Jack Rabbit III Modelers Working Group

Description of the JRIII Modeling Exercise

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Changelog

Version 2.3	Addition of rainout mass fraction, lat/long coordinates of release point and date/times for ammonia releases into Table 1, since Version 1.0. Extra discussion of ammonia liquid rainout in the Desert Tortoise trials (Page 13). Revision of sensitivity tests on rainout in the Desert Tortoise trials (Page 19).
Version 2.4	Clarified that "plume width" means "plume half-width, σ_y" in Table 5 on Page 11, in note "e" accompanying that Table and in Table 6 on Page 12.

Background

The Jack Rabbit III project is being led by the Chemical Security Analysis Center (CSAC) of US Department of Homeland Security and the Defense Threat Reduction Agency (DTRA) of US Department of Defense and will involve large-scale anhydrous ammonia release experiments in 2023 and 2024. The project follows on from the successful Jack Rabbit I and II programs in 2010 and 2015-2016. The experiments are being conducted to improve threat assessment of Toxic Industrial Chemicals (TICs), to fill critical scientific data gaps, to test new technologies and provide training opportunities for first responders.

Aims

The aim of this initial Jack Rabbit III modeling exercise is to evaluate the performance of atmospheric dispersion models using data from previous ammonia release experiments, to help us understand the accuracy of models that may be used to design the Jack Rabbit III trials. The exercise also provides an opportunity to run sensitivity tests with models, to identify important model input parameters that may need to be carefully assessed or measured in the Jack Rabbit III trials. It is not a competition but a collaborative effort, with the ultimate goal of improving toxic industrial chemical modeling tools in general.

Methodology

The work will involve testing models using data from the Desert Tortoise and FLADIS ammonia trials, conducted in 1983 and 1993-4. The rationale for selecting these trials and details of the method that we propose to use for the comparison exercise are described in the Appendix.

It is recognized that some modeling teams may have more resources than others and therefore different levels of outputs are requested: a mandatory basic set of model outputs, and optionally a more comprehensive set of outputs. It is hoped that all participants will be able to produce the mandatory set of outputs and those with sufficient resources will be able to provide more comprehensive results.

Participation

The exercise is not being funded by the exercise coordinators, CSAC nor DTRA. The work is voluntary, to be conducted on a "best endeavors" basis. Participation in the exercise is welcomed from government agencies, national laboratories, research corporations, universities, the oil/gas/chemical industry and engineering consultancies. All classes of model predictions are welcome, including models used for emergency planning and response, for regulatory purposes and for research, e.g., nomograms, integral models, Lagrangian and CFD models.

Benefits

The main benefits to participation in the exercise is that it provides an opportunity to benchmark models against existing ammonia field trial data, and to share knowledge and experience with other world experts. The intention is to publish the jointly-authored findings in one or more conference papers and in a peer-reviewed journal.

The focal point for discussions about Jack Rabbit III will be the annual George Mason University conference on atmospheric transport and dispersion modeling. Further details of the exercise described here will be given at the 25th annual meeting, which is being held online on 2-4 November 2021 (http://camp.cos.gmu.edu/).

Appendix – Description of Modeling Exercise

The exercise will be run using a similar methodology to the Jack Rabbit II model inter-comparison exercise (for details, see the Atmospheric Environment journal special issue[1]). Modelers are provided with a set of model input parameters and they are invited to submit to the coordinators of the exercise their model predictions in a preferred format. The coordinators will then collate the results and compare model predictions to the data. The findings will be shared with the modelers and later published in conference and journal publications. Details of the model inputs/outputs are provided below.

The Desert Tortoise and FLADIS trials have been analyzed extensively in several previously published papers, reports and model validation databases. Some of model inputs and measured values documented in these various literature sources exhibit small differences, due to differences in post-processing methods and interpretation. There may also be some typographical errors. The coordinators of this Jack Rabbit III exercise have cross-referenced several literature sources to check for errors. Details are provided below.

Rationale for choice of trials

The trials chosen for this exercise are:

- Desert Tortoise: Trials 1, 2 and 4 (DT1, DT2, DT4)
- FLADIS: Trials 9, 16 and 24 (FLADIS9, FLADIS16, FLADIS24)

The rationale for selecting these ammonia trials has been to test dispersion models for a range of conditions whilst keeping the exercise relatively simple and not too onerous.

The Desert Tortoise trials are the largest-scale atmospheric dispersion experiments conducted to date on pressure-liquefied ammonia. They involved releases of between 10 and 41 tonnes of ammonia, release rates of between 81 and 133 kg/s and gas concentrations measured downwind[2] at distances of 100 m and 800 m. Releases were directed horizontally from a height of 0.79 m and some liquid ammonia rained-out on the ground.

The FLADIS trials were much smaller in scale, with pressure-liquefied ammonia discharge rates of between 0.25 and 0.55 kg/s. The releases selected here were all directed horizontally from a height of 1.5 m and there was no rainout of liquid ammonia on the ground. Concentrations were measured at distances of approximately 20 m, 70 m and 240 m, which enables analysis of transition from dense to passive dispersion. The 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.

All of the trials selected here were included in the SMEDIS database (Carissimo *et al*., 2001), with the exception of DT4. One of the advantages of selecting these trials is that the SMEDIS project calculated equivalent source conditions for models that are only capable of simulating single-phase (vapor-only) releases. The partners in the SMEDIS project also carefully vetted the datasets.

[1] https://www.sciencedirect.com/journal/atmospheric-environment/special-issue/10FRFPWRB27

[2] In addition to the two rows of sensors at 100 m and 800 m, a number of portable sensors were located at distances of 1.4 km, 2.8 km and 5.5 km, though there were too few sensors at these locations to determine maximum arc-wise concentrations.

The reason for including DT4, in addition to the trials in the SMEDIS database, is that the Frenchman Flat area of the Department of Energy's Nevada test site was saturated with water due to heavy rainfall in preceding days during the DT1 and DT2 trials. There were numerous small pools of water present on the ground in both tests, which gradually dried up during the third test and had completely dried up by the last test (DT4). Ammonia is water reactive and to avoid possible issues associated with interaction between the released ammonia and any surface water, trial DT4 has been included in this model evaluation exercise. Moreover, DT4 was the largest release of all the trials.

