	2836.92	607.80	2480.14



a) b)

Figure 27. a) Maximum dispersion footprint for scenario 4 during summer b) Maximum dispersion footprint for scenario 4 during winter

6.2.3.1. Maximum dispersion footprint at 15.8 m height

Raising the release height from 4.3 m to 15.8 m increases the maximum footprint in every case but preserves the overall hierarchy of scenarios. Semi refrigerated ammonia still produces much longer maximum footprints than fully refrigerated ammonia, and the footprints in winter are still longer than the summer footprints.

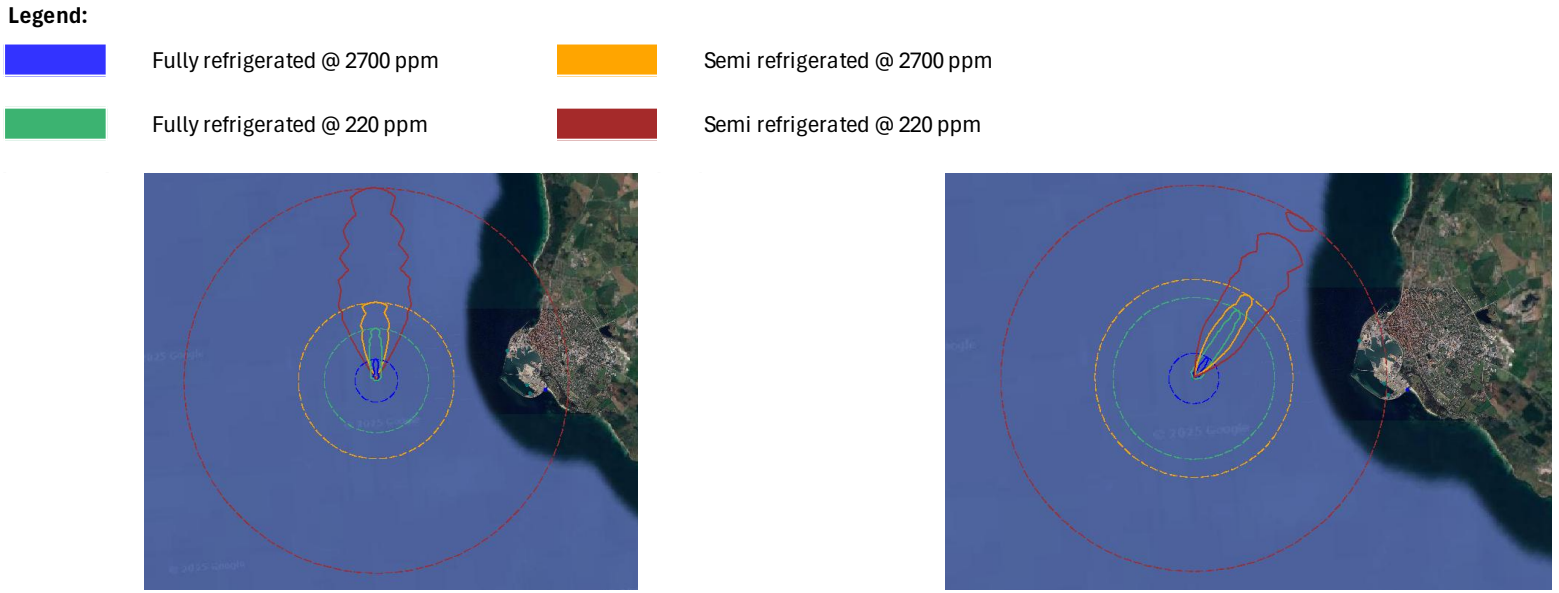
The main differences come from the higher release elevation strengthening the downwind reach, particularly for fully refrigerated ammonia. At 15.8 m, fully refrigerated maximum footprints increase at both 220 ppm and 2700 ppm in summer and winter. For semi refrigerated ammonia, the change at 220 ppm is more moderate. The maximum footprints are already very long at 4.3 m and grow only slightly when the release is raised, since the cloud is already strongly airborne over water. At 2700 ppm the effect of height on semi refrigerated ammonia is mixed. In summer the maximum footprint changes only marginally, while in winter it becomes noticeably longer at 15.8 m. Overall, the higher elevation reinforces long range transport, especially for fully refrigerated and winter semi refrigerated releases, without altering the basic ordering of scenarios observed at 4.3 m.

Table 24. Maximum dispersion footprint for scenario 4 at 15.8 m height

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Maximum dispersion footprint at 220 ppm (m)	2132.57	6587.19	2610.03	5452.11
Maximum dispersion footprint at 2700 ppm (m)	895.77	2753.73	819.14	2823.42

6.2.4. Maximum dispersion footprint at site

The maximum dispersion footprint may appear large. This reflects the envelope of all travelling detached vapour clouds over open water. Even with that understanding, the figures below indicate that ammonia bunkering operations would benefit from a greater offshore standoff so that the outer contours remain seaward and away from the port shoreline.



a) b)

Figure 28. a) Maximum dispersion footprint for scenario 4.1 and 4.2 b) Maximum dispersion footprint for scenario 4.3 and 4.4

6.2.5. Lethality at site

For this scenario the lethality maps are shown only at the site. The contours shown in Figure 29 and **Error! Reference source not found.** at both thresholds are compact and remain offshore. In case of a release, the cloud may reach the shoreline, but it may not extend inland. Compared with Figure 28, the risk to onshore areas is markedly reduced.

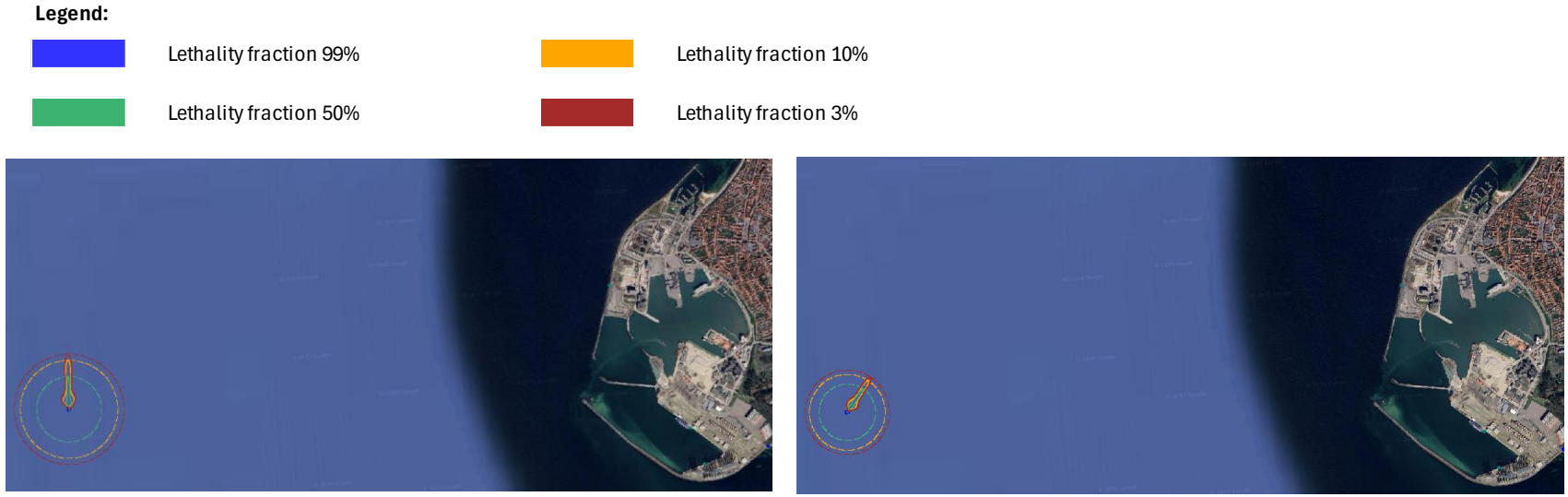


Figure 29. a) Toxic outdoor probit footprint for scenario 4.1 for fully refrigerated ammonia during summer b) Toxic outdoor probit footprint for scenario 4.3 for fully refrigerated ammonia during winter

6.3. Scenario 5 – Release on land, PTS

The following section is applicable for scenario 5:

- Terminal/pipeline-to-ship (PTS) alongside Quay 33

For all these scenarios, it is considered that the dispersion phenomena occur on land.

