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DRIFT MODELLING OF THE DESERT TORTOISE AND FLADIS AMMONIA TRIALS FOR THE JACK RABBIT III MODEL INTER-COMPARISON EXERCISE

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Abstract:
As part of the Jack Rabbit III (JRIII) project, a Modelers Working Group (MWG) has been coordinating an international model inter-comparison exercise using data from six pressure-liquefied ammonia release experiments from the Desert Tortoise (1983) and FLADIS (1993-4) trials. The aim of the collaborative modelling exercise has been to understand the capabilities and limitations of models that could be used to design the new JRIII trials (e.g., to design suitable sensor placement). This paper focuses on DRIFT integral model results that have been produced for the exercise. The coordinators of the modelling exercise provided participants with baseline input parameters, plus suggestions of possible sensitivity tests based on analysis of uncertainties in the Desert Tortoise and FLADIS trials. These included ranges of values for the rainout fraction, wind speed, Monin-Obukhov length, and relative humidity. To investigate the impact of these uncertainties, HSE used a Gaussian process emulator to perform a global sensitivity analysis on DRIFT. Results are presented here to show how the variable model inputs affect the predicted concentrations at different downwind distances in the dispersing plume. The baseline set of DRIFT predictions are shown to be in good agreement with the experimental data, with over half of the centreline concentrations within a factor of two of the measurements. One trial from the Desert Tortoise experimental programme was selected for sensitivity analysis. Sensitivity analysis shows that the predicted concentrations are strongly affected by the wind speed and atmospheric stability. The rainout fraction has a modest effect and its importance gradually diminishes with distance downwind. Relative humidity is shown to have very little influence, despite the fact that DRIFT takes into account reactions between ammonia and atmospheric water vapour. The exercise provides insight into the predictive capabilities of DRIFT for simulating pressure-liquefied ammonia releases.

Key words: *Jack Rabbit III, dispersion modelling, Gaussian process emulator, sensitivity analysis, ammonia***.**

INTRODUCTION

As part of the Jack Rabbit III (JRIII) project, a Modelers Working Group (MWG) have been coordinating an international model inter-comparison exercise using data from six previous pressure-liquefied ammonia release experiments. These six experiments were taken from the Desert Tortoise (1983) and FLADIS (1993-4) trials (Goldwire *et al*., 1985; Nielsen *et al*., 1994). Coordinators of the modelling exercise provided participants with a set of baseline input parameters for the six trials. Also included were suggestions of sensitivity tests that could be investigated, based on analysis of uncertainties in the experiments. These included ranges of values for four model inputs: liquid rainout, wind speed, Monin-Obukhov length, and relative humidity. The aim of the exercise was to assess the performance of dispersion models and to investigate their sensitivity to variability in certain model input parameters.

This paper focuses on the DRIFT integral model results that have been produced for the exercise. In addition to simulating the base case for validation against experimental results, a total of 150 other simulations were run to construct a Gaussian process emulator and perform a global sensitivity analysis. Instead of varying one parameter at a time and fixing all other model inputs, each of these 150 simulations varied all four input parameters simultaneously. The emulator was then used to identify model inputs that had a significant influence on the downwind dispersion behaviour. Results are presented here to show how the variable model inputs influenced the predicted concentrations at different downwind distances in the dispersing plume.

METHODOLOGY

Desert Tortoise and FLADIS

Table 1 presents conditions for the selected Desert Tortoise and FLADIS trials, which were mostly taken from the SMEDIS database (Carissimo *et al*., 2001). The table here only includes inputs required by DRIFT, but MWG participants were provided with more information as some dispersion models require different inputs. All six trials involved horizontal releases of pressure-liquefied ammonia, and for the purpose of this study 100% liquid has been assumed at the exit nozzle which is consistent with the normal assumption for a padded release, but does not account for flashing that may have been induced by pressure losses, e.g. due to the presence of a knee-bend immediately upstream of the exit orifice in Desert Tortoise. There was a considerable difference in the amount of ammonia released between Desert Tortoise and FLADIS, with the former trials involving release rates of 80 to 117 kg s^{-1}, whilst FLADIS involved release rates of only 0.3 to 0.5 kg s^{-1}. The atmospheric weather conditions were also quite different. The Desert Tortoise trials were conducted in the Nevada desert on a lake bed, which was normally dry, although rain on previous days meant that surface water was present in trials DT1 and DT2. The FLADIS trials were conducted in Sweden, close to the Öresund strait, at a test site with some vegetation (10 - 30 cm high grass). The influence of test site location is evident in Table 1; the FLADIS trials had a larger aerodynamic surface roughness and increased humidity. Additionally, buildings upwind of the FLADIS release were reported to contribute to the atmospheric turbulence. There was no rain-out of liquid ammonia in the FLADIS tests, compared to 5% estimated rainout in the Desert Tortoise trials.

