PROTECTING PEOPLE AND PLACES FOR 50 YEARS HSE

Recent Atmospheric Dispersion Modelling Research Activities at HSE

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29th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling, Fairfax, Virginia, 24-25 June 2025

Outline

- Jack Rabbit III
  - Status update on model inter-comparison exercise and journal paper
- DRIFT model evaluation protocol
- Summary of HSE's contributions to the MODISAFE (CBRN) project
- The Skylark CO_2 project
- Spills of ammonia onto water
  - ARISE and SafeAm projects
- Future HSE research topics
- Recent and future activities of the ADMLC

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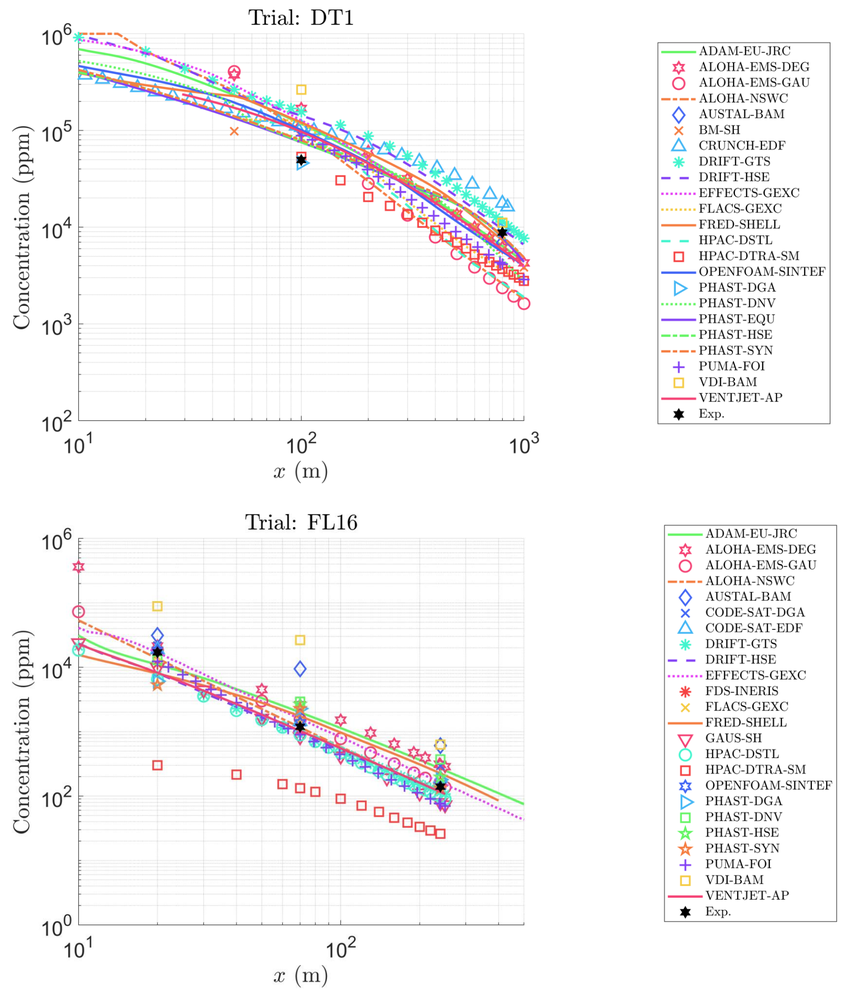
JRIII modelling exercise

- The Jack Rabbit III Modellers Working Group conducted a modelling exercise in 2021-24
- Undertaken to assess the performance of atmospheric dispersion models for simulating releases of pressure-liquefied ammonia
- 21 independent modelling teams participated in the exercise
- Approaches included: (i) empirically-based nomograms; (ii) integral; (iii) Gaussian puff; (iv) Lagrangian; (v) CFD models
- Draft journal paper due to be submitted to Atmospheric Environment X imminently



Arc-max concentration predictions for the Desert Tortoise DT1 trial (top), and FLADIS 16 trial (bottom)