One of the challenges experienced in the previous Jack Rabbit II model inter-comparison exercise was that the experiments were conducted in the early morning, when the atmosphere was transitioning from stable to unstable conditions (see Hanna, 2021). As the chlorine cloud drifted downwind past the arcs of sensors, the characteristics of the atmospheric boundary layer changed, the wind speed near the ground often increased significantly and the wind also changed direction. These shifts made comparisons between model predictions and measurements complicated and subject to uncertainties. The Desert Tortoise trials DT1 and DT2 were conducted during the day between 11 am and 5 pm in the presence of neutral atmospheric conditions (Pasquill Class D). DT4 was conducted in late afternoon at around 6 pm with a low sun angle and moderately stable conditions (Pasquill Class D-E). FLADIS Trials 9 and 24 were conducted in the afternoon at around 2 pm and 4 pm, whilst FLADIS Trial 16 was conducted at around 8 pm with a wind speed of around 6 m/s when atmospheric conditions were neutral. The issues experienced in Jack Rabbit II with the changing atmospheric boundary layer conditions should therefore be less of a problem with the Desert Tortoise and FLADIS trials.

Model Input Conditions

The table below provides the set of input conditions to be used for this modeling exercise. Explanatory notes are provided to highlight where discrepancies exist in the values given in the literature.

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

		DT1	DT2	DT4	FLADIS9	FLADIS16	FLADIS24
Orifice diameter	m	0.081[a]	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[b]	bara	10.1	11.2	11.8	6.93[c]	7.98[c]	5.70[c]
	barg	9.22	10.3	10.9	5.91	6.96	4.69
Release rate	kg/s	80.0[d]	117[e]	108[f]	0.40	0.27	0.46
Release duration	s	126	255	381	900	1200[g]	600
Rainout mass fraction[p]	%	5	5	5	0	0	0
Site average wind speed	m/s	7.42	5.76	4.51[h]	6.1[i]	4.4	4.9[j]
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[k]	D	D-E	C-D[l]
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[m]		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[n]		24/8/83	29/8/83	6/9/83	7/8/93	13/8/93	30/8/94
Start time (local)[o]	h:m	16:37	11:20	15:37	14:39	19:51	16:06

[a] The value of 3.29 inches on Page 6 of the Goldwire *et al*. (1985) report is assumed to be a typographical error. Later in Table 6 of the Goldwire *et al*. (1985) report the orifice diameter was given as 3.19 inches, which was the value used by the SMEDIS and MDA[3] databases and is the value used here. The REDIPHEM database incorrectly stated the diameter as 0.095 m, which was instead the diameter of the orifice in the DT2, DT3 and DT4 trials according to Goldwire *et al*. (1985)

[b] The atmospheric pressure was relatively low in the Desert Tortoise trials and care should be taken when using gauge and absolute pressures (gauge pressure = absolute pressure – atmospheric pressure on the day of the test). The exit temperature and pressure in the Desert Tortoise trials was measured 1 m upstream of the orifice (Goldwire *et al*., 1985). Therefore there may have been a further drop in pressure from the stated exit pressure values before the ammonia reached the orifice. In the FLADIS trials, the temperature and pressure were measured close to the orifice, so there is less uncertainty in release conditions (see Nielsen *et al*., 1994).

[c] The FLADIS reports did not state if measured pressures were absolute or gauge. However, Nielsen *et al*. (1997) noted that the boiling point at the exit pressure was slightly less than the measured exit temperature, which (having checked the ammonia saturation vapor pressure curve) implies that the measured exit pressure was an absolute pressure.

[d] The value of 80 kg/s used here is taken from Table 20 in the Goldwire *et al*. (1985) report. The SMEDIS database gave this same value and the MDA database gave a similar value of 79.7 kg/s. The REDIPHEM database gave the release rate as 81

[3] Modelers Data Archive – see Hanna *et al*. (1993) and the more recent GMU presentation by Chang and Hanna (2016).

kg/s, which may originate from dividing the total mass released by the release duration. According to Table 6 in Goldwire *et al*. (1985) these values are 10200 kg and 126 s, giving an average release rate of 10200/126 = 81 kg/s.

[e] The release rate of 117 kg/s is taken here from Table 20 in the Goldwire *et al*. (1985) report. The same value is given in the REDIPHEM database, but the SMEDIS and MDA databases instead give a value of 112 kg/s. According to Table 6 in the Goldwire *et al*. (1985) report, the total mass released was 29900 kg over a duration of 255 s, which gives an average release rate of 117 kg/s.

[f] The release rate of 108 kg/s is the value given in Table 20 in the Goldwire *et al*. (1985) report and the same value was given in the REDIPHEM database. The MDA database instead gave a value of 96.7 kg/s. According to Table 6 in the Goldwire *et al*. (1985) report, the total mass released was 41100 kg over a duration of 381 s, which gives an average release rate of 41100 / 381 = 108 kg/s.

[g] Nielsen and Ott (1996a) gave a value of 1200 s, while the SMEDIS and REDIPHEM databases gave it as 1140 s. Since these are effectively continuous releases, the precise value is not important.

[h] The wind speed of 4.51 m/s is taken from the Goldwire *et al*. (1985) report and the same value was given in the MDA database. The REDIPHEM database gave a different value of 5.5 m/s.

[i] The wind speed of 6.1 m/s is taken from the Nielsen and Ott (1996a) report and Nielsen *et al*. (1997) paper. The SMEDIS and REDIPHEM database instead gave it as 5.6 m/s. File "INFO.TXT" in the FLADIS dataset in folder FLADEXP\TRIAL009\DOC\ stated "the wind speed at 10 m was approximately 5.6 m/s".

[j] The value of 4.9 m/s used here is taken from Nielsen and Ott (1996a) and Nielsen *et al*. (1997). The SMEDIS and REDIPHEM databases gave a different wind speed of 5.03 m/s. File "INFO.TXT" in the FLADIS dataset in folder FLADEXP\TRIAL024\DOC\ stated "the wind speed at 10 m was approximately 5.0 m/s".

[k] The Goldwire *et al*. (1985) report and the MDA and REDIPHEM databases all gave the Pasquill stability as Class E, but the Golder (1976) plot suggests the conditions were within Class D, close to Class E. It is therefore given as Class D-E here.

[l] The SMEDIS and REDIPHEM databases gave Pasquill Class C for FLADIS24 but according to the Golder (1976) plot, the conditions are exactly on the borderline between Classes C and D, so it is marked here as Class C-D.

[m] Approximate latitude and longitude of the release point are given in degrees, minutes and seconds (top line) and degrees and decimal minutes (bottom line). The Desert Tortoise location was estimated by matching the map of the Nevada Test Site given by Goldwire *et al*. (1985) to aerial views of the Nevada Test Site from Google Maps. The FLADIS release coordinates were taken from the KMZ file provided by Morten Nielsen that can be downloaded from here: https://xnet.hsl.gov.uk/fileshare/public/3385/approximate-fladis-release-point.kmz.