Table 1 Model input conditions for the Desert Tortoise and FLADIS trials.

	DT1	**DT2**	**DT4**	**FL09**	**FL16**	**FL24**
Orifice diameter (m)	0.081	0.0945	0.0945	0.0063	0.004	0.0063
Release height (m)	0.79	0.79	0.79	1.5	1.5	1.5
Exit temperature (K)	294.65	293.25	297.25	286.85	290.25	282.6
Exit pressure (bara)	10.1	11.2	11.8	6.93	7.98	5.70
Release rate (kg s^{-1})	80.0	117.0	108.0	0.40	0.27	0.46
Release duration (s)	126	255	381	900	1200	600
Rainout mass fraction (%)	5	5	5	0	0	0
Wind speed (m s^{-1})	7.42	5.76	4.51	6.1	4.4	4.9
at reference height (m)	2	2	2	10	10	10
Friction velocity (m s^{-1})	0.442	0.339	0.286	0.44	0.41	0.405
Surface roughness (m)	0.003	0.003	0.003	0.04	0.04	0.04
Monin-Obukhov length (m)	92.7	94.7	45.2	348	138	-77
Ambient temperature (K)	301.95	303.55	305.55	288.65	289.65	290.65
at reference height (m)	0.82	0.82	0.82	1.5	1.5	1.5
Ambient pressure (bara)	0.909	0.909	0.903	1.02	1.02	1.013
Relative humidity (%)	13.2	17.5	21.3	86	62	53.6
Averaging time (s)	80	160	300	600	600	400

DRIFT

The Desert Tortoise and FLADIS experiments were modelled 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 (Cruse *et al*. 2016, Coldrick and Webber, 2017). A mathematical description of DRIFT can be found in the report by Tickle and Carlisle (2008). DRIFT was also used previously to model the Jack Rabbit II chlorine trials (Gant *et al*., 2021).

The Desert Tortoise and FLADIS ammonia jet releases were modelled using the two-phase jet model in DRIFT. The model accounts for condensation of water vapour from the air in the cold jet, reactions between ammonia and water, and evaporation of aerosol droplets that contain a fraction of liquid water and ammonia. The baseline set of simulations used a rainout fraction of 5% for Desert Tortoise, and 0% for FLADIS. Rainout was modelled as deposition of liquid ammonia onto the ground at the source, with the deposited ammonia effectively removed from the simulation (i.e., pool evaporation was not modelled). Atmospheric conditions in DRIFT were specified using the inverse Monin-Obukhov length, friction velocity, and roughness length.

Validation against experimental results

Figure 1 shows the predicted plume centreline (arc-max) concentrations and cloud widths from the six trials against experimental data. Overall, DRIFT was in good agreement with the data, with more than half of the predicted concentrations within a factor of two of the measured values. There was a slight over-prediction in concentration for all three DT trials at the first sensor arc at 100 m but closer agreement to the experimental data at the second sensor arc at 800 m. DRIFT slightly under-predicted concentrations in the FLADIS trials 16 and 24 near the orifice at 20 m and slightly over-predicted them in the far-field at 240 m in the FL09 trial. Predicted cloud widths were in good agreement with the experimental data. The cloud width was taken here to be the distance from the centreline to the point at which concentration dropped to $C_{cl}/\sqrt{e}$, where C_{cl} is the centreline concentration. The results confirmed that DRIFT is capable of modelling horizontal two-phase ammonia jet releases at different scales.