JRIII modelling exercise

Atmospheric dispersion of pressure-liquefied ammonia: results from the Jack Rabbit III model inter-comparison exercise on Desert Tortoise and FLADIS

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[11] European Joint Research Centre (JRC), Ispra, Italy
[12] Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany
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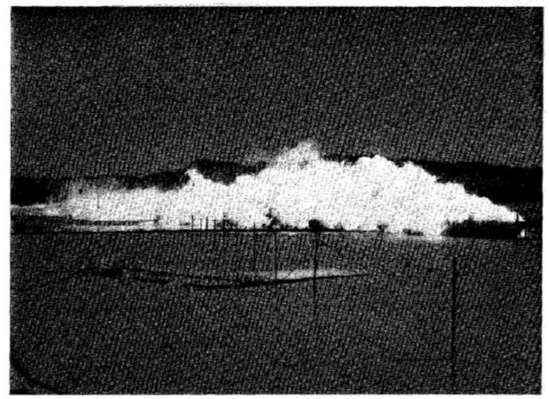
[18] Syngenta, Huddersfield, Yorkshire, UK
[19] Air Products, Allentown, Pennsylvania, USA
[20] Naval Surface Warfare Center Indian Head Division (NSWC IHD), Indian Head, Maryland, USA
[21] Direction Générale de l'Armement (DGA), Paris, France
[22] Shell, London, UK
[23] Equinor, Norway
[24] Emergency Management (EM) Solutions, USA
[25] SINTEF Energy Research, Trondheim, Norway

JRIII modelling exercise

#	Organisation	Model	Model Type				Desert Tortoise			FLADIS		
			A	B	C	D	1	2	4	9	16	24
1	Air Products, USA	Ventjet		■			■	■	■	■	■	■
2	BAM, Germany	AUSTAL			■		■	■	■	■	■	■
3		VDI	■				■	■	■	■	■	■
4	CEREA (EDF/Ecole des Ponts), France	Code-Saturne v7.0				■					■	
5		Crunch v3.1		■			■	■	■			
6	DGA, France	PHAST v8.6		■			■	■	■	■	■	■
7		Code-Saturne v6.0				■				■	■	■
8	DNV, UK	PHAST v8.61		■			■	■	■	■	■	■
9	DSTL, UK	HPAC v6.5			■		■	■	■	■	■	■
10	DTRA, ABQ, USA	HPAC v6.7			■		■	■	■	■	■	■
11	EM Solutions, Inc., USA	ALOHA v5.4.7 Gaussian	■				■	■	■	■	■	■
12		ALOHA v5.4.7 Integral		■			■	■	■	■	■	■
13	Equinor, Norway	PHAST v8.6		■			■	■	■			
14	FOI, Sweden	PUMA			■		■	■	■	■	■	■
15	Gexcon, Netherlands	EFFECTS v11.4		■			■	■	■	■	■	■
16	Gexcon, Norway	FLACS				■	■	■	■	■	■	■
17	GT Science & Software	DRIFT v3.7.19		■			■	■	■	■	■	■
18	Hanna Consultants, USA	Britter & McQuaid WB	■				■	■	■			
19		Gaussian plume model	■							■	■	■
20	HSE, UK	DRIFT v3.7.19		■			■	■	■	■	■	■
21		PHAST v8.4		■			■	■	■	■	■	■
22	INERIS, France	FDS v6.7				■				■	■	■
23	JRC, Italy	ADAM v3.0		■			■	■	■	■	■	■
24	NSWC, USA	RAILCAR-ALOHA	■				■	■	■	■	■	■
25	Shell, UK	FRED 2022		■			■	■	■	■	■	■
26	SINTEF, Norway	OpenFOAM v2206				■	■	■	■	■	■	■
27	Syngenta, UK	PHAST v8.61		■			■	■	■	■	■	■

Note: Model Type: A = Empirically-based nomograms/Gaussian plume model; B = Integral model; C = Gaussian puff/Lagrangian model; D = CFD. Shading in the right six columns indicates model was run for that trial. See Glossary for the full names of the organisations and models.