6.3.1. Released mass

Table 25 reports the released mass for scenario 5, the release of ammonia during the bunkering method of terminal/pipeline-to-ship (PTS). The total mass is higher than in Table 12 because, in addition to the immediate release, the pipeline inventory on the release side is also discharged. After the isolation valve closes, the trapped inventory between the leak and the valve continues to vent, so the total mass released is larger than in scenario 3.

For fully refrigerated ammonia the qualitative behaviour is very similar to that in scenario 3. Only a relatively small amount of the released mass appears in the initial vapour cloud and most of the inventory forms a pool on the ground. Winter still shifts a little more mass into the vapour cloud and a little less into the pool than summer, and after one hour the winter pool is slightly smaller, which means a slightly larger fraction of the pool has vapourised.

Semi refrigerated ammonia behaves differently, and this is where the main change in trend appears compared with scenario 3. In the STS bunkering operation, the summer release is entirely vapour with no pool at all, and in winter only a small pool forms, with very little liquid left after one hour. In that configuration the semi refrigerated line is relatively short and highly flashing throughout most of the discharge. Almost all of the inventory is released while the pressure is still high and the fluid is strongly two phase but very vapour rich. Under those conditions the jet remains mostly airborne and Phast assigns essentially all of the mass to the vapour cloud in summer and only a small amount to the pool in winter.

In the current PTS scenario, semi refrigerated ammonia releases always form a substantial pool in both seasons. In summer a larger share of the release appears immediately in the vapour cloud and the pool is correspondingly smaller than in winter, but the pool is now a significant part of the inventory, and several hundred kilograms of liquid remain on the ground after one hour in both cases. Here the semi refrigerated ammonia line includes a larger inventory in the terminal or pipeline system, so the release lasts longer and spans a wider range of pressures as the line depressurises. Early in the event the behaviour resembles the STS case, with a strongly flashing, vapour rich jet. As the pressure falls, the flash fraction decreases, the flow becomes more liquid rich and droplet momentum is reduced. In Phast, lower pressure phase generates much more rainout, so a substantial pool builds up on the ground. Because the total inventory is larger and the release spends more time in this liquid dominated regime, a much greater mass accumulates in the pool and several tonnes remain available to evapourate, with a few hundred

kilograms still present after one hour.

These behaviours are due to the scenario used in Phast. As stated in Table 10, the Phast scenario used for scenarios 1, 2, 3 and 4 is “Pressure vessel – Short pipe release”, whereas “Long pipeline – Location specific breach” was used for scenario 5.

In the “Pressure vessel – Short pipe release” scenario Phast treats the upstream side as a pressurised source feeding a short line with negligible friction losses, so the discharge occurs at high pressure with high jet momentum and strong entrainment. The result is a high release pressure with stronger initial jet momentum and air entrainment. This consideration is applied because, for a short pipe, friction losses are assumed to be negligible.

“Long pipeline – Location specific breach” uses pumped inflow. This model fixes the pumped inflow equal to the line’s flow rate, solves the hydraulics to obtain the pressure profile along the pipe, and uses the local pressure at the breach for the discharge.

In summary, the fixed flow short pipe case produces larger early footprints due to higher discharge momentum, while the long pipeline case yields smaller early distances and different timing because of pressure losses and reduced momentum. This change in source behaviour between STS and PTS, in particular the formation of a substantial semi refrigerated pool in PTS, underlies the differences seen in the dispersion footprints and lethality distances for scenario 5 compared with scenarios 1–3.

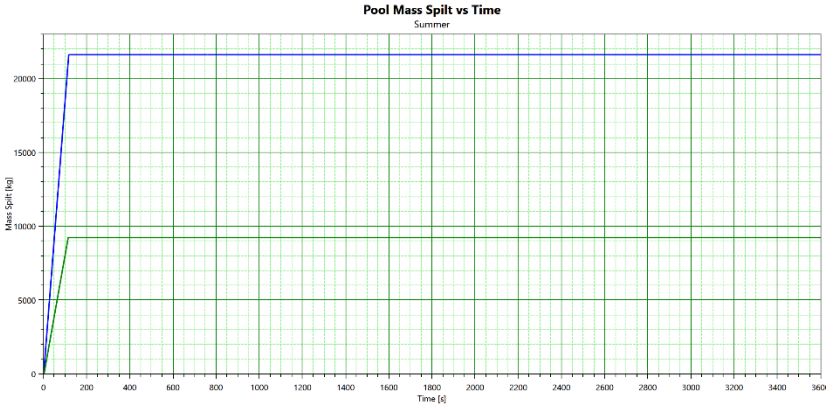
Table 25. Mass balance for scenario 5.

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Total mass released (kg)	24148.89	23313.08	24148.89	23313.08
Mass released as vapour cloud (kg)	2532.23	14082.36	2735.83	13029.02
Total mass released as a pool (kg)	21616.66	9230.72	21413.06	10284.06
Mass vapourized from the pool (kg)	19824.77	8507.23	19760.15	9540.86
Mass remaining in pool after 1 h (kg)	1791.89	723.49	1652.91	743.20

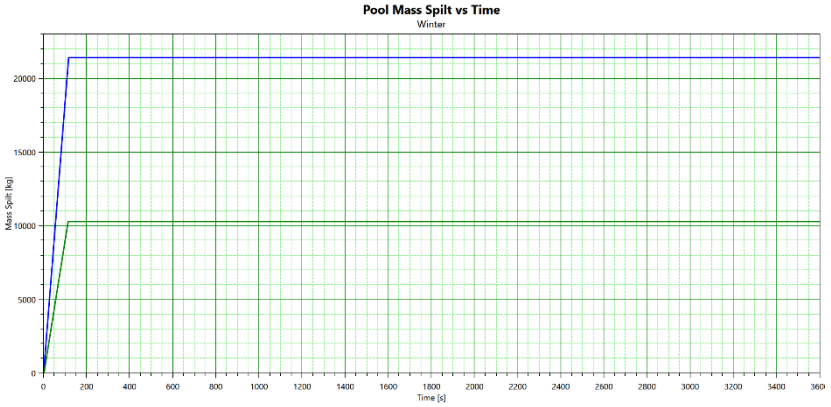
Legend:

Fully refrigerated

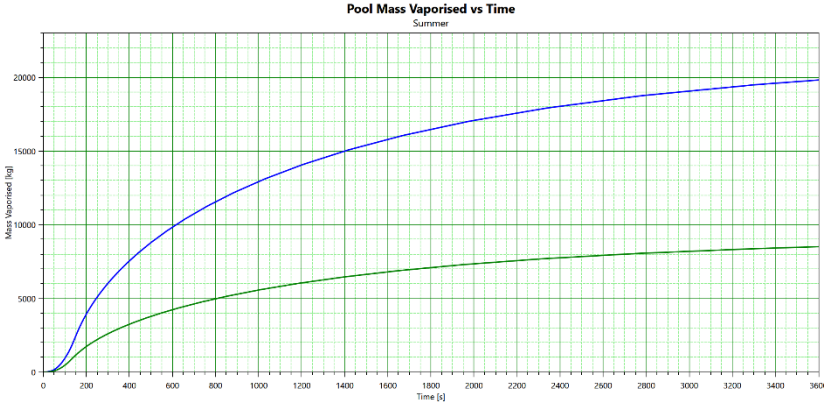
Semi refrigerated


Pool Mass Spilt vs Time
Summer
Mass Spilt [kg]
Time [s]

