# Analyzing ammonia dispersion under varying atmospheric conditions using DRIFT

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### An introduction to HSE

- The Health and Safety Executive (HSE) is Britain's national regulator for workplace health and safety
  - Includes onshore/offshore pipelines, chemical/oil/gas infrastructure, offshore platforms etc.
  - Activities: evidence gathering, policy development,
     consultation, regulation, incident investigation, enforcement
  - HSE acts as an enabling regulator, supporting the introduction of new technologies
  - 2400 total staff (800 scientists and engineers)
  - Budget: 60% from Government, 40% from external income





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### HSE Science and Research Centre, Buxton

- 400 staff, 550-acre test site
- Scientific support to HSE and other Government departments
- "Shared research" or joint-industry projects co-funded by HSE
- Bespoke consultancy on a commercial basis
- HSE Annual Science Review 2024





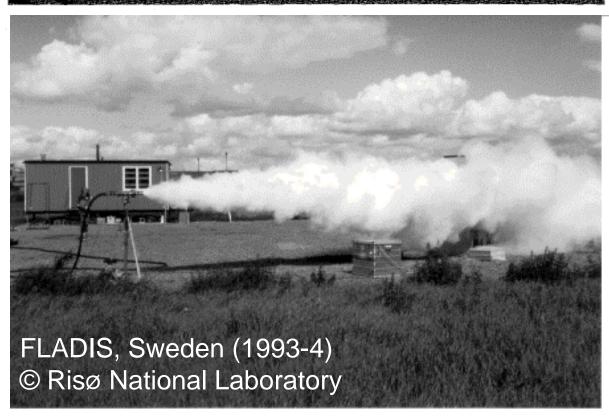
### Ammonia in the context of Net Zero

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- Easier to liquefy ammonia for bulk storage and transport than hydrogen
- Liquid ammonia has higher energy density than liquid hydrogen
- Hydrogen vector: ammonia cracked to hydrogen, with nitrogen released to air
- Ammonia currently produced/stored/shipped in large quantities
  - Existing technologies, standards, procedures available for ammonia (unlike hydrogen)
- Ammonia widely seen as best option for decarbonising shipping fuel
- Cheaper to import green hydrogen from the Middle East as ammonia than produce green hydrogen in the UK

- https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachm ent\_data/file/880826/HS420\_-\_Ecuity\_-\_Ammonia\_to\_Green\_Hydrogen.pdf
- https://www.ammoniaenergy.org/articles/ammonia-for-power-a-literature-review/

	Hydrogen	Ammonia
Boiling point	-253 °C	-33 °C
Energy density (cryo. liquid)	9 MJ/liter	16 MJ/liter





### **Ammonia Dispersion**

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- Release of pressure-liquefied ammonia results in a two-phase flashing jet
- Ambient air mixes into the cloud, resulting in some interesting behaviour:
  - Water vapor in the entrained air condenses as liquid water, releasing latent heat in the process
  - Liquid droplets comprising a mixture of water and ammonia form a non-ideal solution, releasing heat of mixing