Desert Tortoise ammonia release, Nevada, USA, 1983

FLADIS ammonia release, Sweden, 1993-1994

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DRIFT Model Evaluation Protocol

- The gas dispersion model DRIFT 3 has been developed by ESR Technology for HSE (Tickle and Carlisle, 2015) and is used for both regulatory and research purposes
- Development of DRIFT 3 is ongoing and model enhancements include:
  - Inclusion of a pool re-evaporation option to add the concentration from a direct source to the concentration from an evaporating pool
  - Changes to the grounded jet model to suppress initial spreading, for better agreement with the wall jet data of Davis and Winarto (1980) https://doi.org/10.1017/S0022112080001607
  - Modifications to the transition from jet to wind-blown spreading and to the entrainment to better match the Desert Tortoise trials
  - Switch to using a fit to the Tillner-Roth and Friend (1998) correlation for the ammonia-water interaction coefficients https://doi.org/10.1063/1.556015
  - Modifications to the vapour deposition model to include new user inputs of surface resistance and a fixed vapour deposition velocity

Tickle, G. A., and Carlisle, J. E. (2015). *DRIFT Version 3.7.3: Mathematical Model Description*. ESR Technology Report ESR/UC000417/001/Issue 3. Available from https://esrtechnology.com/safety-risk/what-we-do/software/drift/hse-software-support-2022-2025/

DRIFT Model Evaluation Protocol

- Each new version of DRIFT must be thoroughly evaluated before being rolled out for use by HSE, to ensure it is fit for purpose
- Previous versions were evaluated using the Liquefied Natural Gas (LNG) Model Evaluation Protocol (MEP) for dense gas dispersion models (Ivings *et al*., 2016)
- A DRIFT Model Evaluation Protocol has now been developed, which has been designed to test the full range of DRIFT's capabilities
- The DRIFT MEP contains scientific assessment, verification, validation and a user-oriented assessment
- The scientific assessment has been broadened to cover additional topics, including
  - Buoyant lift-off and buoyant rise
  - Deposition
  - Re-evaporation
  - Chemical reactions with moist air

Additional datasets used from:

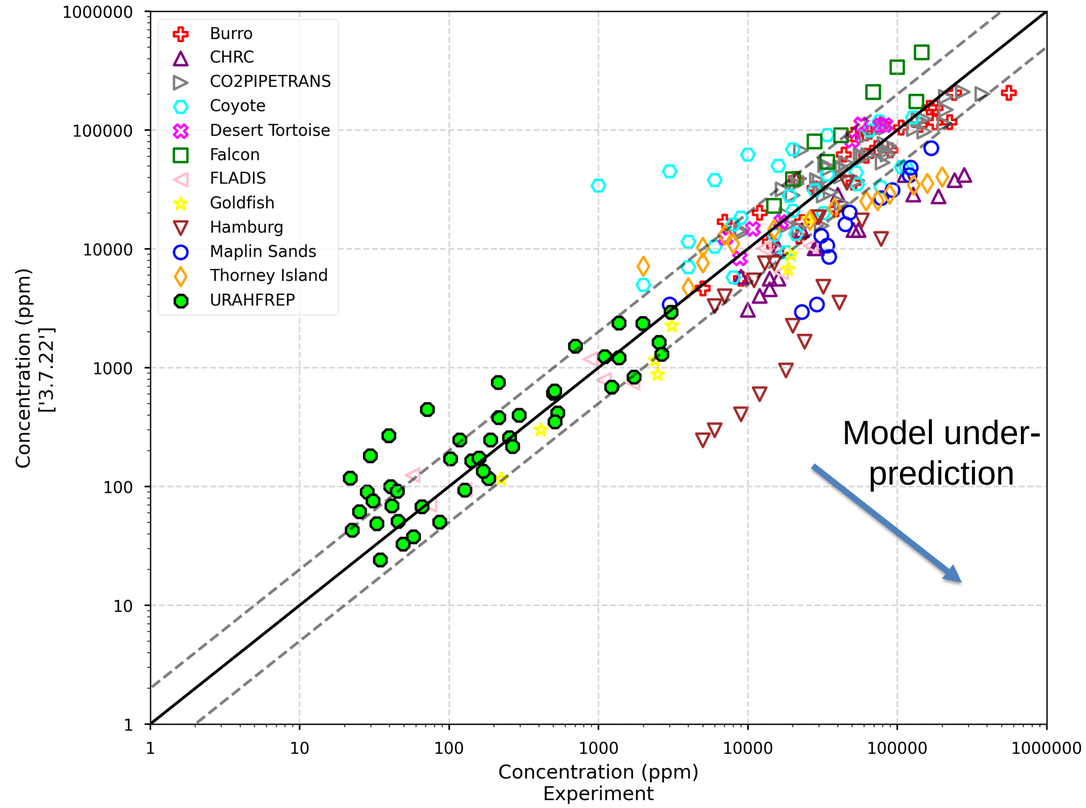
CO2PIPETRANS, CO_2	Goldfish, HF
Desert Tortoise, NH_3	Jack Rabbit II, Chlorine
FLADIS, NH_3	URAHFREP, HF