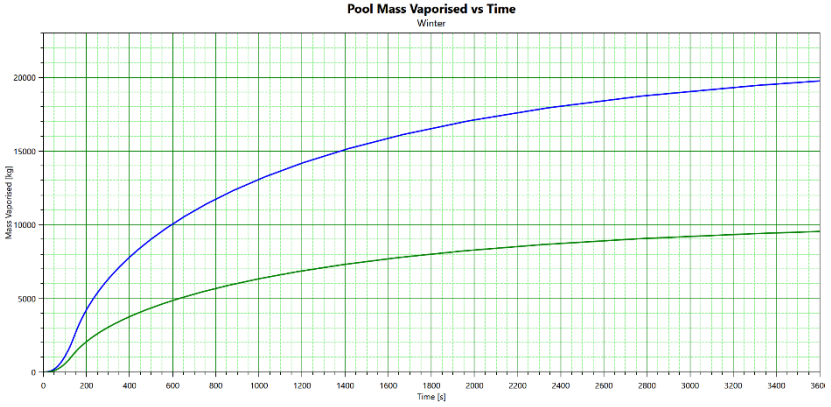
a)


Pool Mass Spilt vs Time
Winter
Mass Spilt [kg]
Time [s]

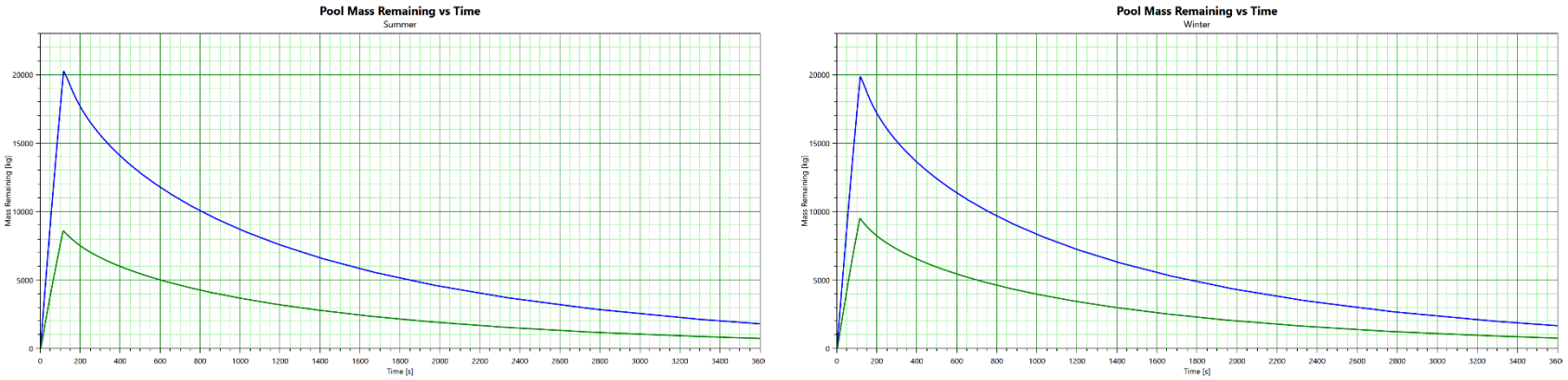
b)


Pool Mass Vaporised vs Time
Summer
Mass Vaporised [kg]
Time [s]

c)


Pool Mass Vaporised vs Time
Winter
Mass Vaporised [kg]
Time [s]

d)



e) f)

Figure 30. Ammonia pool mass split for scenario 5. a) Pool mass split vs time during summer b) Pool mass split vs time during winter c) Pool mass vapourized vs time during summer d) Pool mass vapourized vs time during winter e) Pool mass remaining vs time during summer f) Pool mass remaining vs time during winter

6.3.2. Dispersion

According to Table 26, the main trend between semi refrigerated and fully refrigerated ammonia is that semi refrigerated clouds reach farther at early times, while fully refrigerated clouds are more persistent, which is consistent with Table 14. Seasonally, winter mainly extends the early reach of the cloud, while summer tends to sustain it for slightly longer.

Compared with the STS scenarios at the same height in Table 14, the PTS dispersion keeps the same basic hierarchy. At 220 ppm, semi refrigerated ammonia still reaches farther than fully refrigerated at early times, and fully refrigerated clouds remain more persistent later in the event. At 2700 ppm, semi refrigerated releases again have the longest footprint at the very beginning, while fully refrigerated releases retain shorter but more durable high concentration footprints. In both STS and PTS, winter footprints are longer than summer footprints at about 2–5 minutes, and the 220 ppm footprints are always longer than the 2700 ppm footprints for the same case.

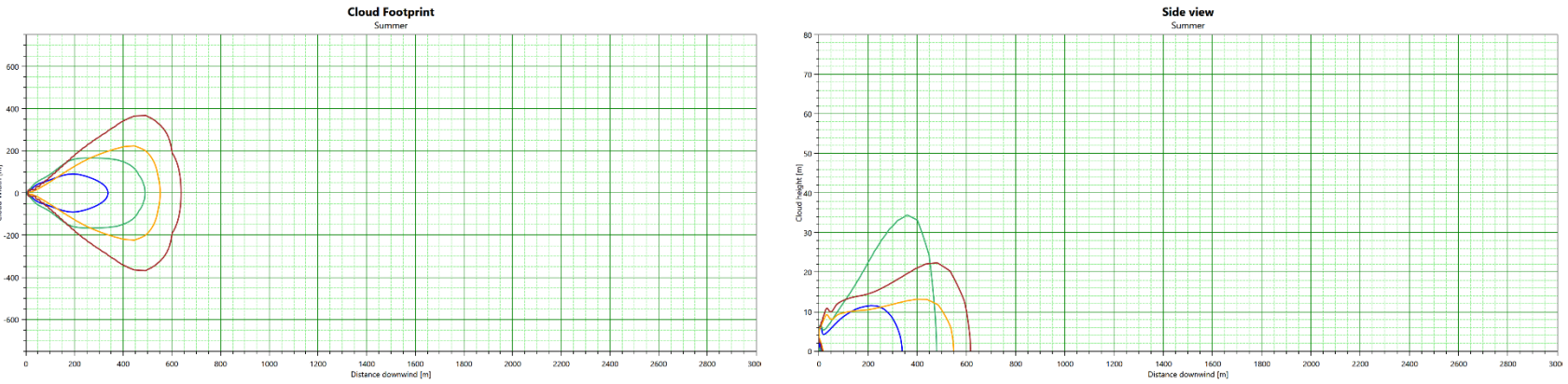
The main differences are in how long the semi refrigerated clouds remain above the thresholds and how far the fully refrigerated clouds extend at intermediate times. In the STS case, the semi refrigerated cloud at 220 ppm grows rapidly to its maximum distance and then disappears or becomes very short by around 10 minutes, and at 2700 ppm it is essentially a very intense but short lived plume that vanishes after the first time step. In the PTS case, the semi refrigerated cloud still reaches similar distances at 2–5 minutes, but now retains a finite 220 ppm footprint at about 10 and 30 minutes and shows measurable 2700 ppm distances out to about 30 minutes in summer. This reflects the larger inventory and the more sustained pool source in PTS, which continue feeding vapour into the cloud after the initial flashing phase.