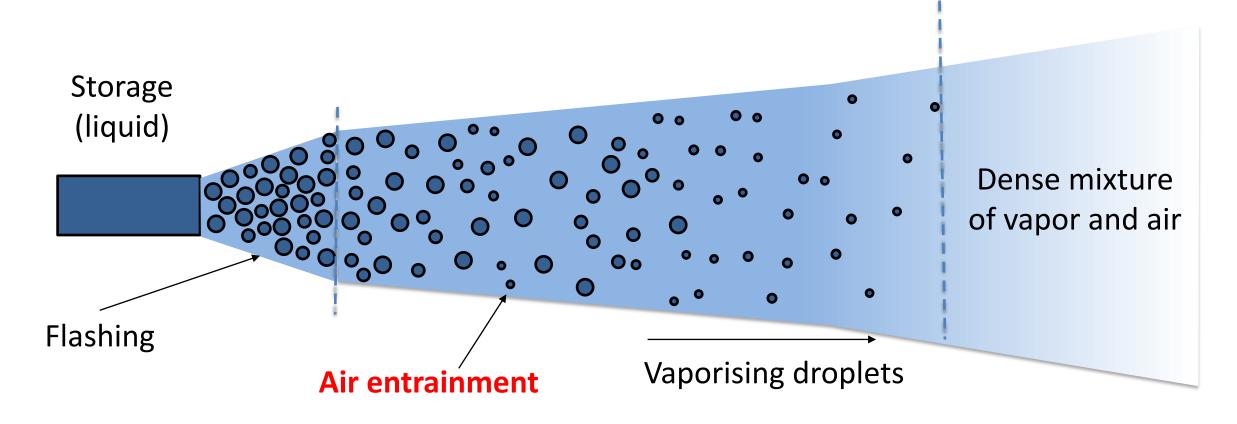


Figure: schematic of ammonia dispersion from a pressurized vessel

 The thermodynamic interactions of ammonia with water potentially make ammonia dispersion in a moist atmosphere sensitive to humidity and temperature

\*Recent experiments on both pressurized and refrigerated releases:

Dharmavaram, S., Carroll, M.J., Lutostansky, E.M., McCormack, D., Chester, A. and Allason, D., 2023. Red Squirrel Tests: Air Products' ammonia field experiments. *Process Safety Progress*, *42*(3), pp.481-498.

#### **Ammonia Incidents**

#### Beach Park, Illinois (2019)

- Release of anhydrous ammonia from a nurse tank configuration, in Beach Park, Illinois, USA. 25 April 2019<sup>1</sup>. Roughly 1.5 tons of ammonia released
- 83 people taken to hospital, 14 admitted, 8 in intensive care unit, no deaths
- Video of the dense cloud: IL ammonia spill 4-25-19 -YouTube



**Figure**: Aerial photo after the release. Approximate release location marked with a star

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#### Dakar, Senegal (1992)

- In 1992 at a peanut oil mill in Dakar Senegal, a road tanker ruptured, releasing approximately 22 tonnes of liquid ammonia
- A repaired weld failed due to overpressures
- The cloud engulfed neighboring offices and restaurants
- Over 1000 injured and 129 fatalities



*Figure*: part of the road tanker<sup>2</sup>. Diameter: ~7 feet.

- 1. https://www.chicagotribune.com/suburbs/lake-county-news-sun/ct-lns-ammonia-spill-no-charges-st-0626-20190625-ikztowsrhfhwhgym3lryjk4v2m-story.html
- 2. French Ministry of the Environment 2006. "Explosion of an ammonia tank, March 24, 1992, Dakar, Senegal". DPPR/SEI/BARPI ARIA No. 3485. https://ammonia.co.nz/wp-content/uploads/2021/10/Senegal1992-1.pdf. (accessed 19 March 2024).

### Methodology- Idealized Cases

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- In this study we simulate two different types of release:
  - Long-duration release, typical of a hole in a vessel
  - Instantaneous release from a catastrophic failure
- The long-duration release is based on conditions found in Desert Tortoise trial 1
- The two cases studied are somewhat idealized representations of what can happen during loss of containment. However, both release scenarios contribute knowledge to how a release of ammonia interacts with the environment, and how this affects downwind dispersion
- Atmospheric sensitivity parameters:
  - Temperature range: 0 to 30 °C
  - Relative humidity range: 0 to 80 %

Parameter	Unit	Long-duration	Instantaneous
Source type	-	Momentum jet	Catastrophic
Orifice diameter	m	0.081	-
	inch	3.19	-
Temperature	°C	21.5	-33.34
Release pressure	Pa	1.01E+06	101325
	psi	146.5	14.7
Release rate	kg/s	80	-
Release duration	S	10000	-
Inventory	tonne	-	20
Release location	m	(0, 0, 1)	(0, 0, 0)

**Table**: Geometry and source conditions for the two types of release

## Methodology- DRIFT Model



- Both release scenarios are modeled using DRIFT version 3.7.19
- DRIFT (Dispersion of Releases Involving Flammables or Toxics) is a gas dispersion model, originally developed by the UK Atomic Energy Authority (UKAEA), and subsequently maintained by ESR Technology, with the support of the UK Health and Safety Executive (HSE)
- DRIFT is used within HSE to model atmospheric dispersion of toxic and flammable substances for the purpose of providing public safety advice on hazardous substance consent applications and land-use planning
- Model evaluation of DRIFT has been undertaken for a variety of release scenarios<sup>1</sup>. A mathematical description of DRIFT is presented in Tickle and Carlisle (2008)<sup>2</sup>

