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SUMMARY OF RESULTS FROM THE JACK RABBIT III INTERNATIONAL MODEL INTER-COMPARISON EXERCISE ON DESERT TORTOISE AND FLADIS

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Abstract: A series of new experiments involving large-scale releases of anhydrous ammonia are currently being planned for 2024 and 2025, known as the Jack Rabbit III trials (JRIII). The aim of the project is to address gaps in modelling methodologies and emergency response procedures. To support the project, an international model inter-comparison exercise was initiated in 2021 to evaluate the performance of atmospheric dispersion models using data from the Desert Tortoise and FLADIS trials. The objective of the collaborative modelling exercise was to understand the capabilities and limitations of models that could be used to design the new JRIII trials (e.g., suitable sensor placement). Dispersion modelling teams from around the world were invited to participate on a voluntary basis. The exercise followed a similar successful model inter-comparison exercise conducted in 2019-20 on the Jack Rabbit II chlorine dispersion dataset. The coordinators of the JRIII inter-comparison exercise provided a set of model inputs for the participants to use and requested model predictions to be provided to them in a standardized format. Twenty independent modelling teams from North America and Europe provided results using a range of different models (i.e., empirically-based nomograms, integral, Gaussian puff, and computational fluid dynamics models). The agreement between model predictions and measurements varied considerably between different models. Given appropriate inputs, most models generally predicted concentrations that agreed well with the data. Useful insights were gained through discussions between participants involved in the exercise.

Key words: *Jack Rabbit III, Desert Tortoise, FLADIS, anhydrous ammonia, two-phase jets, dispersion*

INTRODUCTION

The worldwide use of ammonia as an agricultural fertilizer, chemical feedstock and refrigerant has been growing in recent years and is forecast to increase significantly in the coming decades with the use of ammonia as a renewable energy vector. It is important to ensure the safety and security of this ammonia infrastructure, which requires an understanding of the potential consequences of ammonia releases. Atmospheric dispersion models and their source term models are critical to that effort. These models must be verified, validated and properly tested, before being used for emergency response, regulatory risk assessments and incident investigation. Ammonia is both acutely toxic and flammable. Its 10-minute Acute Exposure Guideline Levels are 2,700 ppm for life threatening effects or death (AEGL-3) and 220 ppm for irreversible effects and/or impaired escape (AEGL-2). Its lower and upper flammability limits are 16% and 27% by volume, respectively.

To improve our understanding of potential ammonia risks and address critical knowledge gaps (Hanna *et al.*, 2021), CSAC and DTRA are currently planning a series of large-scale anhydrous ammonia release experiments, known as the Jack Rabbit III trials (JRIII). To support the JRIII project, an initial collaborative modelling exercise was launched in 2021 to understand the strengths and weaknesses of atmospheric dispersion models using existing data for ammonia releases from previous experiments. The aim was to assess the accuracy of models that may be used to design the JRIII trials (e.g., for sensor placement). A secondary goal was to run model sensitivity tests to identify important parameters that may need to be carefully controlled or measured in the JRIII trials. Modelling experts from defence agencies, government laboratories, industry and consultancies in North America and Europe were invited to participate on a voluntary basis. Each group was asked to provide dispersion model predictions for six previous field-scale ammonia release experiments. The exercise was not a competition but a collaborative effort, with the ultimate goal of improving toxic industrial chemical modelling tools.

DESCRIPTION OF MODELLING EXERCISE AND EXPERIMENTAL DATASETS

The six previous field trials selected for the modelling exercise were taken from the Desert Tortoise and FLADIS experiments (Goldwire et al., 1985; Nielsen and Ott, 1996). Data for these trials was primarily sourced from the SMEDIS dataset (Carissimo *et al*. 2001). All inputs were carefully checked and cross-referenced against the original data reports and other literature. In some cases, minor adjustments were made to the SMEDIS values. Modellers were provided with a full description of the trials, including a summary of model inputs (Table 1) and suggestions for sensitivity tests that could be run to examine uncertainties. The modellers were requested to submit the results to the coordinators of the exercise (Joe Chang and Simon Gant) in a standardized format, to facilitate cross-plotting of the results.

The Desert Tortoise trials took place in 1983 at the Nevada Test Site, Nevada, USA. To date, they are the largest-scale atmospheric dispersion experiments conducted on pressure-liquefied ammonia. They involved releases of between 10 and 41 metric tonnes of ammonia, release rates of between 81 kg/s and 133 kg/s and gas concentrations measured downwind primarily at distances of 100 m and 800 m. Releases were directed horizontally from a height of 0.79 m across flat, open terrain. The test series consisted of four trials. Three of these were selected for the JRIII exercise (trials DT1, DT2 and DT4). In trials DT1 and DT2, there was some standing water present at the test site due to rainfall on the preceding days. This had evaporated by the time that trial DT4 was conducted. Some liquid ammonia in the two-phase jets rained-out on the ground in all of the trials and formed an evaporating pool. There are different accounts in the literature for the rain-out fraction, which vary between 5% and 36% of the total mass of ammonia released. One of the challenges in assessing the precise amount of rainout was the presence of standing water in the early trials.

