APPENDIX L

Modelling Ammonia in the Marine Environment



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Reference: Ammonia Marine Spill Modelling Summary

INTRODUCTION

A review and modelling of the dissolution and dispersion of an ammonia spill in the marine environment has been completed as background information to the ecological risk assessment.

Liquified ammonia is carried to the export marine terminal through a 24-inch pipe at approximately ambient pressure (101.325 kPa) and sufficiently low temperatures to keep the ammonia in its liquid state, or approximately -33.3 °C. A hypothetical release from the transport piping may result in a release of low temperature liquid ammonia into the marine environment.

Upon release and interaction with sea water, a portion of the spilled ammonia will rapidly vapourize. Due to the miscibility of ammonia and water, ammonia readily mixes with water, and so the ammonia that does not vapourize will diffuse into the marine environment. The diffusing ammonia will also undergo a chemical reaction with water that will release heat and form ammonium hydroxide. The portion of ammonia that remains as the reaction reaches equilibrium – also known as un-ionized ammonia (NH₃) – is the primary contributor to ammonia's toxicity to plant and animal life in the marine environment.

The purpose of this memo is to outline the methodology and assumptions used in estimating the un-ionized ammonia concentration in the vicinity of a liquid ammonia release.

METHODS AND ASSUMPTIONS

Source Considerations

To estimate the spatial extents of un-ionized ammonia associated with a plausible worst-case release, a catastrophic failure of the 24" diameter liquid ammonia transfer piping was considered. The approximate layout of the facility and marine export infrastructure is shown in Figure 1. The tanker was assumed to be approximately 80 to 100 m offshore, and the release was assumed to occur between the tanker and the shoreline.

The spill was assumed to release at the facility to tanker transfer rate of 1,786 kg/s. It was assumed that an operator would be able to close an emergency shut down valve (ESDV) within 15 minutes of the release occurring. Experimental observations and numerical modelling studies have indicated that between 60% and 70% of the ammonia released into the marine environment will go into solution while the remainder evaporates into the atmosphere (Raj and Reid 1978). For the purpose of this study, it was assumed that 70% of the spilled ammonia (or 1250 kg/s) enters the water during a release.

As the ammonia mixes and disperses, a chemical reaction will occur that will create ammonium hydroxide, the reaction is described by Equation 1. The equilibrium conditions for this reaction depend on parameters including the temperature, pH and salinity of the sea water (CCME 2010).

$$NH_3 + H_20 \Rightarrow NH_4^+ + 0H^-$$
 Equation 1

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The typical ranges of temperature, pH, and salinity in the Strait of Canso are shown in Table 1, along with the impacts on NH_3 concentration, and the parameter values used in the study. Empirical correlations can be used to estimate the un-ionized ammonia concentration based on these environmental parameters and the total ammonia (Free Ammonia Calculator (hamzasreef.com)). Based on the parameter values used in the study, it is estimated that there are 26.044 g of NH_3 for every 1000 g of "total" ammonia in the water column. This conversion rate is used to estimate the concentration of un-ionized ammonia in the dispersing waterbased plume.



Figure 1 Approximate Layout of the Facility and Marine Transport Infrastructure

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Parameter	Units	Range in the Canso Strait	Value used in Study	Impact on NH₃ concentration
Temperature	°C	6.6 to 16.4	16.4	NH₃ increases with temperature
рН	-log(H+)	7.88 to 8.03	8.03	NH₃ increases with pH
Salinity	g/kg	29.41 to 31.76	29.41	NH₃ decreases with increasing Salinity

Table 1 Parameters Affecting NH₃ Concentration

Dispersion Modelling

The dispersion of ammonia in the sea water was estimated using the OpenFOAM Computation Fluid Dynamics (CFD) Toolbox. OpenFOAM solves the mass, momentum energy and species transport equations to provide an estimate of the concentrations resulting from the release. The model was run in steady state mode that assumes a longer release time than would occur for the actual release which would end when the ESDV closes. Additionally, the modelling was completed using the K-Omega SST turbulence model to close the system of equations.

OpenFOAM allows for an explicit definition of the 3-dimensional (3D) geometry associated with the study. An image depicting the 3D geometry used for the modelling is provided Figure 2. The upper portion of the figure shows the sea floor boundary and the location of the tanker, and the lower portion of the image provides additional detail in the area closer to the spill. The vertical scale is exaggerated to enhance the depiction.

The sea current will carry and diffuse the ammonia away from the release site. The currents in the Strait of Canso have average speeds of 0.1 m/s to 0.2 m/s and peak velocities ranging from 0.3 m/s to 0.6 m/s (CBCL 2015). This study considered two scenarios, one scenario with typical currents of less than 0.2 m/s, and another scenario with average currents of approximately 0.6 m/s.

Consequence Criteria

The British Columbia Approved Water Quality Guidelines provide long-term chronic guidelines and acute-short term guidelines for un-ionized ammonia. The chronic guidelines are designed to protect against sub-lethal effects from continuous or indefinite exposure to a contaminant (BCMOE 2021). The acute guidelines are designed to project against severe effects such as lethality over a specified short-term exposure, typically assumed to be less than 96 hours (BCMOE 2021). As in the case of the estimated un-ionized ammonia in the water column, the consequence criteria for un-ionized ammonia depend on water temperature, salinity and pH. With consideration of the water properties in the Strait of Canso, the guideline concentration criteria were based on:

- Water Temperature of 20 C,
- pH of 8, and
- Salinity of 30 g/kg.

The resulting chronic and acute guidelines are 1.1 mg/L and 7.3 mg/L respectively.

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The persistence of the contaminant is an additional concern when considering a toxic exposure. The release was assumed to terminate after 15 minutes, after which the current will continue to dilute the ammonia concentration. The exposure time was estimated based on the turbulence and speed of the current near the location of the release. The current speed impacts the time it takes for fresh (clean) sea water to enter the region of elevated concentrations and the turbulence levels enhance the mixing of fresh sea water into the region of elevated concentrations.



Figure 2 Geometry Used in the Spill Dispersion Modelling

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RESULTS

Concentration Predictions

The estimated extents for the typical (<0.2 m/s) and high current (~0,6 m/s) scenarios are provided in Figure 3 and Figure 4, respectively. There is little predicted impact of current speed on the extents of the plume and a slight impact on the downstream location, with the higher current speed shifting the plume slightly downstream. This indicates that the turbulence levels are similar for both current speeds as is anticipated in shallower regions of the channel.



Figure 3 Predicted Unionized Ammonia Concentrations Associated with the Typical Current Speed Scenario (< 0.2 m/s)

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1.1	7.3	25	50	100	

Figure 4 Predicted Unionized Ammonia Concentrations Associated with the High Current Speed Scenario (~0.6 m/s)

Ammonia Plume Persistence

The plume area and approximate distance extents, along with the local volume averaged current speed, are provided in Table 2, for the channel current speed cases considered. Based on these parameters, the predicted persistence durations are estimated to be 117 and 20 minutes after the ESDV closes, for the typical and high current speed scenarios respectively. The estimated durations are consistent with consideration of the acute exposure guidelines to assess impacted regions.

Table 2	Parameters Affecting NH ₃ Concentration
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Deveryon	Units	Strait of Canso Current Speed Scenario		
Parameter		Typical (< 0.2 m/s)	High (~0.6 m/s)	
Plume Areal Extent (to 1.1 mg/L)	m²	7749.2	7751.3	
Approximate Width	m	60	60	
Length	m	129.15	129.19	
Volume Average Speed (local)	m/s	0.018	0.106	
Time	minutes	117	20	

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STANTEC CONSULTING LTD.

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