- 1. Coldrick, S. and D. Webber, 2017: Evaluation of the DRIFT gas dispersion model version 3.6.4. HSE Research Report RR1100. https://www.hse.gov.uk/research/rrhtm/rr1100.htm (accessed 07 March 2024).
- 2. Tickle, G. and J. Carlisle, 2008: Extension of the dense gas dispersion model DRIFT to include buoyant lift-off and buoyant rise. HSE Research Report RR629. https://www.hse.gov.uk/research/rrhtm/rr629.htm. (accessed 07 March 2024).

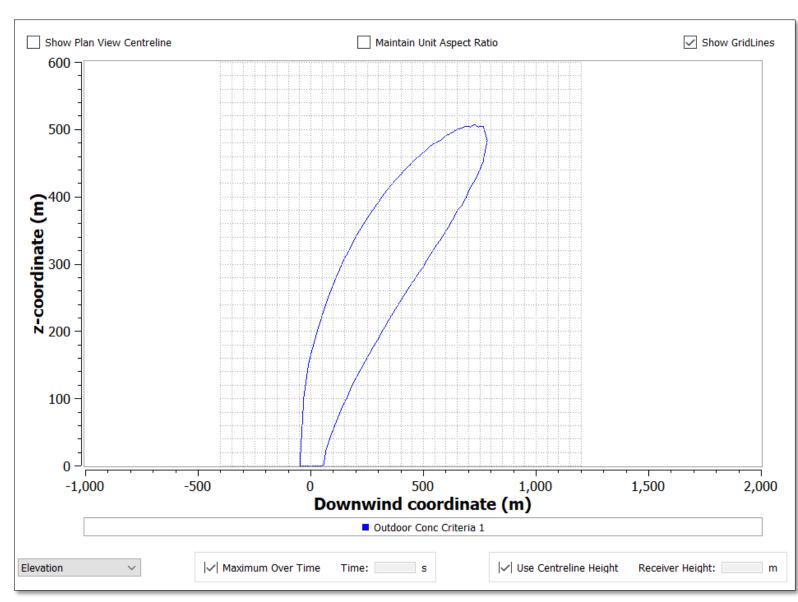


Figure: the DRIFT GUI displaying results

#### Results

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- Concentration is plotted as a function of downwind distance
- A select number of cases have been chosen to illustrate the difference between the two types of release
- The instantaneous release produces concentrations near the source that are nearly two orders of magnitude lower than the long-duration leak
  - This is due to the use of a long time-average (600 s) for a short duration release
- For the instantaneous case, lower ambient temperatures lead to higher concentrations in the region < 10 m. However, the opposite is true for > 10 m, where higher ambient temperatures produce higher concentrations

**Figure**: Concentration profiles at a height of 1 m averaged over 600 seconds. A black diamond marker represents the simulation results reported in Dharmavaram and Pattabathula<sup>1</sup>

<sup>10&</sup>lt;sup>5</sup>

(Ed)