The FLADIS trials took place in Landskrona, Sweden, in 1993-1994. They were much smaller in scale than Desert Tortoise, with pressure-liquefied ammonia discharge rates of between 0.25 kg/s and 0.55 kg/s. There were 27 trials in the test series and three were selected for the JRIII modelling exercise (trials FLADIS9, FLADIS16 and FLADIS24). These three trials all involved releases directed horizontally from a height of 1.5 m, with no rainout of liquid ammonia on the ground (due to the release height and the scale of the release). Concentrations were measured at distances of approximately 20 m, 70 m and 240 m. The ambient humidity in the FLADIS trials was higher and more representative of a damp European climate than the arid high-altitude Nevada Test Site used for the Desert Tortoise trials.

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

		DT1	DT2	DT4	FLADIS9	FLADIS16	FLADIS24
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	°C	21.5	20.1	24.1	13.7	17.1	9.45
Exit pressure	bara	10.1	11.2	11.8	6.93	7.98	5.70
	barg	9.22	10.3	10.9	5.91	6.96	4.69
Release rate	kg/s	80.0	117	108	0.40	0.27	0.46
Release duration	s	126	255	381	900	1200[g]	600
Rainout mass fraction	%	5	5	5	0	0	0
Site average wind speed	m/s	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	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
Pasquill stability class	-	D	D	D-E	D	D-E	C-D
Ambient temperature	°C	28.8	30.4	32.4	15.5	16.5	17.5
at reference height	m	0.82	0.82	0.82	1.5	1.5	1.5
Ambient pressure	bar	0.909	0.910	0.903	1.020	1.020	1.013
Relative humidity	%	13.2	17.5	21.3	86	62	53.6
Averaging time for mean values	s	80	160	300	600	600	400
Approx. coordinates of release point		36°48’05.8” N 115°57’35.7” W			55°51’37.0” N 12°50’34.8 E		
		36.801607, -115.959929			55.860278, 12.843000		
Date of release		24/8/83	29/8/83	6/9/83	7/8/93	13/8/93	30/8/94
Start time (local)	h:m	16:37	11:20	15:37	14:39	19:51	16:06

In both the Desert Tortoise and FLADIS trials, a nitrogen padding system was used to force liquid ammonia from the storage vessel(s) through pipework to the release orifice. This meant that for all of the selected trials, the ammonia liquid mass fraction at the orifice was effectively 100%. Some of the models used by participants in the modelling exercise could not directly simulate the resulting two-phase jets and required vapour-only source conditions. A set of equivalent vapour-only conditions were provided to the modelling exercise participants, using the methodology adopted in the SMEDIS project (i.e., assuming conservation of mass, momentum and enthalpy). Some modellers chose to use these conditions, whilst others used their own preferred methods of calculating vapour-only source conditions.

The list of participants in the exercise and details of the models used are summarized in Table 2. They included 3 sets of results from empirically-based nomograms and/or Gaussian plume models, 11 sets of integral model predictions, 6 sets of Gaussian puff or Lagrangian models and 4 sets of CFD results. Some models were run for only selected Desert Tortoise or FLADIS trials, rather than all six trials.

RESULTS

Predicted maximum arc-wise concentrations are compared to measured values for trials DT1 and FLADIS9 in Figure 1 (enlarged versions of these graphs will be made available in the slides presented at the conference). A similar degree of spread in results was observed between the three Desert Tortoise trials and the three FLADIS trials. The range in predictions spanned roughly between one and two orders of magnitude about the measurements with a tendency for models to over-predict at 100 m and under-predict at 800 m in the Desert Tortoise trials, and with less spatial bias in the FLADIS trials.

#	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	DGA, France	PHAST v8.6										
5		Code-Saturne v6.0										
6	DNV, UK	PHAST v8.61										
7	DSTL, UK	HPAC v6.5										
8	DTRA, ABQ, USA	HPAC v6.7										
9	DTRA, Fort Belvoir, USA	HPAC										
10	EDF/Ecole des Ponts, France	Code-Saturne v7.0										
11		Crunch v3.1										
12	FFI, Norway	ARGOS v9.10										
13	FOI, Sweden	PUMA										
14	Gexcon, Netherlands	EFFECTS v11.4										
15	Gexcon, Norway	FLACS										
16	GT Science & Software	DRIFT v3.7.19										
17	Hanna Consultants, USA	Britter & McQuaid WB										
18		Gaussian plume model										
19	HSE, UK	DRIFT v3.7.12										
20		PHAST v8.4										
21	INERIS, France	FDS v6.7										
22	JRC, Italy	ADAM v3.0										
23	NSWC, USA	RAILCAR-ALOHA										
24	Shell, UK	FRED 2022										
25	Syngenta, UK	PHAST v8.61										

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.