[n] Dates are in European format of day/month/year. Dates/times for Desert Tortoise are taken from Goldwire *et al*. (1985) and for FLADIS from Nielsen *et al*. (1997).

[o] The start times of the releases are given in local time. The Desert Tortoise trials were undertaken in Pacific Daylight Time (PDT) which is UTC-08:00. The FLADIS experiments were conducted in Sweden in summer and therefore are UTC+02:00.

[p] For details, see the later discussion of ammonia liquid rainout in the Desert Tortoise trials on Page 13.

Ammonia liquid mass fraction at the orifice

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 orifice. For all of the trials selected here, it can be assumed that the ammonia liquid mass fraction at the orifice was 1.0, i.e., pure liquid, as specified in the SMEDIS and REDIPHEM databases.

Goldwire *et al*. (1985) noted that the orifice plate used in the Desert Tortoise trials was sized to ensure the ammonia flow remained liquid until reaching the orifice plate, whereupon it flashed to a mixture of vapor and droplets.

Spicer and Miller (2018) noted that photographs of the Desert Tortoise tests showed that there was an elbow in the pipework a short distance upstream of the orifice plate (around 30 cm, equivalent to two pipe diameters). Guidance for placement of relief valves recommends any turbulence causing devices, such as elbows, are kept at least 10 pipe diameters upstream of the relief device to avoid it affecting the flow rate. Spicer and Miller (2018) suggested therefore that the presence of the elbow near the orifice in the Desert Tortoise trials probably caused a reduction in the release rate due to turbulence and flashing of the fluid. This matched the behavior seen with their model predictions, where the metastable liquid model overpredicted the release rate. Predictions with their alternative homogeneous equilibrium model were more consistent with the observations.

As noted above in comment "b", the exit pressure and temperature in the Desert Tortoise trials were measured 1 m upstream of the orifice. Therefore, there could have been some drop in pressure along the 1 m pipe length before the ammonia reached the orifice.

Nielsen *et al*. (1997) described a method to determine the liquid mass fraction of ammonia at the orifice in the FLADIS trials, based on the measured exit temperature and pressure. For Trials 9, 16 and 24, this method gave liquid mass fractions of 0.999, 1.0 and 0.997, respectively.

Terrain

The terrain for both the Desert Tortoise and FLADIS trials can be modelled as flat and unobstructed. The Frenchman Flat area used in the Desert Tortoise trials was an extremely flat (normally) dry lake bed approximately 4-6 km long and 3 km wide (Goldwire *et al*., 1985).

The FLADIS trials took place at the Hydro-Care test site in Landskrona, Sweden. A map of the facility is shown in Figure 1. Modeling by CERC (Edmunds and Britter, 1994) indicated that the presence of some buildings upwind from the release point may have affected the dispersion behavior. For this reason, Nielsen *et al*. (1997) recommended that modelers use the measured wind and turbulence fields rather than parameters of a surface layer in equilibrium (see "Modeling Uncertainties" below).

Equivalent Source Conditions

The following equivalent source conditions for the DT1, DT2, FLADIS9, FLADIS16 and FLADIS24 trials are taken from the SMEDIS database (Carissimo *et al*., 2001). The SMEDIS data files and accompanying reports and papers are all available on the ADMLC website[4]. The method used to determine the source conditions is described in Appendix 4 of the SMEDIS Model Evaluation Protocol (CERC, 2000). DT4 was not included in the SMEDIS database.

[4] See https://admlc.com/smedis-dataset/. The equivalent source terms are in files "equivsrc.txt", distributed in zip files "batch1_24.zip", "batch2_24.zip" and "batch3_24.zip".

Table 2 Equivalent source conditions for the Desert Tortoise trials, taken from the SMEDIS database

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Temperature (K)	Half-width (m)
DT1	51.0	7.5	13	205	6.40
DT2	48.3	6.0	13	205	8.40

Note: The source term refers to the distance at which no liquid remains in the plume. The source size has been specified this time as a rectangular window of height = the half-width.

Table 3 Equivalent source conditions for the end of the flashing phase in the FLADIS trials, taken from the SMEDIS database

Trial	Flash Fraction	Density (kg/m^3)	Temperature (K)	Diameter (m)	Velocity (m/s)
FLADIS9	0.16	5.69	239.7	0.04	65.17
FLADIS16	0.17	-	239.7	0.031	65.85
FLADIS24	0.17	-	239.7	0.045	55.87

Table 4 Equivalent source conditions at the location where all the ammonia liquid has vaporized for the FLADIS trials, taken from the SMEDIS database

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Density (kg/m^3)	Temperature (K)	Diameter (m)
FLADIS9	4.2	4.75	12	1.67	203.7	0.88
FLADIS16	3.1	5.12	12	1.64	203.9	0.73
FLADIS24	4.4	4.22	12	1.64	204.0	1.06