10<sup>7</sup>

10<sup>8</sup>

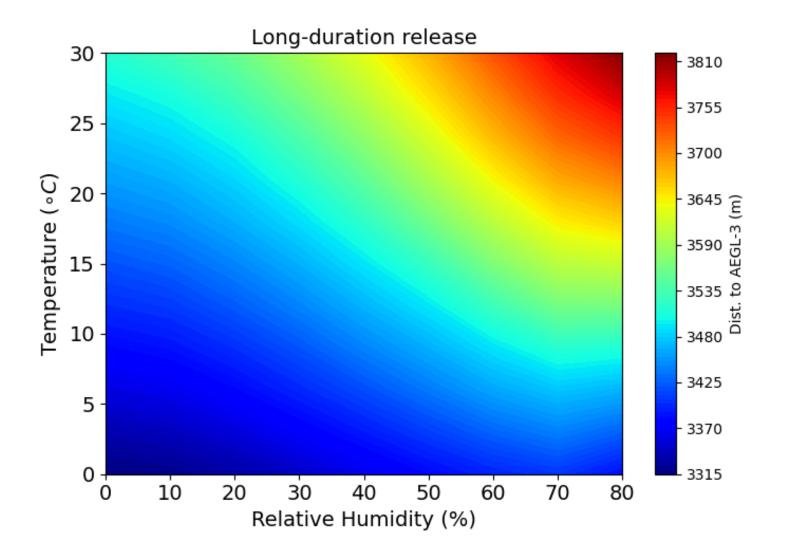
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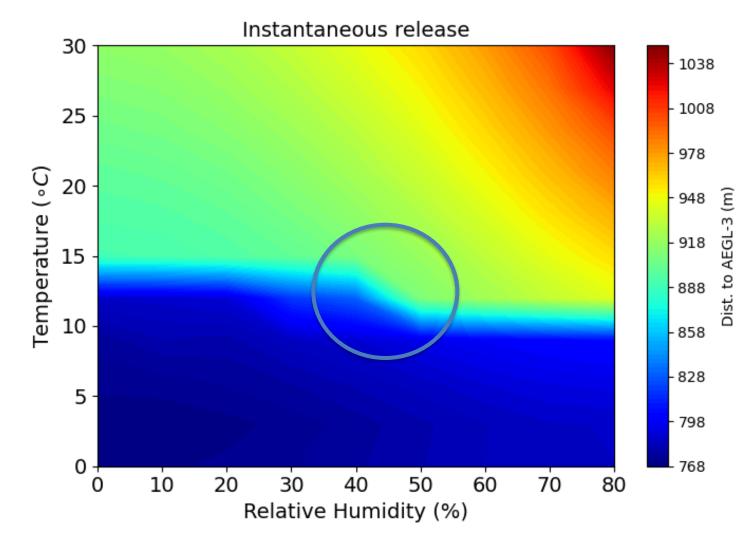
<sup>1.</sup> Dharmavaram, S. and Pattabathula, V., The Dakar Ammonia Accident: Analysis of the Worst Incident at an Anhydrous Ammonia User. https://www.uvu.edu/es/docs/paper4a© Crowndakar Haccident\_final.pdf. (accessed 19 March 2024).

#### Results

- The distance to AEGL-3 (2700 ppm) is plotted for a range of temperatures and relative humidities
- Increasing the temperature from 0 to 30 °C and the relative humidity from 0 to 80% leads to an increase in the distance to AEGL-3 of:
  - 15% for the long-duration release
  - 35% for the instantaneous release
- The ambient temperature and relative humidity have a greater effect on the instantaneous release, in relative terms
- In the long-duration case, the distance to AEGL-3 increases as both temperature and relative humidity increases. The distribution is smooth, unlike the contour produced for the instantaneous case where there is a sharp transition in the temperature range 10 to 15 °C

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**Figure**: Contours of distance to AEGL-3 for a long-duration release (top) and instantaneous release (bottom)

