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PHAST 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, an international model inter-comparison exercise has been conducted where a number of dispersion modelling groups have simulated the Desert Tortoise and FLADIS ammonia trials. The objective of this work has been to understand the strengths and weaknesses of models that may be used to design the forthcoming JRIII ammonia experiments. This paper presents the dispersion modelling undertaken by four organisations: the UK's Health and Safety Executive (HSE), DNV, Syngenta and DGA Maîtrise NRBC (DGA), who all used the DNV Phast dispersion model. Although HSE do not use Phast for regulatory purposes, the organisation recognises that Phast and other integral models are widely used by industry and that it is good practice to keep abreast of current science and to participate in exercises such as this. The initial results produced by each group were based on the same experimental input data, but the methods used to derive the dispersion results were all developed independently. The results show that, overall, the predictions were in good agreement with measured concentrations in the Desert Tortoise trials and were in mixed agreement when compared to the FLADIS trial data. Results from the different organisations were within a factor of two of each other for the Desert Tortoise trials and a factor of four for all the FLADIS trials. The main cause of discrepancy in the results for the FLADIS trials was the specification of exit pressures and temperatures that resulted in vapour source conditions being used in some Phast runs and saturated liquid source conditions in others. Suggestions are given on the modelling approach that should be used when using Phast to simulate the future JRIII pressure-liquefied ammonia release trials.

Keywords: *Jack Rabbit III, Desert Tortoise, FLADIS, ammonia, dispersion modelling, Phast*

INTRODUCTION

Part of the strategy for reducing the effects from climate change is based on a shift from fossil fuels towards renewable energy and alternative energy sources. Recently, the focus has been on hydrogen-based infrastructure but the use of green (zero-carbon) ammonia can also contribute towards meeting climate targets. The adoption of ammonia as a clean fuel subsequently means that more ammonia will be present throughout the distribution network and that accidents may become more frequent. Understanding the ways in which ammonia infrastructure can fail and the corresponding consequences is important to ensure safe usage.

An effective way of understanding the consequences (and associated risks) with chemical storage and transport is through experiment. A series of large-scale experiments involving the release of anhydrous ammonia are currently being planned, known as the Jack Rabbit III (JRIII) trials. An international modelling comparison exercise has been completed prior to the experiments taking place. The aim of this exercise was to identify any modelling knowledge gaps and to understand the effect of using different approaches for modelling releases of ammonia. Previous experiments were used as a benchmark; source term data for three Desert Tortoise (DT) (Goldwire *et al*., 1985) and three FLADIS (FL) (Nielsen and Ott, 1996) trials were supplied to ensure that each organisation began their analysis with the same input data for their model of choice. This way, any differences in the results would reflect the characteristics of the type of model used, the method employed and the assumptions that were applied. Another aim of this work was to determine the most appropriate method for modelling ammonia releases. Any new knowledge gained from this exercise will inform the setup of the future JRIII experimental work. Four organisations used DNV's Phast model to perform the analysis: the UK's Health and Safety Executive (HSE), DNV, Syngenta and DGA Maîtrise NRBC (DGA). This paper examines the modelling approaches taken by the four groups and focuses on the results for the DT1 and FL09 trials. Modelling results for all six trials will be given in the conference presentation.

PHAST MODELLING APPROACHES

Table 1 summarises the input conditions that were provided to the participants involved in the JRIII modelling exercise. HSE used all the data in Table 1 and assumed a leak in a pressurised vessel using version 8.4 of Phast to represent the DT1 and FL09 releases. The mass flow rate predicted by Phast differed slightly from the value given in Table 1. Therefore, a user-defined source was created based on the results of the source term generated by Phast but with the release duration and mass flow rate edited to match the values given in Table 1. Phast was then run with the user-defined source. For DT1, concentrations were output at a height of 1 m, which matched the height of the lowest sensors in the Desert Tortoise experiments. For FLADIS, the sensors were at different heights on the three measurement arcs in the experiments. Three spot values at different heights (matching the sensor heights in the experiments) were therefore output from Phast for FL09.