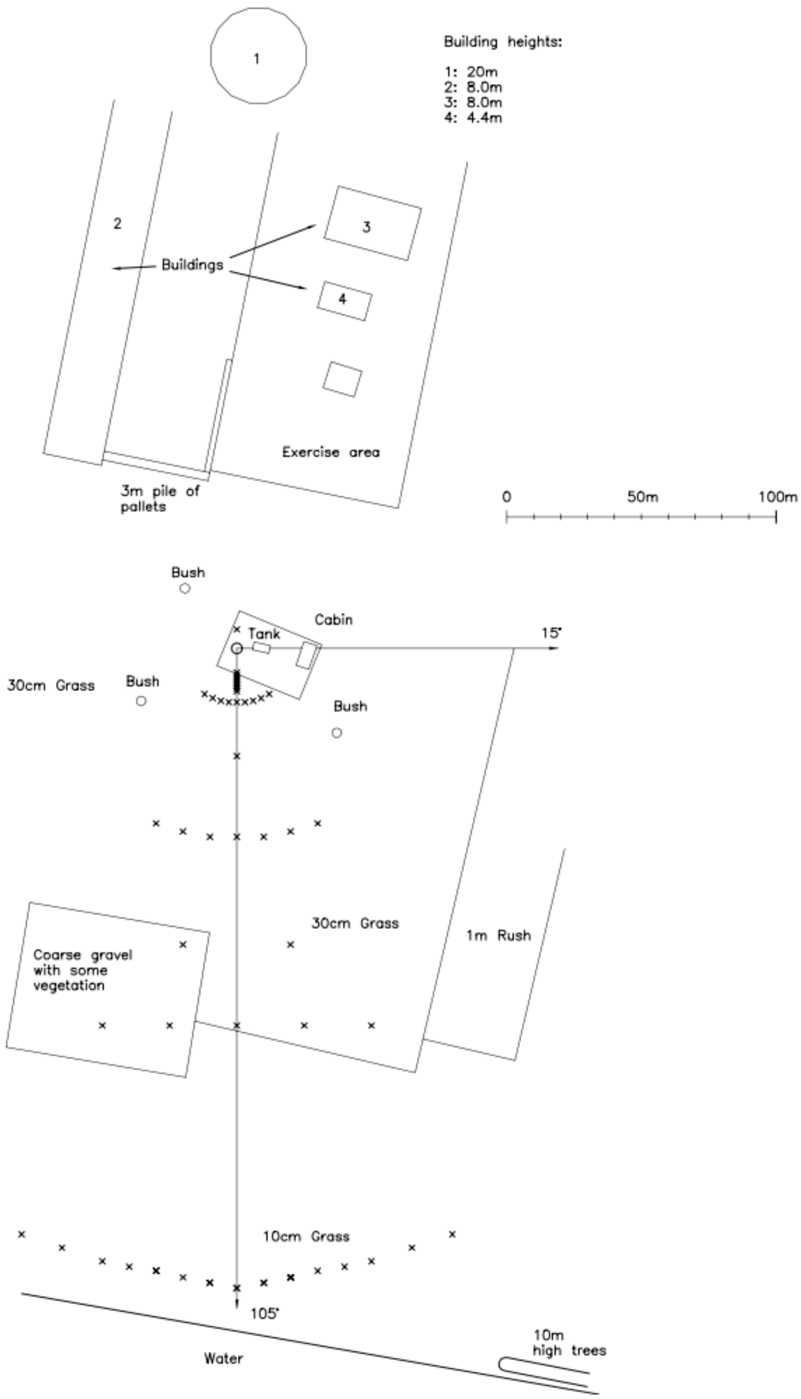

Figure 1 Map of the FLADIS test site including the array of measurement positions and the coordinate system. The building labelled 1 is of a conical shape. From Nielsen *et al*. (1994)

Requested Model Outputs

The mandatory requirement for participants of this modeling exercise is to provide a table of predicted arc-max concentrations versus distance for all six trials given in Table 1. By "arc-max" we mean the maximum ammonia concentration at that given radial distance downwind from the source, at any height or circumferential location (i.e., the plume centerline concentration).

Some models cannot easily output arc-max values without significant post-processing. The height of the sensors that recorded the maximum concentrations in the Desert Tortoise trials was 1.0 m at both the 100 m and 800 m arcs (see the SMEDIS and MDA databases for details). In the FLADIS trials, the height of the maximum concentrations was 0.1 m, 0.5 m and 1.5 m at the 20 m, 70 m and 238 m (or 240 m) arcs, respectively (see Table 4 in Nielsen *et al*., 1997). Modelers can optionally output concentrations at these heights if the arc-max values are too difficult to produce.

In the FLADIS trials, concentrations were determined by Nielsen *et al*. (1997) using both fixed and moving frames of reference. Modelers should use a fixed frame of reference for the mandatory outputs in this exercise.

Modelers are requested to provide a CSV or Microsoft Excel file with two columns of data for each trial: one column with the distance (in m) and one with the concentration (in ppm by volume). The aim is to plot curves of model predictions versus distance to compare to the measurements and other model predictions. It is useful to plot a continuous curve of predicted concentration with distance, rather than just spot values at the sensor arcs. If possible, modelers should therefore output arc-max concentrations at sufficient number of points extending from the source to a maximum distance of 1000 m for Desert Tortoise and 250 m for the FLADIS trials, to enable a smooth curve of concentration versus distance to be drawn.

The averaging times for these predicted arc-max concentrations are different in each trial and vary from 80 to 600 seconds – see Table 1.

In the Desert Tortoise trials, the concentration was measured at 100 m using sensors with a heated element that vaporized any ammonia droplets, so the measured concentration was the sum of both ammonia vapor and aerosol components. Modelers should output equivalent values if possible. The other concentration sensors in the Desert Tortoise and FLADIS trials measured solely the vapor concentration, though the aerosol component should be negligible in those cases anyway.

In addition to the CSV or Excel files that are submitted to the coordinators of the exercise, modelers are asked to provide a short description of their modeling approach, including:

- Name and version of model
- Description of any deviations from the prescribed model input conditions given in Table 1 (e.g., use of standard atmospheric pressure in the model instead of the prescribed value)
- Description of the output values, especially if they differ from the requested arc-max values (e.g., vapor concentrations output at height of X m that do not take into account the aerosol concentration).

The measured arc-max concentration in the Desert Tortoise and FLADIS trials are available in the SMEDIS and MDA databases and are provided below in Tables 5 and 6 for reference.

Table 5 Measured arc-max concentrations and plume half-widths in the Desert Tortoise trials using the long averaging time given in Table 1

	Distance	**Height**	**DT1[b]**	**DT2[c]**	**DT4[d]**
Arc-max concentration (ppm) [a]	100 m	1 m	49,490	82,920	57,300
	800 m	1 m	8,790	10,910	16,678
Plume half-width, σ_y (m) [e]	100 m	1 m	13.7	15.9	15.7
	800 m	1 m	74.5	93.6	86.0

[a] Concentrations measured at 100 m were the sum of vapor and aerosol components

[b] Values shown here are from the SMEDIS database. There are minor discrepancies with the MDA database, which gives concentrations of 49,943 ppm and 8,843 ppm, and plume widths of 11.8 m and 61.8 m at the 100 m and 800 m arcs, respectively.

[c] Values shown here are from the SMEDIS database. There are minor discrepancies with the MDA database, which gives concentrations of 83,203 ppm and 10,804 ppm, and plume widths of 14.7 m and 88.2 m at the 100 m and 800 m arcs, respectively.

[d] Values shown here are from the MDA database. The SMEDIS database does not contain data for DT4.

[e] The SMEDIS database determined the plume half-width, σ_y, from the moments of the concentration distribution across the arc of sensors (see CERC, 2000), whilst the MDA measured σ_y as the distance from the center of the plume to the point where the concentration fell to EXP(-0.5) times the concentration at the center of the plume. For a Gaussian distribution, these two methods give identical results.