For fully refrigerated ammonia, the PTS scenario also produces somewhat longer 220 ppm and 2700 ppm footprints at intermediate times than

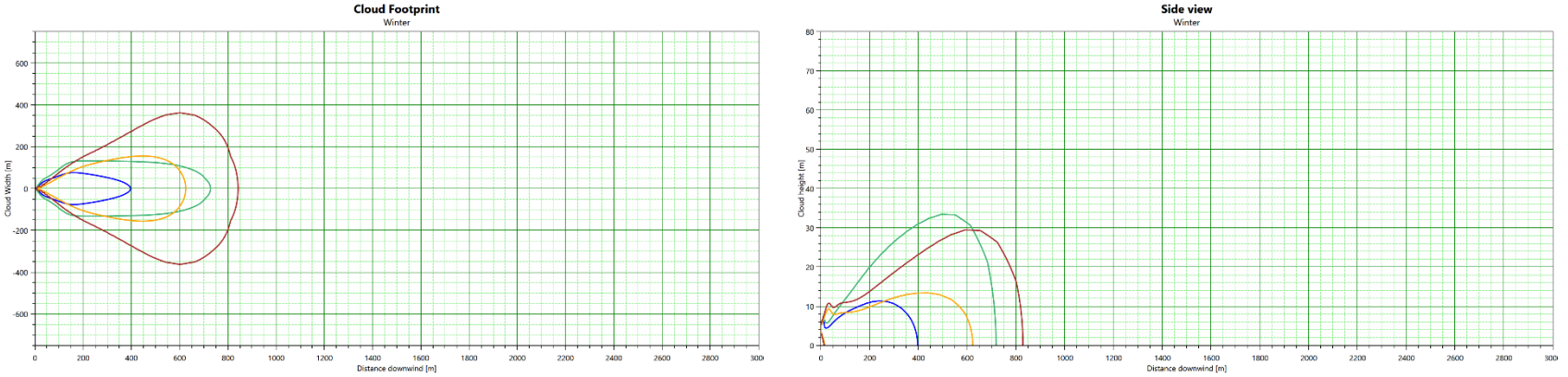
STS, while preserving the same seasonal behaviour. Winter still gives the longest early footprints, but in both seasons the PTS clouds at 220 ppm extend farther around 5–10 minutes than the corresponding STS clouds, before contracting to a few hundred metres and eventually disappearing.

Table 26. Dispersion footprint for scenario 5

	Time (s)	Summer		Time (s)	Winter	
		Fully refrigerated	Semi refrigerated		Fully refrigerated	Semi refrigerated
Dispersion footprint at 220 ppm (m)	106	489.48	637.42	105	727.67	842.92
	318	1329.58	1574.51	314	1869.31	2333.42
	601	579.77	422.53	594	598.21	464.75
	1802	295.30	258.26	1815	251.08	245.03
	3533	0	0	3489	0	0
Dispersion footprint at 2700 ppm (m)	106	336.94	552.02	105	396.17	624.91
	318	193.93	188.93	314	164.10	177.35
	601	168.46	159.06	594	130.78	142.45
	1802	80.25	88.36	1815	0	0
	3533	0	0	3489	0	0



a) b)



c) d)

Figure 31. Cloud footprints for scenario 5. a) Dispersion footprint during summer, time step=106 seconds, b) Dispersion sideview during summer, time step=106 seconds, c) Dispersion footprint during winter, time step=105 seconds, d) Dispersion sideview during winter, time step=105 seconds.

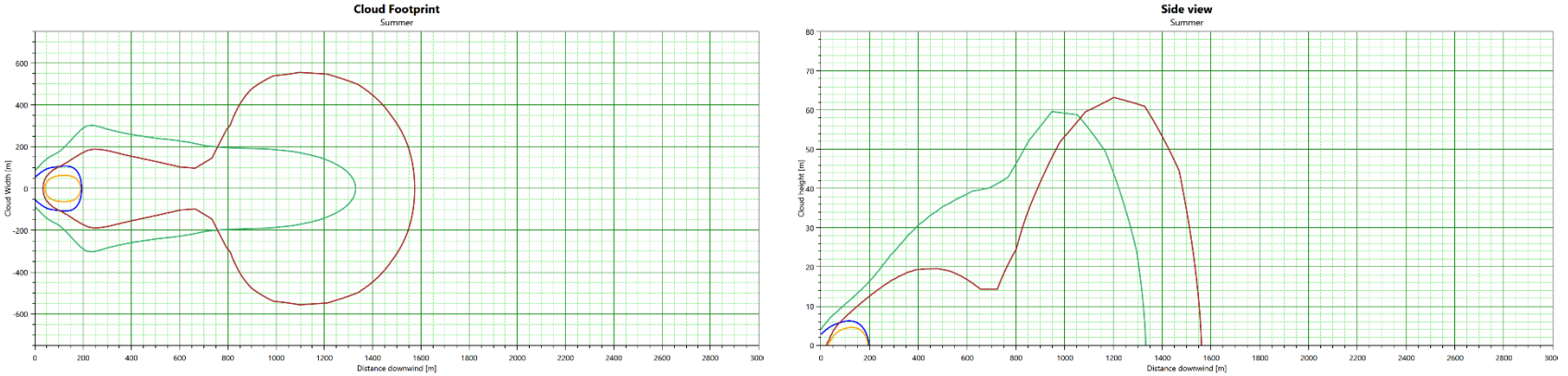
Legend:

Fully refrigerated @ 2700 ppm

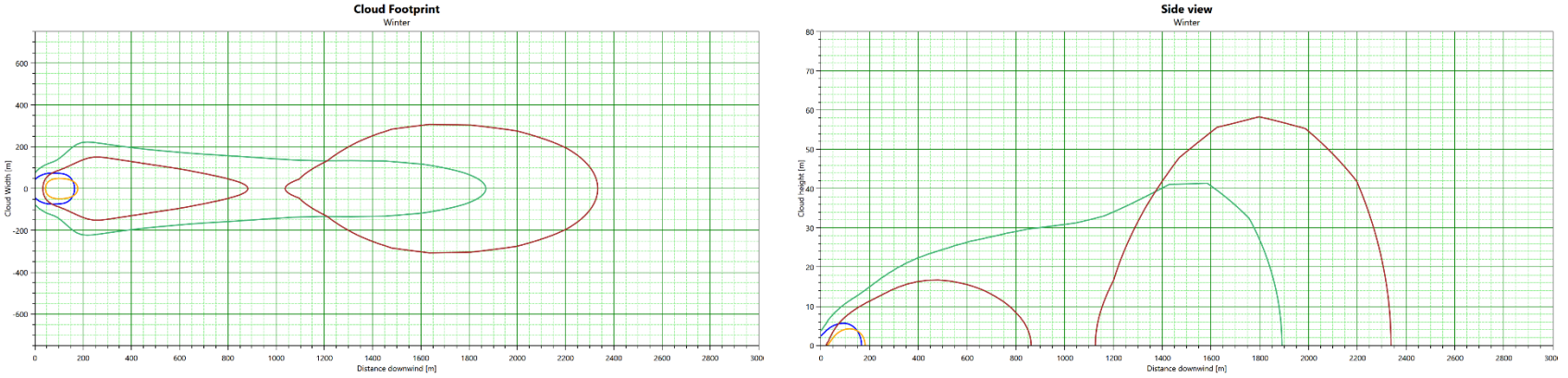
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a) b)



c) d)

Figure 32. Cloud footprints for scenario 5. a) Dispersion footprint during summer, time step=318 seconds, b) Dispersion sideview during summer, time step=318 seconds, c) Dispersion footprint during winter, time step=314 seconds, d) Dispersion sideview during winter, time step=314 seconds.