Table 1. Supplied orifice input data for Desert Tortoise trial 1 (DT1) and FLADIS trial 9 (FL09)

Input	DT1	FL09
Orifice diameter (m)	0.081	0.0063
Release height (m)	0.79	1.5
Exit temperature (°C)	21.5	13.7
Exit pressure (barg)	9.22	5.91
Release rate (kg/s)	80	0.4
Release duration (s)	126	900
Site average wind speed (m/s)	7.42	6.1
at reference height (m)	2	10
Surface roughness (m)	0.003	0.04
Pasquill stability class	D	D
Ambient air temperature (°C)	28.8	15.5
Ambient air pressure (bar)	0.909	1.02
Relative humidity (%)	13.2	86
Averaging time for mean values (s)	80	600

DNV used the latest version of Phast (v8.61) and modelled the Desert Tortoise and FLADIS trials using user-defined sources rather than the software's in-built source models. The post-expansion liquid fraction and velocity source conditions were taken from the SMEDIS database (Carissimo *et al*., 2001). The droplet diameter was calculated by setting up separate leak scenarios in Phast using the default isentropic atmospheric expansion model and the modified CCPS droplet correlation. The resulting predicted droplet diameter was then used as an input to the user-defined source for the Phast runs. The modified CCPS correlation has previously been shown to provide predictions in good agreement against experimental rainout data (see, for example, Witlox *et al.,* 2007).

Syngenta modelled the Desert Tortoise and FLADIS trials using the leak in a pressure vessel model in Phast Version 8.61. The orifice diameter for FL09 (0.0063 m) resulted in a release rate of 0.03 kg/s, which is an order of magnitude lower than the measured release rate. Therefore, Syngenta increased the orifice diameter from 0.0063 m to 0.022 m to obtain the required release rate of 0.4 kg/s.

DGA used Phast version 8.61 and assumed that the ammonia was stored in a pressure vessel using the temperature/bubble point option at ambient temperature which defaulted to a vapour release. The fixed-duration release option was chosen to match the specified release rate in Table 1. This option does not require the input of the orifice diameter, the exit temperature or the exit pressure. The final velocity, liquid fraction and droplet parameters were all calculated by Phast.

Table 2 shows the intermediate data used by each organisation, i.e., the condition of the jet at the point where it has expanded to reach atmospheric pressure. HSE, Syngenta and DGA used Phast to calculate the final post-expansion velocity, liquid fraction and droplet diameter while DNV used the SMEDIS database.

Table 2. Final data after atmospheric expansion for the DT1 and FL09 trials

	Desert Tortoise DT1				FLADIS FL09			
	HSE	**DNV**	**Syngenta**	**DGA**	**HSE**	**DNV**	**Syngenta**	**DGA**
Core averaging time (s)	80	80	80	18.75	600	600	600	18.75
Final velocity (m/s)	246	90.3	246	663	617	65.2	617	624
Liquid fraction	0.825	0.82	0.83	0.09	0.082	0.84	0.08	0.09
Droplet diameter (µm)	83.7	107	83.7	0.94	0.91	144	0.9	0.9

For DT1, the HSE, DNV and Syngenta source conditions given in Table 2 were broadly similar, with a post-expansion liquid fraction of around 82% and a relatively large droplet size of around 80 – 110 µm. HSE used a higher final velocity than DNV (246 m/s versus 90 m/s), which HSE calculated using the default Phast isentropic expansion model. The DGA source conditions were quite different for DT1, with a liquid fraction of just 9%, a small droplet size of < 1 µm and a high velocity of 663 m/s. The DGA conditions are indicative of a vapour-phase release, although the experimental trials recorded a liquid release (see Figure 1).

For FL09, HSE, Syngenta and DGA all used much higher final velocities (> 600 m/s), lower liquid fractions (< 10%) and smaller droplet diameters (< 1 µm) as compared to the conditions used by DNV. The cause of this significant difference in source conditions was related to the exit pressure and temperature, specified in Table 1. Figure 1 plots these exit pressures and temperatures on the phase diagram. This shows that the Desert Tortoise conditions sit within the liquid region but the FLADIS conditions fall close to the saturation line. FL16 sits just on the liquid side but FL09 and FL24 fall into the vapour phase, according to the DIPPR saturation curve (which is used by Phast). The NIST saturation vapour pressure curve is included for comparison purposes and falls slightly below the DIPPR curve. All six experimental trials were saturated liquid releases with a liquid fraction at the orifice close to 100% liquid. The fact that the FL09 and FL24 points fall below the DIPPR saturation curve may be due to non-equilibrium effects or the pressures and temperatures being recorded at slightly different locations in the orifice. The consequence of using these exit pressures and temperatures to setup the Phast source conditions is that trials FL09 and FL24 were modelled as vapour releases by HSE, Syngenta and DGA. By using the SMEDIS source conditions, DNV used more appropriate source conditions for representing a saturated liquid release.