Table 6 Measured arc-max concentrations and plume widths in the FLADIS trials using the long averaging time given in Table 1 and a fixed frame of reference.

	Distance	Height	FLADIS9	FLADIS16	FLADIS24
Arc-max concentration (ppm)	20 m	0.1 m	14,190	17,010	28,180
	70 m	0.5 m	1,100	1,190	2,610
	238 m (240 m)[a]	1.5 m	70	140	70
Plume half-width, σ_y (m)	20 m	0.1 m	3.54	4.00	3.50
	70 m	0.5 m	12.4	11.9	10.0
	238 m (240 m)[a]	1.5 m	28.2	21.5	24.0

[a] The “far end dispersion array” in the FLADIS trials was located at 238 m in Trials 9 and 24, and at 240 m in Trial 16 (Nielsen and Ott, 1996a; Nielsen *et al*., 1997). The SMEDIS database gave the distance as 235.5 m in all three trials.

The concentrations and plume half-widths given here are taken from the SMEDIS database. The values given by Nielsen and Ott (1996a) and Nielsen *et al*. (1997) are slightly different, probably because they used different averaging times. The differences are consistent in that the averaging times were slightly shorter and the concentrations slightly higher in the SMEDIS database than in Nielsen and Ott (1996a) and Nielsen *et al*. (1997).

Modeling Uncertainties

This section discusses some of the uncertainties in the Desert Tortoise and FLADIS trials. A summary of possible sensitivity tests that could be undertaken to examine these uncertainties is given in the final sub-section.

Previous work

In their seminal model evaluation study, Hanna *et al*. (1993) provided an example of sensitivity analyses applied to atmospheric dispersion models. They noted that the choice of model input ranges to study should depend on the uncertainties associated with the particular trial of interest, which could relate to the type of instruments, the averaging times, orientation of the wind with the test grid, atmospheric stability and so on. As a starting point, they chose the following ranges of input uncertainties and subsequently applied these to study the DT3 trial (Table 7)

Table 7 Model input ranges by Hanna *et al*. (1993) in their sensitivity analysis

Wind speed (u and du)	the mean ± larger of 0.5 m/s and σ_u
Temperature difference	the mean ± 0.2 °C
Relative humidity	the mean ± 10%
Surface roughness	the mean ± ½ order of magnitude
Source emission rate	the mean ± ½ order of magnitude
Source diameter	the mean ± ½ order of magnitude

Using the SLAB dispersion model, they found that the largest ranges in predicted concentrations for the DT3 trial were due to uncertainties in the wind speed (u), source emission rate and source diameter. The surface roughness had moderate influence. Changes in the wind speed difference (du), temperature difference and relative humidity had little effect.

Standing water in Desert Tortoise trials DT1 and DT2

Goldwire *et al*. (1985) noted that for DT1 the "lake bed was covered with 6-8 inches of water on previous night. Prior to test, wind blew most of the water downwind well past 100 m row. Only pockets of water were in the spill area. Surface water was present from 0.4 to 2.0 km downwind. … spill jet scoured out surface water in vicinity of spill, leaving surface relatively free of water at end of test." And in Trial 2: "lake bed was covered with water on previous night. Prior to test, wind blew some of the water downwind, leaving about 1/2 cm of water on ground in spill area out to central region of the mass flux row."

The effect of this standing water on the dispersion behavior is a source of uncertainty. Entrainment of water from the ground into the high-speed ammonia jet could have increased the humidity in the dispersing cloud. Some dispersion models can take into account the chemical reactivity between ammonia and water vapor. For those models, the effect of standing pools of water could be investigated by increased the ambient humidity in model sensitivity tests.

Another effect of the standing surface water could be to change the surface roughness. The surface roughness value specified for this modelling exercise (z_0 = 0.003 m) was recommended by Goldwire *et al*. (1985) for all of the Desert Tortoise trials. They calculated the value from wind profile measurements at a meteorological tower for each of the Desert Tortoise trials. It falls within the range recommended by the TNO Yellow Book (2005) for atmospheric flows over open water with a fetch of at least 5 km (z_0 = 0.0002 m) and mud flats (z_0 = 0.005 m). Sensitivity tests could potentially be conducted within this range of values, though Hanna *et al*. (1993) reported it had little effect.

Surface water could also have affected the atmospheric stability. Standard Pasquill-Gifford stability classification schemes and Monin-Obukhov boundary layer analysis assume "dry" heat. For example, the Monin-Obukhov scaling length, L, is calculated using just the sensible heat flux, and latent heat effects due to evaporation are assumed to be unimportant. Water vapor has a lower density than dry air. In the Desert Tortoise trials, the vertical flux of water vapor evaporating from the surface of the wet playa may have had a similar effect to the surface being heated by solar radiation (i.e., a reduction in density of the air) – effectively causing unstable stratification. To investigate the possible impact of this, sensitivity tests could be undertaken using model input conditions for less stable atmospheric boundary layers, e.g., changing Pasquill stability class from D to C in Desert Tortoise Trials 1 and 2, or equivalently decreasing in the Monin-Obukhov length from 92.7 m or 94.7 m to -20 m.

Wind speed variability in DT4

Goldwire *et al*. (1985) noted in DT4 that the "test was performed late in the day while winds steadily slowed to 1.3 m/s. Low sun angle affected photography. Cloud remnants returned to test area after 3-4 hours." And also "In the case of DT4, the wind data were not recorded successfully and we used the values which were occasionally and irregularly saved from the real time display. Fortunately, due to the stability of the atmospheric conditions on DT4, this lack of complete data does not lead to appreciable error. More importantly for DT4, the arrival time of gas at the 800 m row suggests that the effects of the strong source jetting may still be present at 800 m. Thus the actual cloud speed at 800 m on that test was likely higher than the ambient wind speed. For the other tests, the ambient wind speeds were considerably higher and the cloud speeds probably had been reduced to the ambient wind speed by the time the clouds reached 800 m."

Because of the issue mentioned above with the failure to record wind speeds, there is no data available on the wind speed for DT4 over the first few minutes following the start of the release to see if the reported reduction in wind speed affected the measured concentrations at the 100 m and 800 m arrays. The variance in the wind speed was also not reported. If the dispersion behavior was dominated by jetting effects in DT4, the falling wind speed may not be a dominant factor. However, sensitivity tests could potentially be conducted to investigate the effect of the falling wind speed.