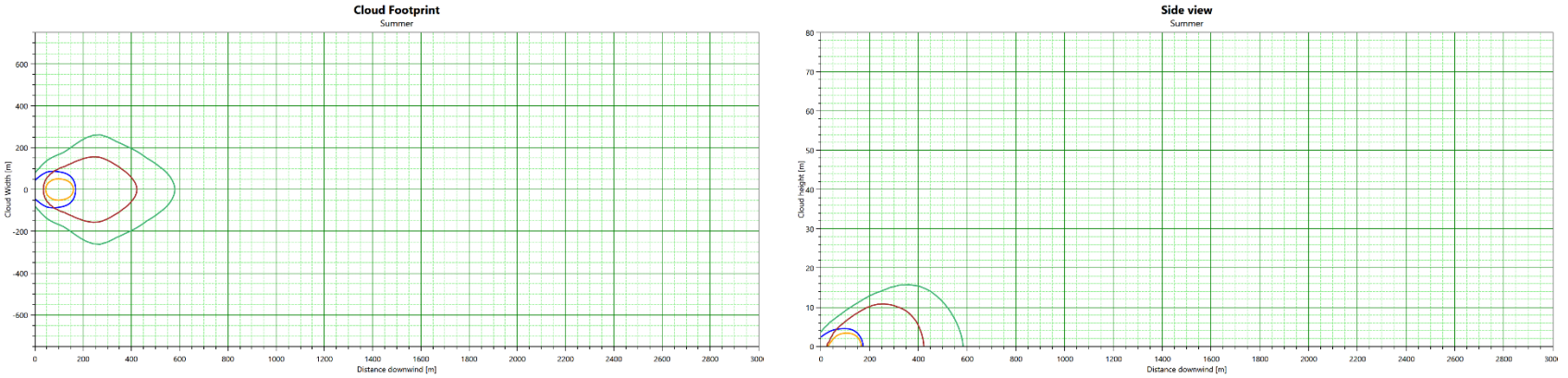
Legend:

Fully refrigerated @ 2700 ppm

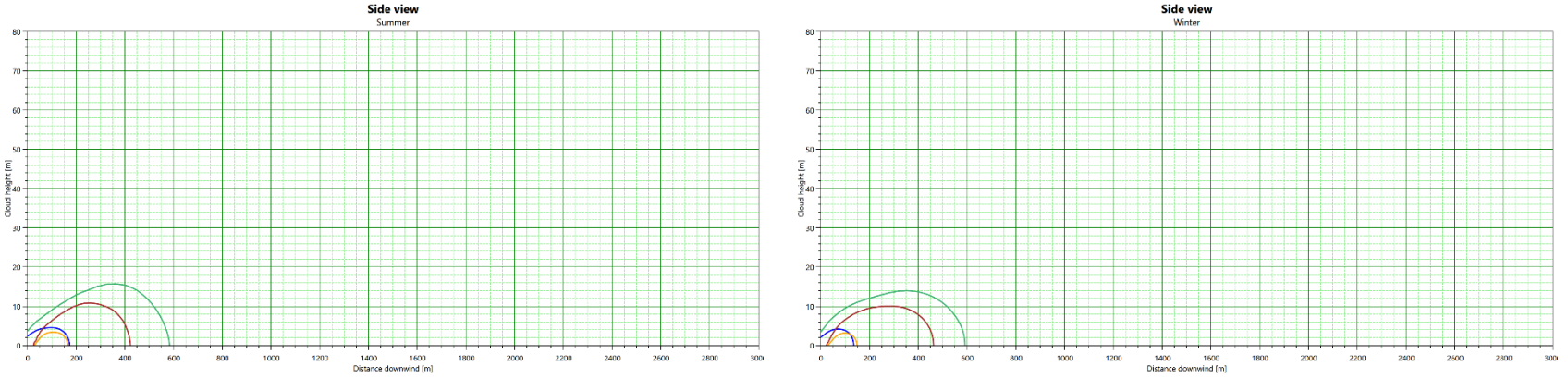
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a) b)



c) d)

Figure 33. Cloud footprints for scenario 5. a) Dispersion footprint during summer, time step=601 seconds, b) Dispersion sideview during summer, time step=601 seconds, c) Dispersion footprint during winter, time step=594 seconds, d) Dispersion sideview during winter, time step=594 seconds.

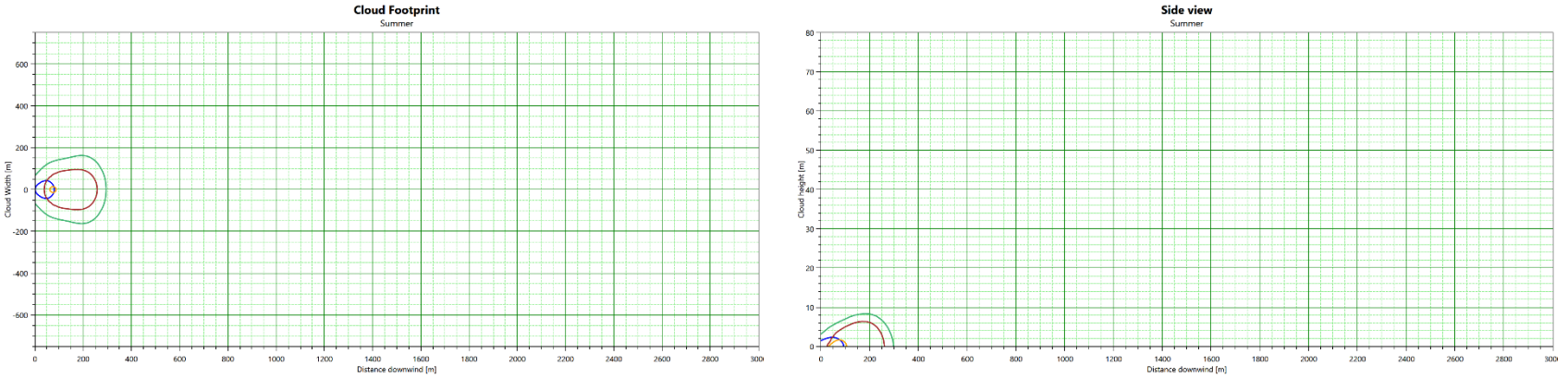
Legend:

Fully refrigerated @ 2700 ppm

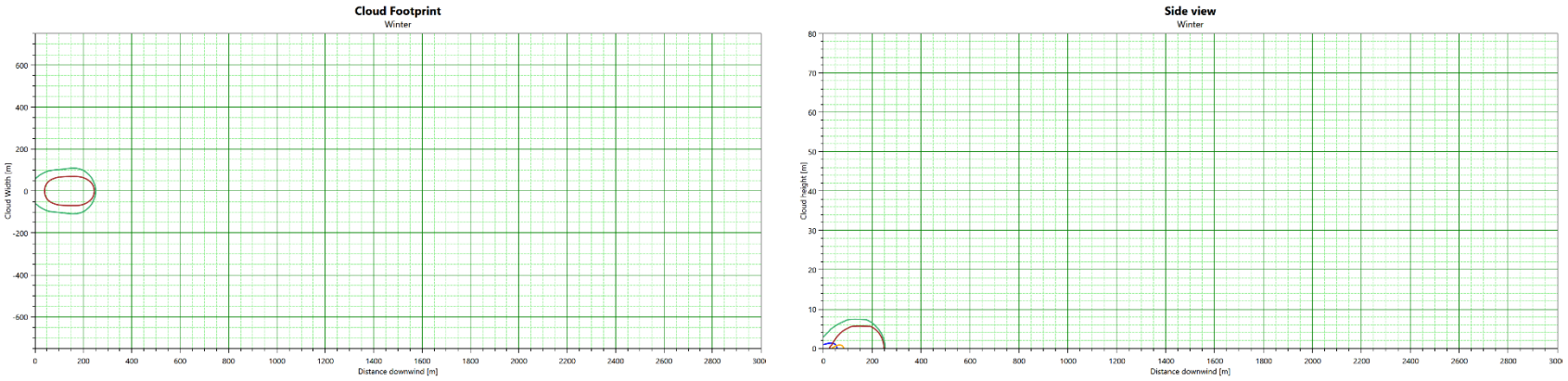
Semi refrigerated @ 2700 ppm

Fully refrigerated @ 220 ppm

Semi refrigerated @ 220 ppm



a) b)



c) d)

Figure 34. Cloud footprints for scenario 5. a) Dispersion footprint during summer, time step=1802 seconds, b) Dispersion sideview during summer, time step=1802 seconds, c) Dispersion footprint during winter, time step=1815 seconds, d) Dispersion sideview during winter, time step=1815 seconds.