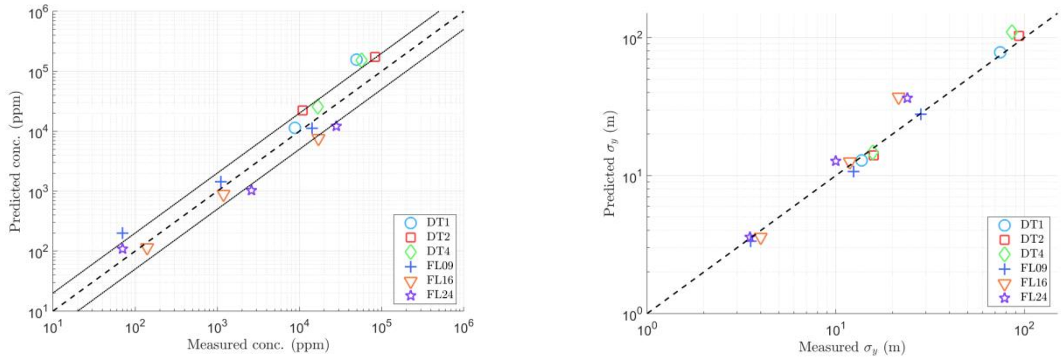

Figure 1 Left: predicted versus measured arc-max concentration for six Desert Tortoise and FLADIS trials. A dashed line indicates where predicted (DRIFT) and measured (experiment) concentration are equal. A solid line above and below indicates the range where measured concentration is a factor of 1/2 and 2 of predicted concentration, respectively. Right: predicted versus measured cloud width σ_y.

SENSITIVITY ANALYSIS OF DT1

DT1 was selected for further analysis, due to the potential similarities between this trial and future JRIII ammonia releases. Four model input parameters were selected for sensitivity analysis: rainout mass fraction, site average wind speed, Monin-Obukhov length, and relative humidity. There were uncertainties associated with these four model inputs in the DT1 trial, due to measurement issues, changing meteorological conditions and the presence of standing water on the test site. Table 2 presents the sensitivity parameters used in the current study. There were different estimates in the literature for the rain-out fraction, which varied between 5% and 36% of the total mass of ammonia released. For the purposes of this study, the baseline value was set at 5% and a range of 0% to 40% was used in the sensitivity analysis. Due to uncertainties arising from the presence of standing water, the relative humidity was varied from 5% to 60% and the atmospheric stability was varied from neutral to slightly unstable conditions, as indicated by the inverse Monin-Obukhov length varying between 0.01 m^{-1} and -0.07 m^{-1}. The measured wind speed of 7.4 m s^{-1} in the DT1 trial was high compared to wind speeds commonly used in regulatory risk assessments (and observed in previous field trials such as Jack Rabbit II). A wide range for one model input can cause it to dominate the results of a sensitivity analysis. Due to these considerations, a range of lower wind speeds between 2 to 6 m s^{-1} were used in the sensitivity analysis. A maximin Latin Hypercube design was used to generate a uniform distribution of parameter values between the minimum and maximum values.

A total of 150 DRIFT simulations were run for DT1 and centreline concentrations were output in the downwind direction at a fixed height of 1 m. Figure 2 plots the predicted concentrations from all 150 DRIFT runs, in addition to the baseline results and experimental data. The spread in predicted concentrations generally increased with distance downwind. At 100 m, all of the predicted concentrations were higher than the measurements (by approximately a factor of 1.5 to 2.5). Further downwind at 800 m, the baseline concentration was in close agreement with the measured concentration, and the 150 runs gave concentrations that spanned roughly half an order-of-magnitude above and below the baseline value. The marked increase in spread of predicted concentrations at a distance of around 50 m coincided with the point where the cloud centreline reached ground level, and the cloud transitioned from a free-jet into a wall-jet, with the cloud spreading along the ground.

Table 2 Model input parameters and assumed range.

Parameter	Min	Max	Base Case
Rainout mass fraction (%)	0	40	5
Site average wind speed (m s^{-1})	2	6	7.4
Inverse M-O length[a], $1/L_a$ (m^{-1})	-0.07	0.01	0.011
Relative humidity (%)	5	60	13.2

[a] The inverse length was used instead of the Monin-Obukhov length L_a to avoid singularities under neutral stability conditions when $1/L_a = 0$.