Ivings, M. J., Gant, S. E., Jagger, S. F., Lea, C. J., Stewart, J. R., and Webber, D. M. (2016). *Evaluating vapor dispersion models for safety analysis of LNG facilities.* Fire Protection Research Foundation Report FPRF-2016-25. Available from https://www.nfpa.org/education-and-research/research/fire-protection-research-foundation/projects-and-reports/lng-model-evaluation-protocol-and-validation-database-update

Performance of DRIFT 3.7.22 against experimental data

- Majority of data within a factor of 2 (see figure)
- Both datasets (peak and averaged) for the field scale experiments are within the acceptance criteria ($\mathrm{MG} \approx 1, \mathrm{VG} \approx 2$)
  - LNG MEP acceptance criteria:

    0.67 < MG < 1.5 ; VG < 3.3 ; FAC2 > 50%
- Wind tunnel concentration data from Hamburg and CHRC underpredicted by DRIFT
- Overall good agreement between DRIFT and experimental data for a range of releases and substances



Averaged concentration data scatter. Solid line indicates where predicted is equal to measured. Dashed lines indicate factor of 2 under- and overprediction.

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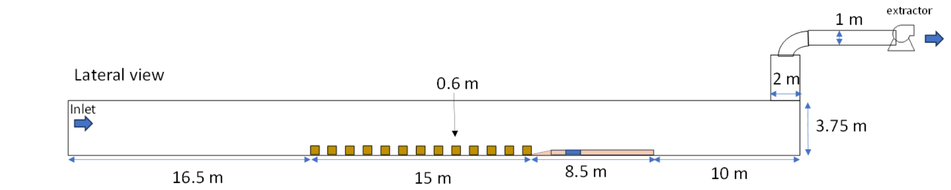
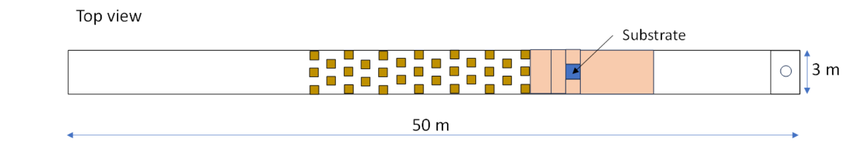
- MODISAFE is an international collaboration researching three topics relevant to atmospheric dispersion of hazardous substances:
  - Evaporation from porous and non-porous substrates
  - Deposition and resuspension
  - Buoyant dispersion in urban areas
- In each research area, new experimental data have been produced, which will be made publicly available (uploaded to the ADMLC website)
- The experimental data have enabled development of Computational Fluid Dynamics (CFD) models and provided a platform for model intercomparison exercises and model validation
- There will be a special session on the MODISAFE project at the HARMO conference in Hamburg, Germany on 15-19 September 2025 www.harmo.org