6.3.3. Maximum dispersion footprint

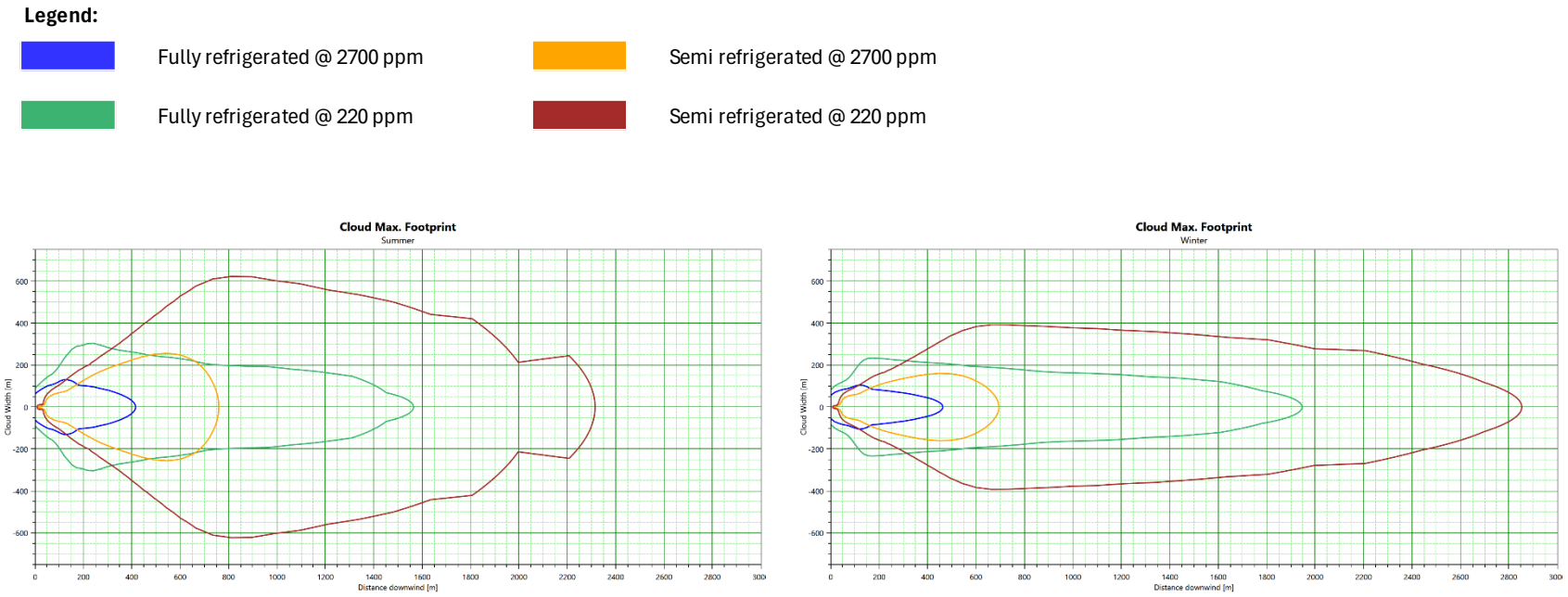
Comparing Table 27 with Table 16, the main hierarchy is unchanged. At both 220 ppm and 2700 ppm, semi refrigerated ammonia still reaches farther than fully refrigerated ammonia. For fully refrigerated ammonia, winter continues to give a longer maximum footprint than summer at 220 ppm and slightly longer footprints at 2700 ppm. For semi refrigerated ammonia, the summer maximum footprint remains longer than the winter footprint at both concentration levels in both scenarios.

The main differences concern how far the clouds travel and how this varies with storage mode and concentration. For fully refrigerated ammonia, changing from STS to PTS increases the maximum footprint at both 220 ppm and 2700 ppm in summer and winter. At 220 ppm the distances grow by several hundred metres, and at 2700 ppm the footprints also extend farther downwind, which reflects the larger inventory and longer release in the pipeline configuration. For semi refrigerated ammonia, the 220 ppm maximum footprints increase only moderately from STS to PTS, so the far field reach is only slightly larger. At 2700 ppm, however, the semi refrigerated footprints become shorter in PTS than in STS, which means the highest concentration region is more confined to the near field, even though the 220 ppm impact range is somewhat extended.

Table 27. Maximum dispersion footprint for scenario 5

	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
Maximum dispersion footprint at 220 ppm (m)	1605.98	2459.56	1990.48	2947.24

Maximum dispersion footprint at 2700 ppm (m)	419.88	759.67	468.97	694.84



a) b)

Figure 35. a) Maximum dispersion footprint for scenario 5 during summer b) Maximum dispersion footprint for scenario 5 during winter.

6.3.4. Maximum dispersion footprint at the site for each scenario

As a reminder, the maximum dispersion footprint is overlaid on a true scale map of the area around the Port of Rønne. The contour shows the outer envelope of all locations reached by the cloud at the stated concentration at any time during the simulation. It is not a time slice or a simultaneous exposure map. Any point inside the contour could experience that concentration at some moment. Elongated lobes may indicate periods when the cloud moved in that direction, while the concentric rings are distance guides only and do not indicate duration or concurrent impact.

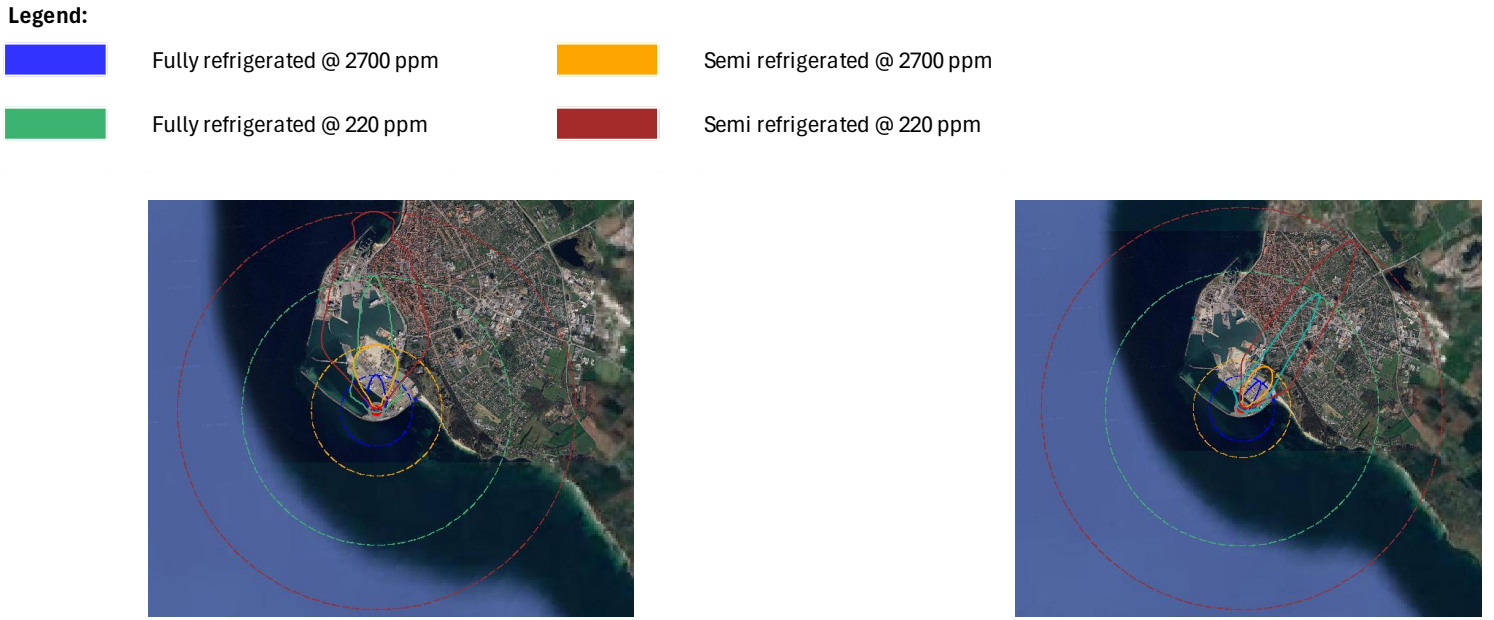


Figure 36. a) Maximum dispersion footprint for scenario 5.1 and 5.2 b) Maximum dispersion footprint for scenario 5.3 and 5.4

