

Jack Rabbit III Modelers Working Group

Equivalent Vapor-Only Source Conditions: Cloud Aspect Ratio for the Desert Tortoise Trials

Version 1.1, 30 March 2022

Simon Gant¹, Rory Hetherington², Alison McGillivray³, Graham Tickle⁴.

¹ UK Health and Safety Executive (simon.gant@hse.gov.uk)

² UK Health and Safety Executive (rory.hetherington@hse.gov.uk)

³ UK Health and Safety Executive (alison.mcgillivray@hse.gov.uk)

⁴ GT Science and Software (graham.tickle@gtscience.co.uk)

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Changelog

Version 1.1 Clarified that “Cloud width, $2\sigma_y$ ” means “Cloud full-width, $2\sigma_y$ ” in Table 4 on Page 12, to avoid confusion with the cloud half-width, σ_y . The nomenclature has also been updated with this clarification on Page 13.

Background

Model input conditions for the Jack Rabbit III inter-comparison exercise on Desert Tortoise and FLADIS were provided in the document “Initial Modeling Exercise (2021-2022)” (File: JRIII initial modeling exercise description v2.3.pdf). Within this document were the equivalent vapor-only conditions, which

were originally provided in the SMEDIS database (Carissimo *et al.*, 2001). However, source conditions for Desert Tortoise trial 4 were absent, because the SMEDIS database did not examine that trial.

On 12 January, a document was circulated to the JR III MWG participants called “Equivalent Vapor-Only Source Conditions for the Desert Tortoise Trials” (File: JR III MWG equivalent source conditions for Desert Tortoise v1.2.pdf) which provided equivalent vapor-only source conditions for the Desert Tortoise trial 4. The calculation of these source conditions was based on the method used in the SMEDIS project, which was described in Appendix 4 of the report by CERC (2000).

Subsequently, Steven Hanna tested these source conditions with the Britter and McQuaid (1988) dispersion model and found that predictions were sensitive to the shape of the equivalent vapor-only source. In the SMEDIS project, the source was specified to be a vertical rectangular window with a width to height aspect ratio of 2 (see Figure 1). Steven questioned the basis of this choice of aspect ratio and asked if there was any data available from the Desert Tortoise experiments that could provide further clarification of the shape of the cloud at a position roughly 50 m downstream from the release point, where the jet was predicted to transition from a two-phase to a vapor-only cloud.

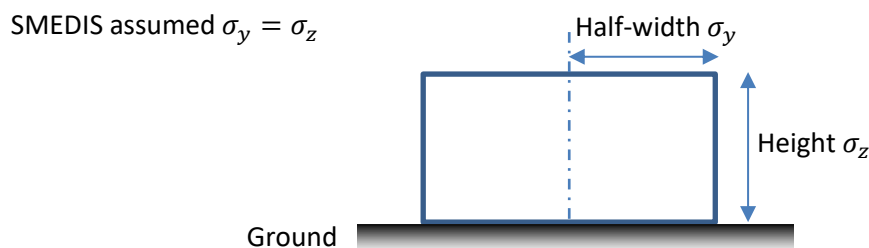


Figure 1 Shape of the equivalent vapor-only source for the Desert Tortoise trials as specified by the SMEDIS project, which consisted of a vertical rectangular window with a width to height aspect ratio of 2

This document summarizes the results of the investigation into this matter. It includes:

- Analysis of video footage from the Desert Tortoise trials
- Analysis of gas concentration measurements at the first line of sensors (at a downstream distance of $x = 100$ m)
- Modelling of the dispersion behavior in the first hundred meters of the Desert Tortoise trials, to understand how measurements at 100 m can be extrapolated back to the equivalent source location at $x \approx 50$ m.

The document concludes with new recommendations for the shape of the equivalent vapor-only source in the Desert Tortoise trials and some suggestions for sensitivity tests.

Desert Tortoise Video Footage

Joe Chang (RAND Corp.) provided the following links to videos of the Desert Tortoise trials:

1. DOE video
 - https://drive.google.com/file/d/1AKINc_ggFiwtz1SF_c9TqDvJhawa8YFD/view?usp=sharing
2. LLNL Desert Tortoise video
 - https://drive.google.com/file/d/1MjuJKluLPP9Qm6AC2Ovy_j_DMMYSIDge/view?usp=sharing

Snapshots taken from these videos are shown in Figures 2 to 4. Whilst the videos provide useful qualitative insight into the dispersion behavior, it is difficult to determine from them any quantitative values of cloud widths and heights. The investigation has therefore focused on the concentrations measured in the Desert Tortoise trials at the first downstream line of sensors at 100 m.