MODISAFE: Evaporation

Experiments

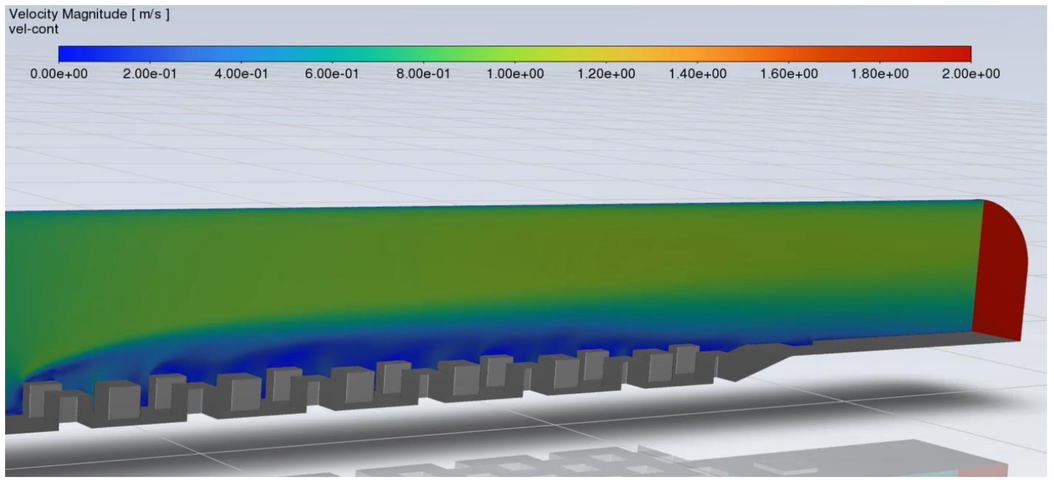
- 30 tests investigating pool evaporation and droplet evaporation on impermeable and permeable substrates in the INERIS fire tunnel
- Varying the substance, substrate, wind speed, pool depth





Modelling

- Integral modelling of pool evaporation using GASP and SLOPS
- CFD modelling to understand fire tunnel flow field
- Inter-model comparison exercise with MODISAFE partners' own codes



MODISAFE: Deposition

- Deposition boundary condition developed in Fluent CFD
- Deposition is handled by experimentally-derived parameters k_s (which controls the flux), and $M_{\max}$ (which determines saturation)
- See the Spicer *et al*. (2021) paper for details of the experiments

Sample	k_s (m/s)	$M_{\max}$ (kg/m²)
Clover	0.0001	0.0002
Rye Grass	0.00008	0.00008
Soil (4% moisture)	0.006	0.003
Soil (12% moisture)	0.004	0.004
Soil (20% moisture)	0.003	0.0015

Initialise

Step 0a: Identify cells neighbouring boundary patch

Step 0b: Set $a_s = 1$ (saturation parameter)

Step 1: Calculate flux into ground

$$f_s = C\ k_s\ a_s$$

Step 2: Accumulate mass (and store)

$$M_s \rightarrow M_s + f_s\ \delta t$$

Step 3: Contaminant sink calculation

Loop **Step 1**

Spicer T.O., Fox S.B., Hicks B.B. (2021) "Preliminary assessment of chlorine reactivity with environmental materials accounting for boundary layer and maximum deposition effects". *Atmospheric Environment* 256, 118274. https://doi.org/10.1016/j.atmosenv.2021.118274.

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Skylark

- Kick-off on 13 May 2025, 3-year duration
  1. CO_2 pipeline craters and source terms – DNV
  2. Wind-tunnel experiments – University of Arkansas
  3. Simple terrain dispersion experiments – DNV
  4. Complex terrain dispersion experiments – DNV
  5. Model validation – HSE
  6. Emergency response – NCEC
  7. Venting – DNV

https://www.dnv.com/article/skylark-pioneering-excellence-in-co2-pipeline-safety-250648/