Ammonia liquid rainout in the Desert Tortoise trials

In the Desert Tortoise trials, some of the liquid ammonia from the jet rained-out and formed a pool on the ground. In Trials DT1 and DT2, there was water present on the ground surface when the tests took place, due to heavy rains on the preceding days. It was therefore difficult to establish how much liquid ammonia rained out. Goldwire *et al*. (1985) noted for DT1 "After spill, a dense, decimeter-high fog came off of the cold ground or ammonia pool in the region exposed to jet impingement" and for DT2 "Elevated pool temperatures in area of maximum ammonia pooling at end of test suggests exothermic reaction of ammonia with water." In the later trials, the surface water on the test site had cleared and it was easier to see the extent of the liquid ammonia pool deposited from the jet. Goldwire *et al*. (1985) noted "Desert Tortoise 4 definitely exhibited a pool on the ground after the test which slowly boiled off and persisted for almost ten minutes. Small puffs of boiled-off gas were seen off and on in the 100 m row to at least 1100 seconds after the start of the spill. Little of this gas was seen at 800 m. A portion of the spilled material was heated directly by the ground, presumably becoming buoyant and passing over the array" and with reference to DT4 "a large pooling on the ground (over 2000 m^2 in extent, and out to 90 m) quickly evaporated, forming a large, low cloud lower than 10 cm high; however, fog continued to form over the inner areas for at least 1200 s".

Goldwire *et al*. (1985) used temperature, concentration and flow speed measurements to calculate the mass flux through the 100 m and 800 m arcs. The anemometers at the two lowest positions were damaged by chemical effects of the ammonia jet and therefore they assumed a flow speed of 10 m/s at these positions in their calculations. They then integrated the calculated mass flux over time to produce the results shown in Table 8. They noted that “the results from the mass balance … will be less than the amount spilled if there [was] pooling of ammonia on the ground, absorption of ammonia into the surface water or soil, or if portions of the cloud did not pass through the array due to large wind shifts or to excessive height of the cloud”.

Table 8 Summary of calculated ammonia mass balance results for the Desert Tortoise trials

Trial	Mass released, m_r (kg)*	Mass calculated as passing through the 100 m arc, m_c (kg)*	Ratio m_r/m_c	Upper bound on rainout mass fraction
1	10,200	8,200	0.80	0.20
2	29,900	19,200	0.64	0.36
4	41,100	28,600	0.70	0.30

* Values from Goldwire *et al*. (1985)

Nielsen (1998) made the following comments on the Goldwire *et al*. (1985) mass flux analysis: “In order to calculate the mass flux through each sensor array, Goldwire *et al*. (1985) extrapolated the concentration to the surface, assuming negligible vertical gradient at the surface and constructed a parabolic fit through the two lowest measurements ... In the light of the propane profiles in figure 41 and the laboratory work of Britter and Snyder (1988), this assumption probably underestimates the ground-level concentrations”. The final column in Table 8 is therefore considered to provide an upper bound on the rainout mass fraction. These values of the rainout mass fraction were previously compared to rainout model predictions by Witlox *et al*. (2013) and Ichard (2012).

A different interpretation of rainout in the Desert Tortoise trials was given by Wheatley (1987) as follows: “No rainout of ammonia was seen in three of the trials. In the fourth trial a liquid pool was formed but it contained only about 10% of the total amount discharged”. The REDIPHEM database gave the pool mass fraction as “0.05 estimated” for all of the Desert Tortoise trials. Justification for this value of 0.05 was given by Nielsen and Ott (1996b) as follows: “According to Koopman *et al*. (1982) some of the liquid deposited in a pool covering up to 2000 m^3, but Koopman *et al*. (1986) state that: 'this pool represented, however, a small percentage of the total liquid spilled'. We interpret this as a rainout mass fraction of 5%”.[5]

Some dispersion models can account for rainout and pool evaporation, whilst other models cannot. Based on the above review of published work on this topic, for the purposes of this Jack Rabbit III modeling exercise it is recommended that if a model can account for rainout then a rainout mass fraction of 5% should be used for all of the Desert Tortoise trials as a baseline case – in line with the REDIPHEM database. Some atmospheric dispersion models feature specific sub-models for liquid rainout (e.g., PHAST), which could alternatively be used. If so, it would be useful to document this approach in the description of the model that is submitted to the coordinators of the exercise, along with details of the predicted rainout fraction. If a dispersion model cannot account for rainout, it is recommended that the stated mass flux given in Table 1 should be used (i.e., without reducing it by 5% to account for rainout). It is furthermore recommended that, if time allows, sensitivity tests be

[5] Their citation of Koopman *et al*. (1982) appears to be a mistake since this reference was a report on the Burro LNG trials. In any case, the Desert Tortoise trials took place in 1983 so the results were unknown in 1982. Instead, the reference was probably meant to be Goldwire *et al*. (1985).

undertaken in which the rainout mass fraction is varied between limits of zero to the upper bounding values given in Table 8 (for models that can account for rainout). A value of zero would enable direct comparison to models that cannot account for rainout. Some models may have the functionality to predict the extent of the ammonia pool. In which case, predictions could also be compared to the reported extent of the wetted area in DT4, i.e., "over 2000 m^2 in extent, and out to 90 m" (Goldwire *et al*., 1985).

Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24

Some models require the Pasquill stability class to specify the atmospheric stability, rather than the Monin-Obukhov length. For DT4, FLADIS16 and FLADIS24, the conditions were borderline between two stability classes, e.g., between D and E in DT4. Sensitivity tests could be undertaken to assess how this impacts the predicted concentrations, i.e., running separate simulations with Class D and E for DT4.

Wind and turbulence profiles in the FLADIS trials

As shown in Figure 1, there were buildings upwind of the release point in the FLADIS trials. The following statement is taken from Nielsen *et al*. (1994): "Because of the upstream buildings, the wind profile is not an equilibrium boundary layer, i.e., the turbulent fluxes will not have a simple relation to the roughness length and wind profile." Nielsen *et al*. (1997) recommended modelers to use measured wind and turbulence fields rather than parameters of a surface layer in equilibrium, due to the effect of upwind building wakes.