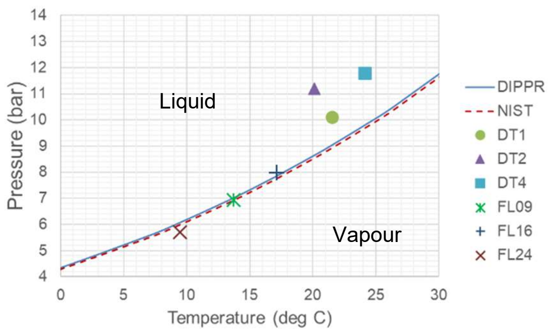

Figure 1. Pressure –temperature phase diagram for ammonia. The markers show the phase at the exit conditions for the Desert Tortoise and FLADIS trials.

The core averaging time is a user-defined input which is often left at the default value of 18.75 s. HSE, DNV and Syngenta changed the core averaging time to match the averaging time for mean values which was provided at the start of the exercise (see Table 1) while DGA kept the default value. DNV recommends setting the core averaging time in Phast to the same value as the averaging time of interest.

RESULTS

Figure 2 shows the results obtained by each organisation for DT1 (left) and FL09 (right). For DT1, HSE, Syngenta and DNV produced predicted concentrations at a height of 1 m, while DGA produced spot values at the two sensor locations. Despite the use of four different methods, there was good agreement between the results obtained for the DT1 trial, and it appears that the results were largely insensitive to the inputs that were varied. When compared to the experimental data (grey diamonds), all of the predictions performed well, but most tended to overpredict the concentration at the first sensor position at 100 m from the release point. The dip at approximately 50 m in DNV's result corresponds to the point where the droplets touched down and there was rainout (concentrations output from Phast include both vapour and liquid components). The droplet trajectories in Phast are based on a single Sauter mean diameter, and they generally track slightly lower than the plume centreline. The far-field DNV concentrations were lower, due to the attenuated mass caused by rainout, which led to an earlier transition from dense to passive dispersion. Although not shown here, there was good overall agreement for the DT2 and DT4 trials, with DT2 showing the closest match out of the three.

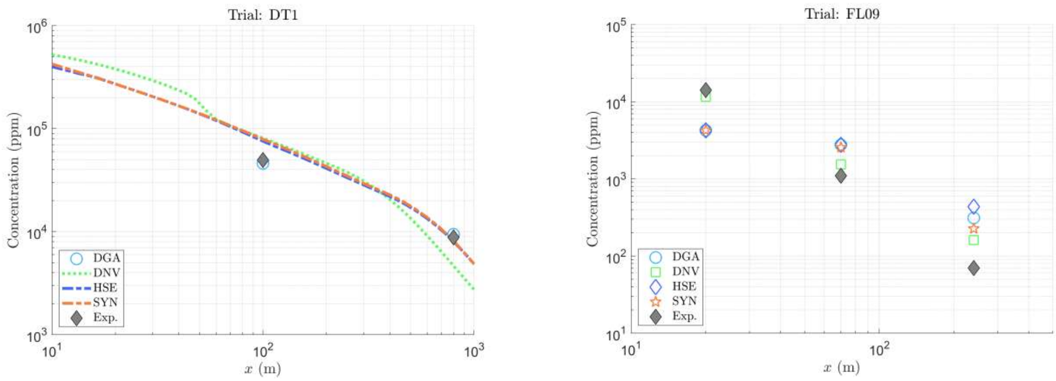

Figure 2. Concentration vs. distance plots for the DT1 (left) and FL09 (right) trials.