Source of images: Allason D., Armstrong K., Barnett J., Cleaver P. and Halford A. “Behaviour of releases of carbon dioxide from pipelines and vents”, Paper IPC2014-33384, Proc. 10th International Pipeline Conference IPC2014, Calgary, Alberta, 29 September – 3 October 2014, © Copyright National Grid / DNV / ASME

http://dx.doi.org/10.1016/j.ijggc.2015.04.001

University of Leeds

Proposed PhD project

Accelerated Fluid Dynamics of CO2 dense gas dispersion in complex terrain

Academic lead: Dr Amirul Khan, School of Civil Engineering, a.khan@leeds.ac.uk
Industrial lead: Dr Simon Gant, Health and Safety Executive (HSE), simon.gant@hse.gov.uk
Co-supervisor(s):
Dr Andrew Ross, School of Earth and Environment, A.N.Ross@leeds.ac.uk, Dr Rory Hetherington, Health and Safety Executive (HSE), rory.hetherington@hse.gov.uk (External)
Project themes:
Clean Energy, Computational & Analytical Tools, Data-driven methods, Multiphysics & Complex Fluids

Carbon Capture and Storage (CCS) is recognised as a crucial element in reaching the target of Net Zero. To support this, an infrastructure of pipelines are required to transport liquid CO2. However, safe operation of pipelines relies on accurately predicting the consequences of a leak or rupture (e.g. 2020 Satartia pipeline release in Mississippi). Key factors in modelling pipeline releases, especially when a risk assessment is undertaken along the full length, include (i) the computational cost of a model and (ii) its capacity to account for complex terrain.

https://fluid-dynamics.leeds.ac.uk/projects/accelerated-fluid-dynamics-of-co2-dense-gas-dispersion-in-complex-terrain/

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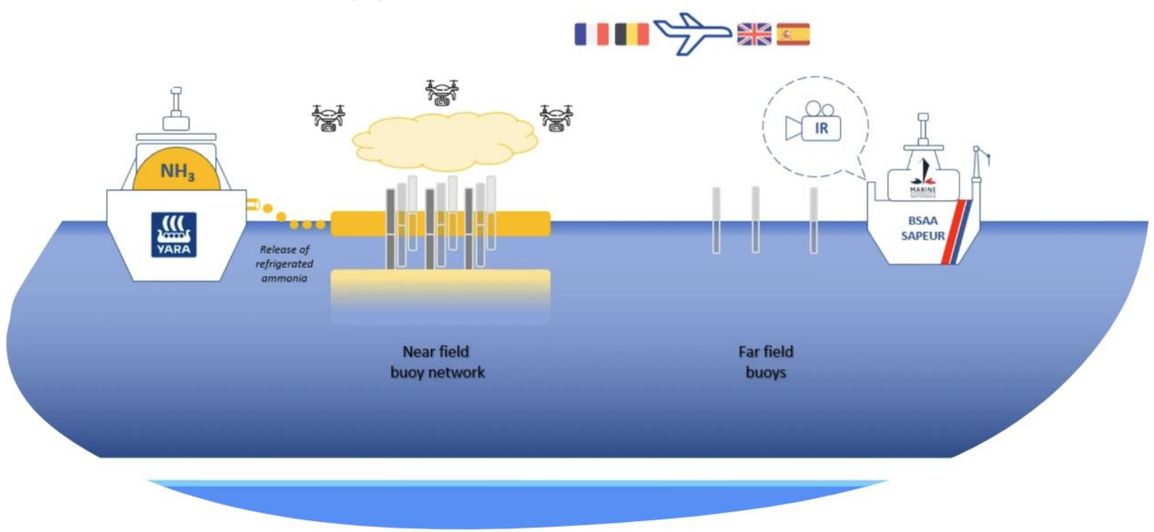
Ammonia spills onto water: ARISE

- HSE is partner in the ARISE Joint Industry Project led by INERIS, CEDRE and Yara Clean Ammonia
- Aims:
  - Conduct multi-tonne spills of ammonia at sea
  - Improve understanding of dispersion in water and air
  - Provide dataset for validation of models
  - Develop methodology for risk assessment for marine applications
- Experiments planned for Sept 2025
- Contacts: Laurent.Ruhlmann@yara.com
  Olivier.Salvi@ineris-developpement.com