The FLADIS dataset included the following note on the aerodynamic roughness length[6]: "The area around the release point was covered by coarse gravel and the rest of the field had 10-30 cm grass with some patches of flowers and nettles. Within the first 100 m of the plume path the previous ammonia releases had caused a withering of the vegetation, especially close to the source. In campaign 2 the grass was shorter at the far end dispersion array than at 10-100 m. The wind and turbulence were affected by the upstream factory so use of the measured wind profiles and turbulence is better than to translate z_0 and u* values to u_{10} or vice versa. If such a dependence is inherent in a model, the optimal model z_0 input may depend on the feature to be examined. Based on wind profiles from the evening of Trial 16 corrected for stability using the measured M-O length and the Psi(z/L) stability correction functions of Businger, the roughness near the centerline mast of the far end dispersion arc was estimated to O(0.02 m). Wind profiles from the neutral dispersion mast during period in campaign 2 with winds from south-west (i.e., without obstructions) have also been examined. This suggested a roughness length of z_0=0.04 m around the neutral dispersion mast."

Turbulence conditions were given in data files distributed with the FLADIS dataset[7] and are summarized in Table 8. In addition, the time-varying measured wind speed, wind direction, temperature etc. are available in the FLADIS dataset[8]. The SMEDIS database also provides a summary of the mean wind speeds and their variance at the reference mast upstream of the release point and at the three downwind arrays.

[6] Source: file "Z0.TXT" in the FLADIS dataset folder r1_doc\FLADEXP\DOC\
[7] Source: file "INFO.TXT" in the FLADIS dataset folder FLADEXP\TRIALxxx\DOC\, where xxx is the trial number.
[8] For details, contact Morten Nielsen (nini@dtu.dk) or Simon Gant (simon.gant@hse.gov.uk).

Table 9 Wind and turbulence conditions for the FLADIS trials

		FLADIS9	FLADIS16	FLADIS24
Friction velocity, u_*	m/s	0.44	0.41	0.405
Monin-Obukhov length, L	m	348	138	-77
Turbulent temperature scale, T_*	C	0.042	0.093	-0.159
σ_u/u_*		2.68	2.30	2.39
σ_v/u_*		3.14	1.92	2.06
σ_w/u_*		1.57	1.22	1.26
σ_T/T_*		8.81	1.85	-1.86

Measurement uncertainty

- **Desert Tortoise - Wind speed**

Goldwire *et al*. (1985) provided the following description of the anemometers used to measure the average wind speed in the Desert Tortoise trials: "The wind field during the Desert Tortoise series of spills was measured by an array of eight or ten 2-axis anemometers mounted at heights of 2 m above the ground. The array covered an area from 1000 m upwind of the spill point to 2800 m downwind, as shown in Fig. 7 and the Experiment Descriptions. Wind speed and direction were measured every second and averaged within each remote station for a 10-sec period. Mean values of speed and direction, and the standard deviation about the mean wind direction for the 10-sec period were calculated and transmitted to the data-recording trailer. … The average wind speed and average direction variability [i.e., the values given above in Table 1] are averages over the entire 2-axis anemometer array (omitting W9) for the three-minute period immediately after the spill valve open signal … The meteorological array consisted of eleven stations with Met-One two-axis, cup-and-vane anemometers (all at a height of 2 m), plus a 20-m tall meteorological tower and station located 50 m upwind of the spill area. The Met-One anemometers had starting thresholds of 0.2 m/s, a response distance constant of 4.6 m, and accuracy of ±1% (~0.7 m/s)."

The accuracy figure here seems to suggest a wind speed of 70 m/s for 1% to give an absolute value of 0.7 m/s. It is unclear if this was a typographical error. The model of the anemometer was not provided, so it is not possible to confirm this with the manufacturer.

- **Desert Tortoise – Temperature**

Goldwire *et al*. (1985) reported that the ambient temperatures on the 10 m high meteorological masts were measured to within ±0.1°C measured using resistive temperature detectors (RTDs) composed of 1000 ohm platinum resistance elements mounted in aspirated solar shields.

Temperatures in the dispersing ammonia cloud were measured using "20-mil diameter, Type K thermocouples with a response time of about one second". Goldwire *et al*. (1985) noted that "The reference junction and amplifiers for the thermocouples tended to drift over the long periods of time in the field. It was not uncommon that the temperature readings throughout the array would incorrectly show a spread of > 5°C. However, the relative temperature variations during vapor cloud passage are felt to be quite accurate (± 0.5°C). Consequently, all of the thermocouple data of the mass flux and dispersion arrays were shifted to correspond to the average value of the G01 RTD pre-spill temperature at 2 m."

- **Desert Tortoise – Ammonia Concentrations**

Gas concentrations and temperatures were measured at seven stations on the 100 m array, at heights of 1 m, 2.5 m and 6 m, and at five stations on the 800 m array at heights of 1 m, 3.5 m and 8.5 m above ground level. The primary means of recording concentrations at 100 m used Mine Safety Appliances (MSA) nondispersive infrared (NDIR) gas sensors. These NDIR gas sensors measured the total ammonia concentration present by passing the ingested gas and aerosol through a heating apparatus to vaporize the aerosol. Concentrations at 800 m were measured primarily using International Sensor Technology (IST) solid state gas sensors which worked over a range of 0 – 3%. They were reported to be "somewhat sensitive" to humidity and the measurements were believed to be reliable to within ±20% (in relative terms). The IST sensors only registered the vapor component of the ammonia cloud. Any aerosol component was not detected.

Goldwire *et al*. (1985) presented comparisons of concentrations measurements from the NDIR and IST sensors to those recoded from Lawrence Livermore National Laboratory Infrared LLNL-IR sensors. These LLNL-IR sensors had a greater dynamic range of gas concentration than the IST sensors and served as a check on sensor calibrations. Comparison of LLNL IR and IST gas sensor results suggested the IST sensors were accurate to ±20% (in relative terms).

When presenting gas concentrations in figures in their report, Goldwire *et al*. (1985) noted: "To reduce noise fluctuations, the gas concentration data were smoothed prior to usage with a 3-second sliding average." For this modelling exercise, the primary means of comparing model predictions to the data for arc-max concentrations uses long time-averages (see Table 1). Modelers could also optionally compare to the short time-averaged concentration data.

- **FLADIS**

The accuracy of measurement equipment used in the FLADIS trials was described in detail in the report by Nielsen *et al*. (1994). In summary, they include:

- Load cells for measuring ammonia release rate: better than 0.5%
- Wind speed from Solent ultrasonic anemometer: ± 1% below 30 m/s for 10 s average
- Ammonia concentration sensors
    - Dräger Polytron NH_3: repeatability better than 5% of measured range
    - Dräger Polytron Ex: repeatability better than 2.5% of measured range
    - UVIC detector: accuracy not given

Most of the concentration sensors were arranged on three arcs at distances of 20 m, 70 m, and 238 m (or 240 m). The horizontal separation of the instruments increased from 3 m on the first arc to 10 m on the last one. About 5 instruments were simultaneously exposed to plume concentrations on each arc.