Significant differences between HPAC results from different groups arose from differences in modelling approach. One group adopted the same methodology commonly applied to requests for Reachback support under operational settings, i.e., using only limited information from Table 1 and making conservative choices of hole sizes, weather conditions etc. Another HPAC group instead used a more complete set of inputs from Table 1. The results from empirically-based nomograms, Gaussian plume and integral models generally showed less scatter about the measurements compared to that shown by Gaussian puff or Lagrangian models (Figure 2). Four independent groups used the PHAST integral model and each group took a slightly different modelling approach, which resulted in minor differences in predicted concentrations. The four CFD models all gave quite similar results (mostly, within a factor of two of each other), despite them each using quite different modelling approaches (e.g., LES versus RANS).

Sensitivity tests were undertaken by some of the modelling groups (results not shown here), which provided useful information. For example, HPAC results were found to be sensitive to both the assumed liquid fraction and atmospheric stability. EFFECTS results were relatively insensitive to rainout and surface roughness. FLACS results showed some sensitivity to the way in which equivalent vapour-only source conditions were derived and how they were implemented in the CFD code (both the shape of the vapour-only source window and the source velocity profile).

Further results, including plume widths and statistical performance measures are provided in the accompanying presentation at the Harmo-21 conference.

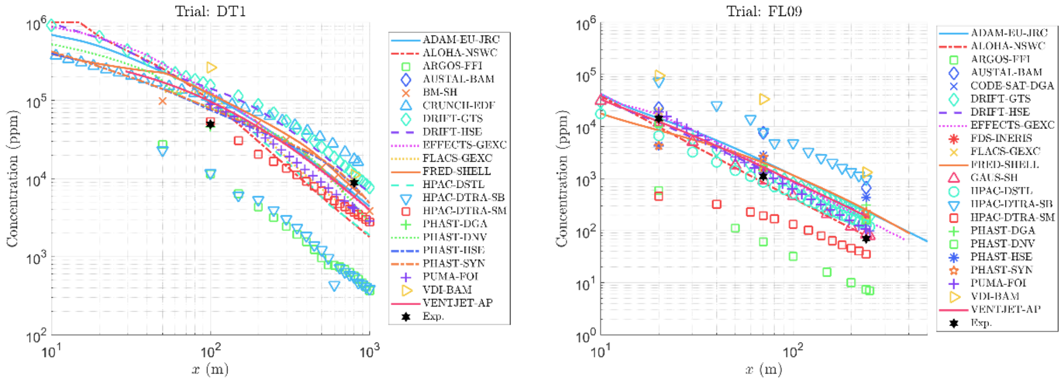

Figure 1. Maximum arc-wise concentrations for trials DT1 and FLADIS9 (all models)

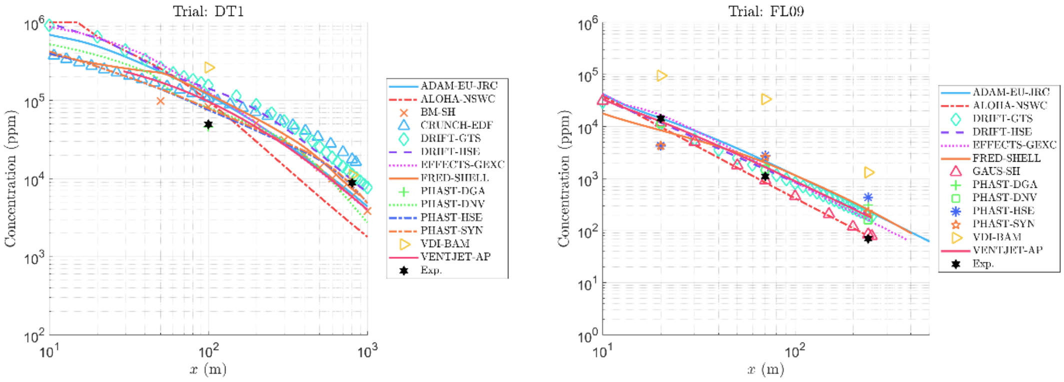

Figure 2. Maximum arc-wise concentrations for trials DT1 and FLADIS9 for empirically-based nomograms, Gaussian plume and integral models only

CONCLUSIONS

A model inter-comparison exercise has been undertaken using data from the Desert Tortoise and FLADIS ammonia trials. A total of 25 sets of model predictions were provided by 20 independent groups. The agreement between model predictions and measurements varied considerably between different models. Given appropriate inputs, most models generally predicted concentrations that agreed well with the data. Useful insights were gained through discussions between participants involved in the exercise into the choice of modelling approach – especially, in cases where different groups used the same model. The modelling exercise and analysis of the Desert Tortoise and FLADIS data provided useful insights into the design of the future JRIII trials. For example, analysis of the Desert Tortoise trials highlighted the need for a greater number of concentration sensors in the far-field than were present in the Desert Tortoise trials to measure the full extent of the hazardous cloud. A future collaborative JRIII modelling exercise may be undertaken to examine a previous large-scale ammonia incident.

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