ARISE
Ammonia Response In Sea Emergencies

www.arise-partnership.org

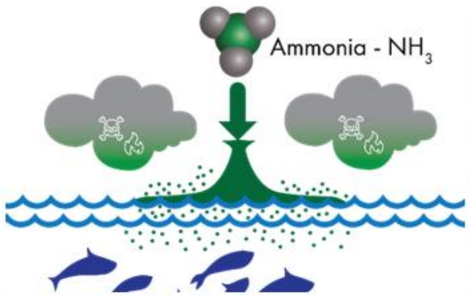


INERIS Cedre YARA Yara Clean Ammonia ONERA museum HSE INERIS Développement IMT Mines Alès SINTEF

Ammonia spills on water: SafeAm

SafeAm

Increased Safety of Ammonia Handling for Maritime Operations



Consortium of 21 partners led by SINTEF

LOWEMISSION, Sjøfartsdirektoratet Norwegian Maritime Authority, Havtil, HSE Health & Safety Executive, KYSTVERKET, DNV, TotalEnergies, WÄRTSILÄ, amon MARITIME, YARA, NTNU, USN University of South-Eastern Norway, equinor, ConocoPhillips

BACKGROUND

- Ammonia (NH_3) is deemed by many as a promising energy carrier to reduce carbon dioxide (CO_2) emissions from transport and a viable solution for global H_2 transport
- Although NH_3 has been safely transported as a chemical in dedicated carriers for decades, the potential large-scale implementation and handling by different users, introduces emerging risks and a potential need for stricter requirements

OBJECTIVE Accelerate the implementation of new value chains for NH_3 as a zero-emission fuel and energy carrier by improving safety systems design and procedures for handling of LNH_3 spills on and into water.

APPROACH AND EXPECTED OUTCOMES

- Experiments on NH_3 spills on and into water (evaporation, dissolution, mixing dynamics)
- Thermophysical modelling of NH_3_water interface, Rapid Phase Transition model, partition ratio model (PIRATE)
- Safety and environmental risk analysis (trade-offs, case studies, input to standards and regulations)

Total budget ca. 18 MNOK
For info: marta.bucelli@sintef.no (project manager)

https://www.sintef.no/en/projects/2023/safeam__increased_safety_of_ammonia_handling_for_maritime_operations

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Potential future HSE dispersion-related research topics

- Understanding hydrogen flammability ranges: ignition and flame propagation
- Buoyancy-induced ventilation in enclosures produced by a hydrogen cloud
- Develop and validate source models for bulk catastrophic storage tank failure of:
  - Liquid hydrogen (recent Air Products experiments at Baker Risk)
  - Refrigerated liquid CO_2 (experiments needed?)
- Dispersion of CO_2 from vents in capture plants, pipelines and offshore installations
  - Vent CO_2 from the underside of offshore platforms rather than from the flare stack?
  - Potential impact of CO_2 on floating support vessels and lifeboats?
- Subsea CO_2 releases
  - Develop and validate models for dispersing waterborne plume of CO_2, absorption into seawater and characteristics of the airborne source of CO_2
  - Large-scale subsea CO_2 release experiments planned in connection with Northern Lights dewatering campaign in 2025 (SINTEF DACOLSS-CO2-NL project)
  - Possible DNV SubCO2 Phase 3 project: subsea CO_2 release experiments in Scotland

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Recent and future activities of the ADMLC

- Atmospheric Dispersion Modelling Liaison Committee www.admlc.com
- One-day conferences:
  - Investigating the impact of applying different grid resolutions of NWP data in atmospheric dispersion modelling, UKHSA, Harwell, UK, 18 Oct 2024
  - Atmospheric dispersion modelling of wildfire smoke, Met Office, Exeter, UK, 13 Feb 2025
  - Future event planned: machine learning applications in dispersion modelling
- ADMLC funded research projects:
  - Review of model evaluation procedures (CERC and Hanna Consultants)
  - Benchmarking nitrogen deposition models (CERC participation in RIVM-led study)
  - Future project planned: impact of climate change on dispersion model predictions used for regulatory impact assessments

Thank you

Any questions?

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