

A mathematical model of a plunging liquid ammonia jet into water, sensitivity analysis and the impact as a source term on airborne and waterborne dispersion model predictions

Sébastien Legrand(1), Gemma Tickle(2), Eirik Holm Fyhn(3), Simon Gant(4), Rory Hetherington(4), Olivier Gentilhomme(5), Ludovic Lepers(1), Thibault Penelon(5), Hans Skarsvag(3)

(1) Royal Belgian Institute of Natural Sciences (RBINS), Brussels, Belgium

(2) GT Science and Software Ltd, Chester, United Kingdom

(3) SINTEF, Trondheim, Norway

(4) HSE, Buxton, United Kingdom

(5) INERIS, Verneuil-en-Halatte, France

Abstract

Global maritime transport of ammonia is expected to grow significantly as the industry pursues net-zero carbon emission objectives. This growth is driven by ammonia's dual role: as an alternative maritime fuel and as a key carrier for hydrogen within the emerging hydrogen supply chain. To sustain this expansion, it is essential to demonstrate the safety of ammonia operations, particularly by assessing potential impacts on people and the environment in the unlikely event of accidental spillage at sea or in ports. Safety demonstrations typically rely on mathematical models that, while often validated against smaller-scale experiments or field trials, incorporate the necessary physics to scale up and predict large-scale scenarios associated with extreme loss-of-containment events.

A hose rupture during an ammonia bunkering operation is considered the most credible spillage scenario. These operations typically involve transferring refrigerated ammonia at rates ranging from 25 to 200 m³/hour. In the event of a rupture, the liquid ammonia would discharge as a high-velocity jet from a height typically between 4 and 10 meters above the waterline. During freefall, the jet may partially break up into droplets, increasing its surface area and accelerating heat transfer. By inertia, the remaining liquid stream will continue its plunge into the water column to a certain depth before dispersing. Upon contact with seawater, a significant fraction of the ammonia will undergo rapid flashing and boil-off due to its very low boiling point and high heat of solution, generating large volumes of cold, toxic vapor. The remaining ammonia will dissolve into the water, and because of its lower density, the aqueous ammonia solution will resurface, where part of the dissolved ammonia will continue to vaporize more slowly. This combination of jet breakup, immediate vapor cloud formation, and delayed evaporation poses serious hazards to personnel and the environment, emphasizing the

need for accurate modelling of jet dynamics, flashing phenomena, and atmospheric and marine dispersion under these extreme conditions.

This paper presents a modular chain of numerical models to simulate this complex hose rupture scenario. The chain begins with an integral model that simulates the dynamics and thermodynamics of the plunging refrigerated ammonia jet. This model builds on similar approaches for mixing in reversing fountain flows, extended to include the thermodynamics of ammonia-water mixing, where rapid flash boil-off is predicted based on vapor-liquid equilibrium and adiabatic mixing assumptions. The second link in the chain is a near-field Lagrangian transport model for dissolved ammonia, accounting for the thermodynamics of aqueous ammonia solutions and slow vaporization. The third link is the marine pollution model OSERIT, which simulates far-field drift and dilution of the aqueous ammonia solution in seawater. Finally, the plunging jet and near-field models provide source terms for atmospheric dispersion models, including the integral gas-dispersion models PHAST and DRIFT, as well as the CFD model OpenFOAM. These models form the fourth link of the modular chain.

A sensitivity analysis was conducted by varying the inputs of the plunging jet model to determine their impact on predictions. Based on these sensitivities, a subset of cases was selected as source-term inputs for near-field and far-field marine spill models and for the different atmospheric dispersion models. The results from these linked models provide theoretical insight into the potential variability of airborne and waterborne hazard extents.

The work presented in this paper forms part of the modelling package of the ARISE joint industry partnership, which focuses on large-scale ammonia releases at sea to enhance safety and response strategies associated with ammonia transport and bunkering operations in marine environments (<https://www.arise-partnership.org/>). Field-scale sea trials involving spills of refrigerated liquid ammonia are planned for 2026, with the prospect of these measurements providing much-needed data for model validation.