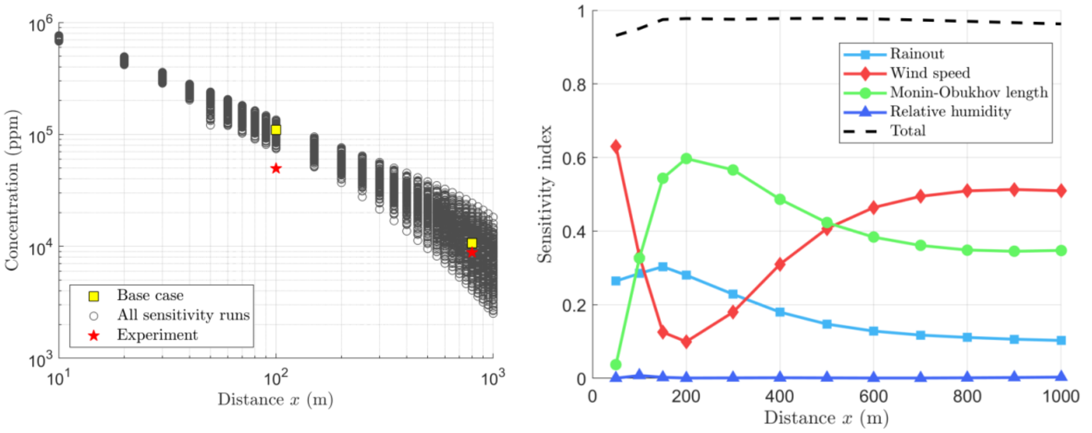

Figure 2 Left: Centreline concentrations at 1 m height for DT1 from DRIFT baseline case and 150 DRIFT sensitivity tests and experimental data. Right: Sensitivity index (i.e., main effect) from GEM analysis of DRIFT runs.

Gaussian Emulation Machine (GEM)

Statistical analysis of DRIFT results was undertaken using the Gaussian Emulation Machine (GEM), v1.1 (Kennedy, 2022). GEM determines which model inputs affected the selected output in terms of the sensitivity index (main effect), i.e., the fraction of total output variance that was due to varying that input. GEM also outputs the total effect for each input, which includes all the interactions between that parameter and other inputs. However, interactions between the four model inputs were found to be negligible (as indicated by the Total line in Figure 2) and they are therefore not discussed further here. The sensitivity index for each variable is plotted as a function of downwind position in Figure 2 (right-hand side). Sensitivity indices are normalised with the total variance and the left-hand plot shows that this total variance increased with distance downwind. It is clear from the right-hand graph that varying the relative humidity between 5% and 60% RH had little influence on the predicted centreline concentrations, compared to varying the other model input parameters. The effect of varying the rainout fraction, wind speed, and Monin-Obukhov changed rapidly within the first 200 m from the source. Overall, the two main dominant inputs were the wind speed and atmospheric stability. The rainout fraction had a more modest effect, and its importance gradually diminished with distance downwind. Figure 2 demonstrates the usefulness of assessing model sensitivity at various downwind distances.

CONCLUSIONS

The DRIFT integral model was used to simulate six trials from the Desert Tortoise (1983) and FLADIS (1993-1994) ammonia field experiments. Good agreement was obtained between predicted centreline concentrations and measured values, with more than half of the DRIFT predicted centreline concentrations within a factor of two of the measurements. A sensitivity analysis was also undertaken on the Desert Tortoise trial DT1, which is expected to be of similar scale and conditions to future JRIII trials. A Gaussian process emulator has been fitted to 150 DRIFT simulations. Four model input parameters were varied and their effect on the predicted centreline concentration was investigated. The range of predicted plume centreline concentrations from the 150 DRIFT runs at the first sensor arc at 100 m were all higher than the experimental measurement. On the second sensor arc at 800 m, the 150 DRIFT runs spanned roughly half an order-of-magnitude above and below the measured centreline concentration. The relative importance of model inputs, such as the wind speed, was shown to vary significantly as a function of downwind position. Unsurprisingly, the two main dominant input parameters were the wind speed and atmospheric stability. The rainout fraction had a modest effect. Varying the relative humidity between 5% and 60% RH had very little influence on the predicted centreline concentrations. The exercise was useful in understanding the predictive capabilities of DRIFT and its sensitivity to four uncertain input parameters. This information will be useful when DRIFT is used to help setup the future JRIII ammonia trials, e.g., to help position sensor arrays.

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