For the FL09 trial, the comparison between predictions and measurements did not show as good agreement as for the DT1 trial. Results for the FL16 and FL24 trials show similar patterns. All of the Phast results underpredicted the measurements in the near-field and overpredicted in the far-field. In the near-field, HSE, Syngenta and DGA obtained similar results, but the DNV predictions were in best agreement with the experimental data. Across all of the FLADIS trials, the model predictions from the different groups varied by up to a factor of four. The maximum over-prediction of measured concentrations was up to a factor of ten. However, this was largely due to the choice of vapour source conditions. The DNV predictions, using appropriate source conditions for a saturated liquid release, were in closer agreement with the measurements with more than half the predictions within a factor of two of the measurements.

Once the analysis presented above was complete, the Phast modellers met to examine the results and compare modelling approaches. From these discussions, the issues relating to modelling vapour phase releases rather than liquid phase releases were identified. HSE, Syngenta and DGA revised their inputs to see how modelling the release as a liquid would affect their results. The simplest way to do this in Phast is to select one of the bubble point options which sets the conditions to saturation. The user then changes the phase to liquid on the "material tab" in the Phast user interface. HSE selected the "temperature/bubble point" option which kept the temperature at 13.7 °C but changed the pressure to 5.94 barg which, although similar to the original input conditions in Table 1 (5.91 barg) meant the correct liquid phase could be selected. When the studies were re-run with the liquid phase selected, the final velocity did not reduce as much as expected. HSE generated a final velocity of 202 m/s (droplet size: 112 µm and liquid fraction: 0.85) which is still significantly higher than DNV's velocity of 65.2 m/s.

During the analysis it became apparent that this high velocity was due to the choice of the atmospheric expansion model. The default option (used by HSE, Syngenta and DGA) selects "conservation of momentum" if rainout is not possible, or typically (for two-phase releases) the "isentropic" expansion method. This latter choice is the default because the CCPS droplet correlation in Phast was derived using an isentropic assumption. However, it does result in artificially high final velocities. Changing the atmospheric expansion method from the default to "conservation of momentum" produces a more realistic and lower final velocity (Witlox and Bowen, 2002; Witlox *et al.*, 2014). Using a liquid release and the "conservation of momentum" option, HSE produced a final velocity of 49.4 m/s (droplet size: 142 µm and liquid fraction: 0.84). If the four organisations had simulated a liquid release using the "conservation of momentum" option, then the agreement between the predictions and against the experimental data would have been much closer.

Three groups used Phast version 8.61 while HSE used version 8.4. A number of changes were made to several Phast dispersion sub-models between these two versions, but these had limited impact on the scenarios modelled here. It is recommended to use the most up to date version of Phast, where possible.

Differences between model predictions and measurements can arise from uncertainty or variability in the experiments. For example, there was standing water on the test site in trials DT1 and DT2, which may have affected the humidity and/or atmospheric stability. Several of the modelling teams performed sensitivity studies to examine the potential impact of these uncertainties. Details are provided in the presentation accompanying this extended abstract at the Harmo conference.

SUGGESTIONS FOR FUTURE PHAST MODELLING OF PRESSURE-LIQUEFIED RELEASES

Improved predictions for pressure-liquefied releases can be obtained using non-default options in Phast. The following recommendations are given for Phast users when simulating pressure-liquefied releases, in addition to the usual Phast recommended practices:

1. Check the specified orifice exit pressures and temperatures on a phase diagram to confirm that the conditions input to Phast produce the expected phase of the ammonia released in the experiments (i.e., liquid or vapour). Also, check the predicted liquid fraction in the Phast results.
2. Set the core averaging time to be the same as the specified averaging time.
3. For cases with rainout, find the initial post-expansion ammonia droplet diameter by running a simulation using the default isentropic expansion model and the CCPS droplet size correlation.
4. Re-run the same Phast case using the conservation of momentum atmospheric expansion model, which gives a more representative post-expansion source velocity.
5. Produce a user-defined source from Step 4 and change the droplet size to that found from Step 3, and then run Phast. This approach will use the best estimate for the release velocity and droplet size.

CONCLUSIONS

Four modelling groups (HSE, DNV, Syngenta and DGA) produced results using Phast for the JRIII modelling exercise on Desert Tortoise and FLADIS. Each group took a slightly different modelling approach. Predictions were generally in mixed agreement with the measurements; there were differences between the Phast predictions of up to a factor of two for Desert Tortoise and a factor of four for the three FLADIS trials as a whole. The causes of these discrepancies were investigated and the exercise provided valuable learning lessons for all the organisations involved in this work.

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