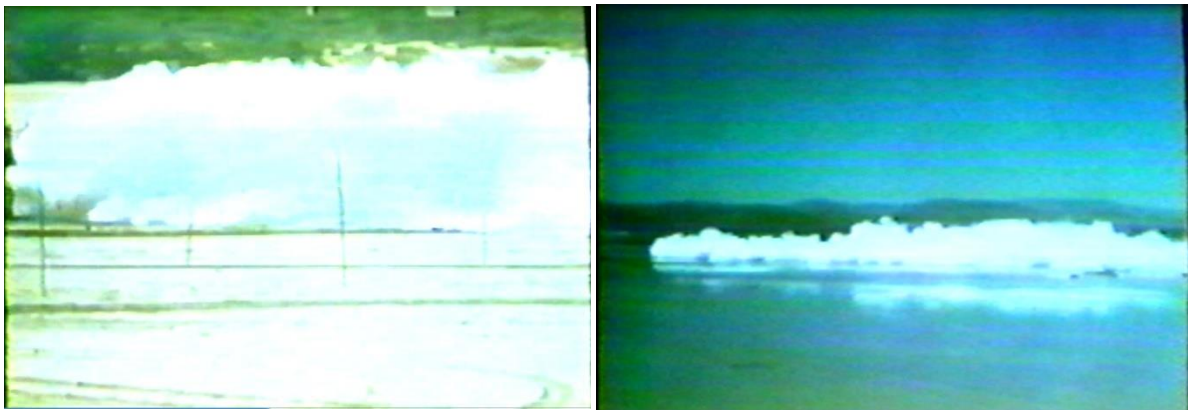


Figure 2 Still images from the DOE video of the Desert Tortoise trials



Figure 3 Still images from the LLNL Desert Tortoise video showing the location of cameras and a snapshot of Trial 2 from the wide upwind camera



Figure 4 Still images of Trial 2 (top) and Trial 4 (bottom) from the LLNL Desert Tortoise video from the wide side camera

Desert Tortoise Concentration Data

Three sources of data were examined in the current work:

1. Raw data files of measured concentrations over time at each sensor, provided by Joe Chang
2. Desert Tortoise data report by Goldwire *et al.* (1983)
3. Spreadsheets of processed data produced by the SMEDIS project (files “dt1.xls” and “dt2.xls” in file “batch1_24.zip”, which can be downloaded from here: <https://admlc.com/smedis-dataset/>)

The raw data (Item 1 above) consisted of ASCII text files of concentrations recorded every 1 s for a total of 1000 time steps, yielding approximately 17 minutes of data for each sensor. The Desert Tortoise trials used two sensor arrays spanning the lateral direction (y) and vertical direction (z) at two downstream positions of $x = 100$ m and 800 m, which were called the mass flux array and dispersion array, respectively. Each line of sensors recorded concentrations at three separate heights. A summary of these sensor locations is given in Table 1.

There were two cases of missing data. Firstly, there were no measurements for the highest of the three sensors on each mast of sensors on the 100 m arc in Trial DT1. This meant that it was not possible to determine the cloud height in that trial. Therefore, no estimation has been provided here of the cloud aspect ratio for DT1 at 100 m.

Secondly, data for one mid-height sensor on the 100 m arc (Sensor G03) was absent in Trial DT2. A linear interpolation using data from the neighboring sensors (G02 and G04) was used here to replace that data.

In line with Goldwire *et al.* (1983), a moving average was applied to smooth the raw data with a window of 3 s. No additional outlier detection and replacement was applied, apart from the aforementioned interpolation onto missing data and moving average. The arrival and departure times of the cloud at each arc were estimated from the times at which 10% and 90% of the total dose (i.e., concentration integrated over time) had been recorded. Concentrations were then time-averaged within this window, i.e.:

$$C = \langle C'(t_1 < t < t_2) \rangle \quad (1)$$

where C' is the instantaneous concentration, t_1 and t_2 are the times taken to record 10% and 90% of the total cumulative dose, respectively, and angled brackets $\langle \rangle$ denote time averaging. This method of determining time-averaged concentrations was used in the SMEDIS project to process the Desert Tortoise data (see Appendix 3 in CERC, 2000).