6.3.5. Lethality

Similar to Table 18, the main qualitative trends are preserved in Table 28. For every lethality level and in both seasons, semi refrigerated ammonia still reaches farther than fully refrigerated ammonia. For a given product and lethality fraction, summer distances remain longer than winter distances, and in both scenarios the distance increases as the lethality fraction becomes smaller, so the lowest lethality level is always farthest from the source.

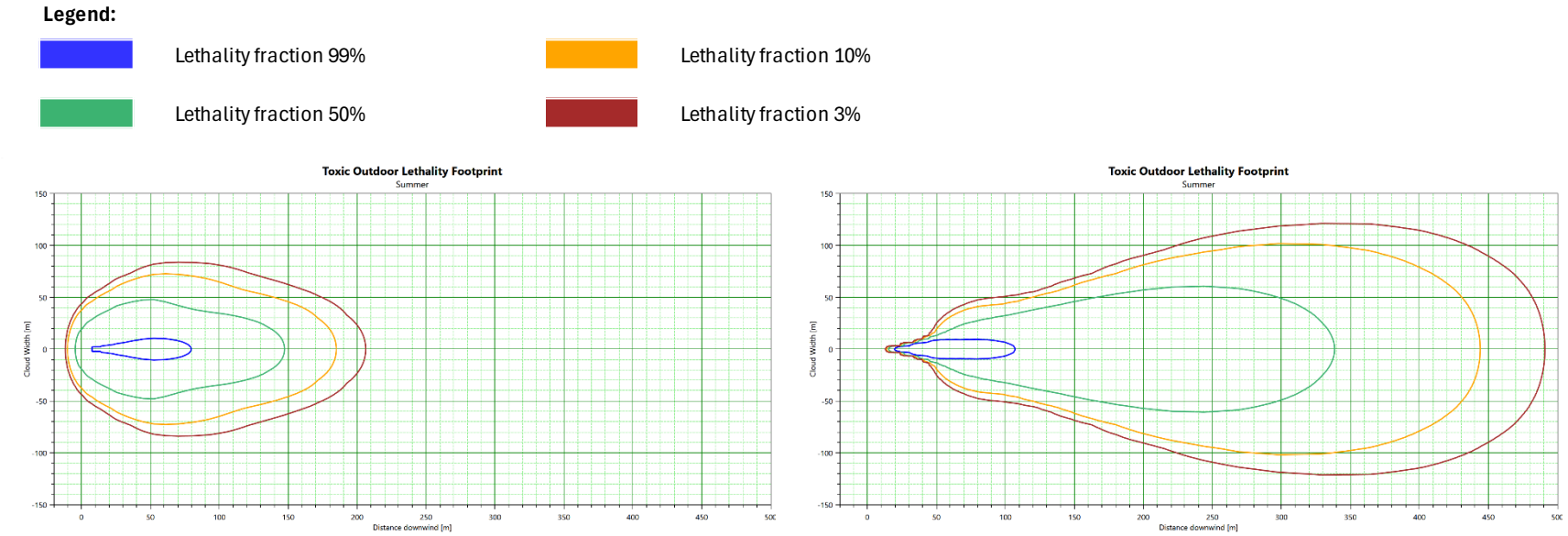
The main differences lie in how the distances change between STS and PTS. For fully refrigerated ammonia, all lethality distances increase in the PTS case at every lethality fraction and in both seasons. The highest lethality distances move farther from the source, and the lowest lethality contours also extend noticeably, reflecting the larger total release and the stronger pool-driven vapour source in the pipeline configuration.

For semi refrigerated ammonia the change is more subtle. At the highest lethality levels the distances are clearly larger in the PTS scenario than in the STS case, showing that the near field doses close to the source are higher when the larger terminal or pipeline inventory is released. At the lowest lethality levels, however, the distances in PTS are somewhat shorter than in STS, in both summer and winter. This is consistent with the mass balance. In PTS a substantial pool now forms and anchors more of the release near the source, so the lethality is more concentrated in the

near and intermediate field, while the very far field impact is slightly reduced compared with the purely airborne STS case.

Table 28. Distances of lethality fractions for scenario 5

Lethality fraction	Summer		Winter	
	Fully refrigerated	Semi refrigerated	Fully refrigerated	Semi refrigerated
99%	79.74	107.33	60.88	86.95
50%	147.34	338.51	125.32	268.79
10%	184.89	444.08	164.87	358.54
3%	206.26	490.97	190.19	400.42



a) b)

Figure 37. a) Toxic outdoor probit footprint for scenario 5 for fully refrigerated ammonia during summer b) Toxic outdoor probit footprint for scenario 5 for semi refrigerated ammonia during summer

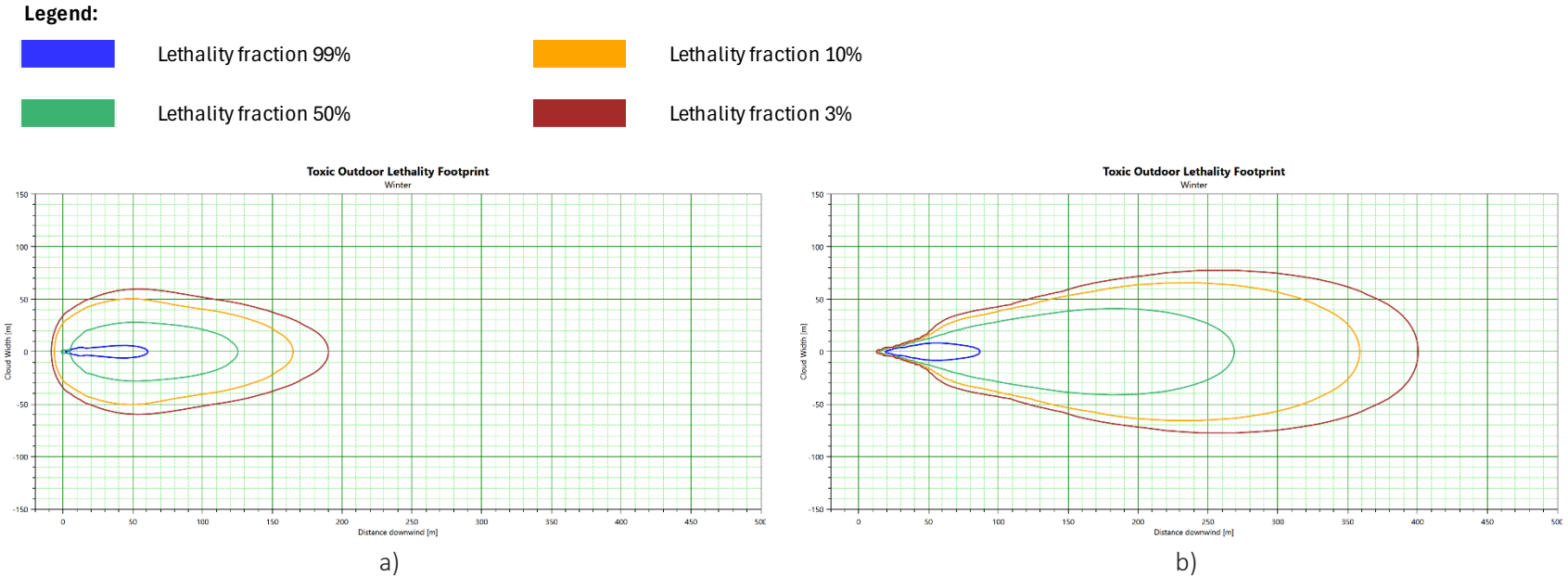


Figure 38. a) Toxic outdoor probit footprint for scenario 5 for fully refrigerated ammonia during winter b) Toxic outdoor probit footprint for scenario 5 for semi refrigerated ammonia during winter

6.3.6. Lethality at site

As with scenarios 1, 2 and 3, the lethality analyses for the Port of Rønne were performed only under fully refrigerated operation, the safer and more plausible case.