- 1.3

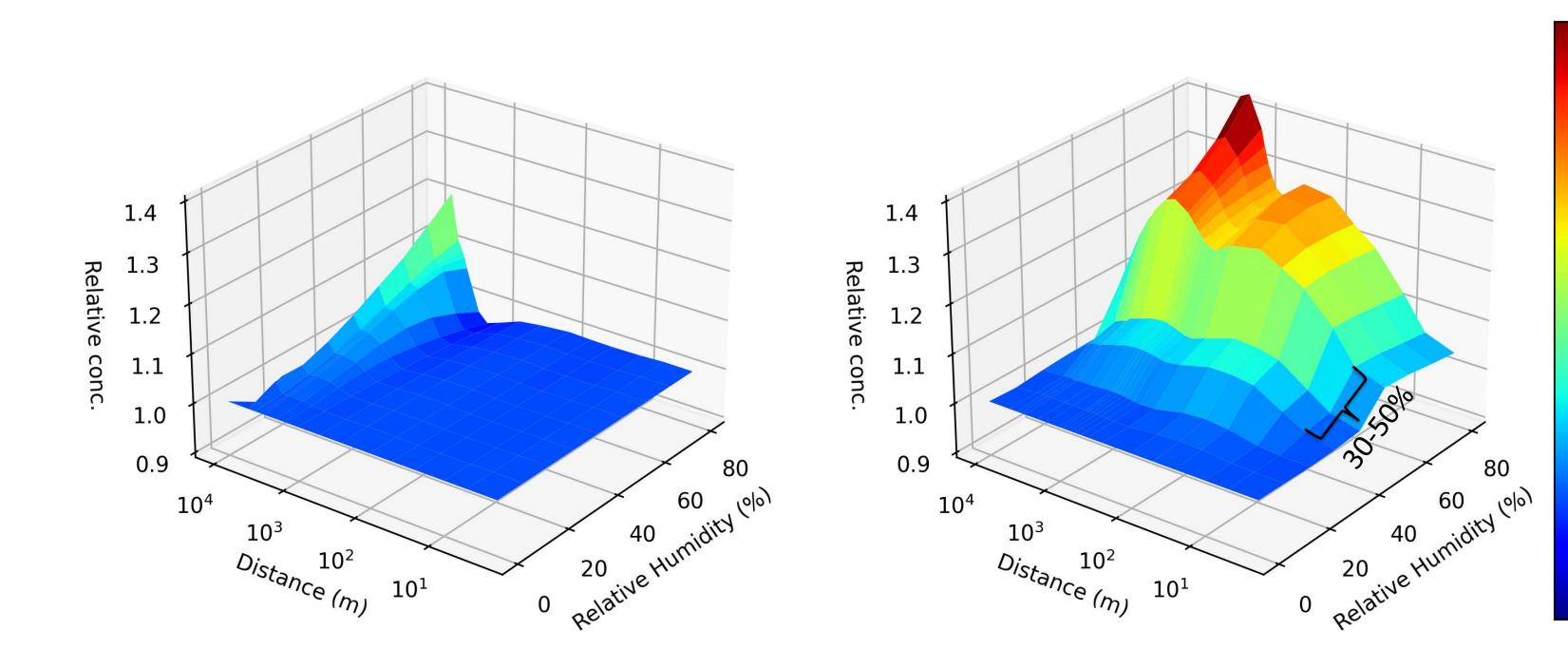
- 1.2

- 1.1

- 1.0

0.9

- To further explore this, we extract the data at ambient temperatures of 12 °C, and plot the relative concentration as a function of distance and relative humidity
- Concentrations are normalized by the 0% humidity case (relative concentration is equal to 1 at 0% RH)
- In the long-duration case, increasing humidity has little effect for < 1 km
- For the instantaneous release, an increase in the relative humidity has a more pronounced effect. In fact, there is a maximum increase in concentration of roughly 40%



**Figure**: Relative concentration profiles as a function of distance and relative humidity for the long-duration release (left), and instantaneous release (right).

### **Conclusions**



- Atmospheric conditions, such as ambient temperature and relative humidity can affect dispersion of toxic chemicals. This is true for ammonia which is hygroscopic and therefore has complex interactions with water vapor present in the atmosphere
- We have simulated ammonia dispersion for two types of release: (i) long-duration, typical of a leak from a hole in a vessel; (ii) instantaneous release, typical of a catastrophic release. These two cases are somewhat idealized representations of what can happen during loss of containment
- The integral model DRIFT has been utilized to predict ammonia dispersion and downwind concentrations for a range of temperatures (0 to 30 °C) and humidities (0 to 80%)
- The distance to AEGL-3 (2700 ppm) has been reported to assess the cloud size
- In general, increasing the temperature and humidity resulted in a greater distance to AEGL-3
- However, when considering a fixed temperature, the effect of varying humidity was dependent on distance from the source
- Concentrations in the far field (> 1 km) for the high humidity case at 12 °C were approximately 20% higher for the long-duration release, and 40% higher for the instantaneous release
- This study has shown that humidity and temperature have a modest effect on ammonia dispersion behavior. The effect is more pronounced for the case of an instantaneous release compared to a longduration release. In addition, the effect is dependent on downwind distance

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Thank you, any questions?

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