The Dräger Polytron Ex catalytic sensors were used to measure high concentrations on the first two arcs and the Dräger Polytron NH_3 electrochemical cells were used on the third arc. The UVIC sensors had a fast response time but were limited to low concentrations in the range 0-2000 ppm and were used on the third arc. High concentrations were also deduced from sonic anemometers with attached thermocouples.

The sensors all measured only the vapor concentration and did not account for the aerosol component (unlike Desert Tortoise NDIR sensors). Nielsen *et al*. (1997) estimated that maximum aerosol liquid fraction would be 2% at the first arc at 20 m, which would give measurement errors less than the sensor accuracy.

To assess measurement accuracy, Nielsen *et al*. (1997) compared concentration measurements using two different types of sensors at nearly identical locations (up to 1 m apart horizontally). The differences in mean concentrations were in the range 10-17% in relative terms (see Table 5 in their paper). The variability was partly attributed to the different temporal response times of the instruments and the spatial separation between sensors.

Uncertainties in the reported mass release rate from the ammonia storage tank were assessed by comparing the time integral of the release rate to the tank weight[9]. The average error in the release rate was reported to be 1.9% for the 4.0 mm nozzle (Trial 16) and 5.2% for the 6.3 mm nozzle (Trials 9 and 24).

Details of some other uncertainties in FLADIS Trials 9, 16 and 24 are mentioned in the narrative description of the trials, which were distributed with the data files[10].

For further details of the accuracy of the FLADIS test equipment, see Nielsen *et al*. (1994).

Summary of Suggested Sensitivity Tests

Based on the above review of modeling uncertainties, several suggestions for optional model sensitivity studies are summarized below. The tables provide the baseline value (from Table 1) and alternative values that could be used in sensitivity tests. The choice of some input values for the sensitivity tests is fairly arbitrary. For example, to assess the impact of water entrained into the jet from the ground in DT1 and DT2, it is suggested to increase the ambient humidity to 50% RH. Other values could be chosen but this is considered a starting point and the suggested values provide a means of comparing the behavior of one model to another, using the same inputs.

1.) Standing water at the Frenchman Flats test site in Desert Tortoise trials DT1 and DT2

		DT1	**DT2**
Relative humidity (%)	Baseline	13.2	17.5
	Sensitivity test	50	50
Monin-Obukhov length (m)	Baseline	92.7	94.7
	Sensitivity test	-20	-20
Pasquill stability class	Baseline	D	D
	Sensitivity test	C	C

[9] The results were described in file “SOUREERR.TXT” distributed with the FLADIS dataset.
[10] Files “INFO.TXT”. Please contact Morten Nielsen or Simon Gant for further information, if interested.

2.) Wind speed variability in DT4

		DT4
Site average wind speed (m/s)	Baseline	4.51
	Sensitivity test	3.0

3.) Ammonia liquid rainout in the Desert Tortoise trials

- For models that have the capability to simulate a fixed fraction of liquid raining out from the jet and depositing to form an evaporating pool on the ground:

		DT1	DT2	DT4
Rainout mass fraction (%)	Baseline	5	5	5
	Sensitivity test (min)	0	0	0
	Sensitivity test (max)	20	36	30

- Tests could also be performed with rainout sub-models (if available)
- Compare predicted size of deposited ammonia pool to observed wetted area, if possible

4.) Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24

- For models that use Pasquill stability class instead of Monin-Obukhov length to specify the model atmospheric boundary layer, the following tests could be undertaken:

		DT4	FLADIS16	FLADIS24
Pasquill stability class	Baseline	D	D	C
	Sensitivity test	E	E	D

5.) Wind and turbulence profiles in the FLADIS trials

- Use wind profiles specified in the SMEDIS database and turbulence conditions specified in Table 8 or those extracted directly from the FLADIS dataset measurements (if possible).

Optional Model Outputs

If modelers have sufficient time, some suggested optional outputs for this exercise are:

1.) Predicted plume widths using a long averaging time (as specified in Table 1). Outputs can be compared to the measured values given in Tables 5 and 6 above.

2.) Arc-max concentrations using a short averaging time of 1 s in Desert Tortoise trials for comparison to data in the MDA database (Hanna *et al.*, 1993).

3.) Arc-max concentrations and plume widths using the moving frame of reference for comparison to data presented in Table 3 of Nielsen and Ott (1996a) or Table 4 of Nielsen *et al.* (1997) (just for the FLADIS trials). Note that the averaging time needed for these predictions is longer than that given in Table 1 – see the final column (T_{obs}/T_{dur}) in Table 3 of Nielsen and Ott (1996a) and Table 4 of Nielsen *et al.* (1997). T_{obs} is the observation (or averaging) time and T_{dur} is the duration of the release, which is given in Table 2 of Nielsen and Ott (1996a) and Nielsen *et al.* (1997).

4.) Mean temperatures on the plume centerline in Desert Tortoise trials DT1 and DT2 and FLADIS Trials 9, 16 and 24. These can be compared to measured values given in the SMEDIS database.

5.) Results from the suggested sensitivity tests described above.

Useful Background Information Sources

- **Desert Tortoise**
  - The original data report of Goldwire *et al*. (1985)
  - Preliminary summary report by Koopman *et al*. (1984)
  - Analysis by Spicer and Havens (1987) and DesAutels and Schulman (2010)
  - Dataset available on request from Joe Chang (jchang@rand.org)

- **FLADIS**
  - Risø reports by Nielsen *et al*. (1994) and Nielsen and Ott (1996a)
  - Journal paper by Nielsen *et al*. (1997)
  - Supporting reports by CERC (Britter, 1994; 1995; Edmunds and Britter, 1994)
  - Analysis by Labovský and Jelemenský (2011)
  - Dataset and Risø reports available from Morten Nielsen (nini@dtu.dk)

- **SMEDIS**
  - Summary paper by Carissimo *et al*. (2001)
  - Report by CERC (2000)
  - Dataset, reports and paper pre-prints available from https://admlc.com/smedis-dataset/

- **REDIPHEM**
  - Risø reports by Nielsen and Ott (1996b) and Nielsen (1998)
  - Dataset and Risø reports available from Morten Nielsen (nini@dtu.dk)

- **MDA**
  - Report by Hanna *et al*. (1993)
  - Conference presentation by Chang and Hanna (2016)
  - Dataset available on request from Joe Chang (jchang@rand.org)

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