In Figure 39, these plots reflect only the probit-based lethality analysis for outdoor dispersion under the stated conditions and do not account for confinement, terrain channelling, building induced recirculation, or accumulation in enclosed spaces, nor other operating or weather conditions.

Legend:

Lethality fraction 99%

Lethality fraction 10%

Lethality fraction 50%

Lethality fraction 3%

a)

b)

Figure 39. a) Toxic outdoor probit footprint for scenario 5.1 for fully refrigerated ammonia during summer b) Toxic outdoor probit footprint for scenario 5.3 for fully refrigerated ammonia during winter

7. CONCLUSIONS

Across all scenarios, the release of semi refrigerated ammonia is consistently more vapour dominated than fully refrigerated ammonia. For a given release, a larger share of the semi refrigerated ammonia inventory appears immediately as a vapour cloud and a smaller share forms a pool. Fully refrigerated ammonia behaves in the opposite way. Only a modest fraction flashes to vapour at release and a large cold liquid pool remains on the ground or on the water surface. Where semi refrigerated pooling does occur, the pool is always smaller and shorter lived than for fully refrigerated ammonia. Fully refrigerated ammonia releases retain a clearly larger liquid inventory after one hour and therefore provide a more sustained source of evaporation.

For the current simulations, it was considered that the total mass released is the same in summer and winter. Seasonal effects act only on how that mass is divided between the initial vapour cloud and the pool and on how quickly the pool evaporates. For fully refrigerated ammonia, winter generally shifts a small additional portion of the release into the vapour cloud and leaves a slightly smaller pool after one hour, so a little more of the pool mass has evaporated. For semi refrigerated ammonia, the direction of the seasonal shift depends on the scenario. For releases on land for STS bunkering, summer can be almost entirely vapour with negligible pooling, while winter produces some rainout and a small pool. In PTS releases and over water, semi refrigerated pooling is present in both seasons but tends to be more pronounced in winter.

For releases over land with an elevation of 4.3 m, semi refrigerated ammonia releases consistently produce longer footprints at early times. The semi refrigerated ammonia cloud is more intense near the source and reaches farther downwind in the first minutes because most of the inventory appears directly as vapour. Fully refrigerated ammonia releases produce shorter footprints initially but maintain detectable clouds for longer. The large pool continues to evaporate after the discharge ends and feeds vapour into the atmosphere, so the cloud persists at both concentration thresholds well beyond the time when semi refrigerated ammonia clouds have largely diluted.

For maximum dispersion footprints, winter generally stretches the cloud farther than summer for fully refrigerated ammonia, especially at the lower concentration threshold. Colder, denser air and stronger winds in winter carry the cloud further downwind before it falls below the threshold, so the winter maximum footprint is usually longer than the summer one in those cases. For semi refrigerated ammonia the picture is more mixed. On land, winter tends to give the longest maximum footprints, similar to the fully refrigerated case. Over open water, however, summer can become dominant at the lower threshold, because the smoother sea surface and summer conditions favour long range persistence of a vapour dominated cloud. Overall, seasonal effects on maximum footprint are noticeable but remain secondary to the influence of storage mode, terrain and release elevation.

Increasing the release height from 4.3 m to 15.8 m makes the cloud more airborne and strengthens its downwind reach, especially for semi refrigerated ammonia. When the release point is raised, vapour and droplets remain aloft longer, entrain more air and travel farther before interacting with the surface. This reduces rainout, increases the initial vapour cloud and lengthens the early dispersion footprints at both concentration thresholds. For fully refrigerated ammonia, a higher release height increases the initial vapour cloud and slightly reduces the pool, but the pool remains the dominant long term source, so the overall time evolution of the cloud is similar. For semi refrigerated ammonia, the effect is stronger. At higher elevation

the two phase jet can remain fully airborne, so rainout is largely suppressed and the cloud behaves like a purely airborne release, with very long footprints at intermediate times and no pool contribution. Despite these changes in magnitude, the qualitative pattern in time is preserved, with an initial expansion to a peak footprint followed by contraction as the cloud dilutes.

The underlying terrain has a clear effect on dispersion. Changing from land to open water increases dispersion footprints at both concentration thresholds for all release types, with the largest increases for semi refrigerated ammonia. The open water surface has much lower roughness than the land terrain used for the quay scenarios. This reduces mechanical turbulence in the surface layer, so dilution is slower and the cloud can be carried farther downwind before it drops below the thresholds. Fully refrigerated ammonia also shows longer footprints over water, but the increase is more modest because its behaviour remains strongly influenced by the pool close to the source. For semi refrigerated ammonia, which is dominated by airborne vapour, the combination of low roughness and sustained advection over water allows the cloud to develop very long footprints at intermediate times.

For a given scenario and season, semi refrigerated ammonia releases consistently produce longer lethal distances than fully refrigerated ammonia releases at the same lethality level. This difference becomes more pronounced for lower lethality levels. Semi refrigerated ammonia releases generate a large vapour cloud that transports a significant toxic dose farther downwind, so the outer lethal contours extend well beyond the fully refrigerated ammonia contours. Fully refrigerated ammonia releases still present substantial lethal ranges but these are more limited. The toxic impact is more tightly linked to the region where the pool driven cloud remains concentrated rather than to long range transport of a purely airborne plume.

Across storage modes and scenarios, summer conditions generally produce longer lethality distances than winter at a given lethality level. This is consistent with the dose based nature of the probit model. In winter, clouds may momentarily reach farther, but stronger winds lead to faster dilution and shorter exposure times at individual locations, which reduces the time integrated dose. In summer, lower wind speeds and more persistent concentrations near the source allow higher doses to accumulate even if the cloud does not travel as far at any instant. Consequently, the lethal contours extend farther in summer than in winter for the same release and storage mode of ammonia.

The effect of terrain on lethality is more about where the impact occurs than about the physics of dose. Over land near the port, lethal contours for fully refrigerated ammonia can extend across operational areas but, under the conditions analysed, remain largely within the port boundary. Over open water at several nautical miles offshore, the same or larger releases produce lethal contours that remain offshore and only approach the shoreline. Although dispersion footprints become longer over water, receptors on land are farther from the source, and the additional travel distance increases dilution and reduces the dose by the time the cloud reaches the coast. For semi refrigerated ammonia, the longer dispersion footprints over water do not translate into proportionally longer onshore lethal distances because much of the toxic impact is taken up over the sea. In practical terms, moving releases offshore shifts the main lethality risk away from populated onshore areas, even though the physical cloud can travel farther over the smoother marine surface.

Overall, fully refrigerated ammonia operation remains both the safer and the more plausible bunkering mode for the Port of Rønne. In the site specific assessments, fully refrigerated ammonia lethality contours remain within the port area and do not intrude into populated zones for the conditions analysed. Overall, the combination of storage mode, release elevation, surface type and season has a systematic and understandable effect on the hazard, and careful selection of bunkering configuration and location can

significantly reduce offsite toxic risk for ammonia.

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