Table 1 Sensor locations for Desert Tortoise trials

	Station	x (m)	y (m)	z_1 (m)	z_2 (m)	z_3 (m)
Mass flux array	G02	100	-45.72	1.0	2.5	6.0 ^a
	G03	100	-30.48	1.0	2.5 ^b	6.0 ^a
	G04	100	-15.24	1.0	2.5	6.0 ^a
	G05	100	0	1.0	3.5	6.0 ^a
	G06	100	15.24	1.0	2.5	6.0 ^a
	G07	100	30.48	1.0	2.5	6.0 ^a
	G08	100	45.72	1.0	2.5	6.0 ^a
Dispersion array	G20	800	-200	1.0	3.5	8.5
	G21	800	-100	1.0	3.5	8.5
	G22	800	0	1.0	3.5	8.5
	G23	800	100	1.0	3.5	8.5
	G24	800	200	1.0	3.5	8.5

Notes:

^a Missing file- no sensor data for the highest arc in trial DT1 available.

^b No sensor data at G03 in the trial DT2.

Cloud Aspect Ratio

The cloud aspect ratio was defined here as follows:

$$AR = \frac{2\sigma_y}{\sigma_z} \quad (2)$$

where σ_y and σ_z are the cloud half-width and height, respectively. Methods to calculate σ_y and σ_z are now discussed.

Cloud Full-Width, $2\sigma_y$

The cloud width can be calculated a few different ways. Firstly, from the method of moments:

$$\sigma_y^2 = \frac{\sum C y^2}{\sum C} - \left[\frac{\sum C y}{\sum C} \right]^2 \quad (3)$$

where the summation is taken over all lateral positions at a fixed height. In the Desert Tortoise trials at the 100 m arc, this height was the lowest sensor height on each mast, which was at a height $z = 1$ m. The cloud width was estimated using the method of moments in the SMEDIS project.

Secondly, the cloud half-width can be defined as the distance from the cloud centerline (the position of maximum concentration, C_m), to the lateral position where the concentration first drops below $C_m/\sqrt{e}$ (see Figure 5). This was the method used in the Modelers Data Archive (Hanna *et al.*, 1993; Chang and Hanna, 2016). It is reported to be less sensitive to outliers than the method of moments. For a Gaussian profile, the two approaches should give identical values of σ_y .

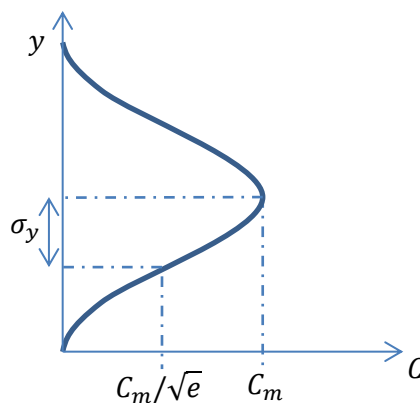


Figure 5 Calculation of σ_y from the concentration distribution

Alternative methods of calculating σ_y include using different threshold values instead of $C_m/\sqrt{e}$. For example, in the Jack Rabbit II model inter-comparison exercise, cloud widths were determined from the experimental data using the positions where concentrations fell to 20 ppm or 200 ppm (Mazzola, 2020).

In the present work, to be consistent with the SMEDIS data used for the modeling exercise, the method of moments was used to calculate the cloud half-width σ_y (Eqn. 3). Calculated values of the cloud half-width, σ_y , are given in Table 2 along with values from the SMEDIS and MDA databases. Interestingly, there is closer agreement between the present results and the MDA values, despite the present work using the same calculation method as SMEDIS.

As a cross-check on these calculated cloud widths, Figure 6 shows contour plots of the measured concentrations over time on the lowest sensors on the 100 m arc. Trial DT1 produced a compact cloud with a fast drop off in concentrations at approximately $t = 150$ s. This was due to the shorter release

time of $T = 126$ (s) for DT1, compared to $T = 255$ (s) and $T = 381$ (s) for DT2 and DT4, respectively. Figure 6 shows that the cloud width was largest in Trial DT4, which is consistent with the calculated σ_y given in Table 2.

Table 2 Mean values of cloud half-width σ_y from the present work and the SMEDIS and MDA databases

	DT1	DT2	DT4
Present work	11.7	14.8	16.0
SMEDIS database	13.7	15.9	N/A ^a
MDA	11.8	14.7	15.7

^a The SMEDIS database does not contain data for DT4.

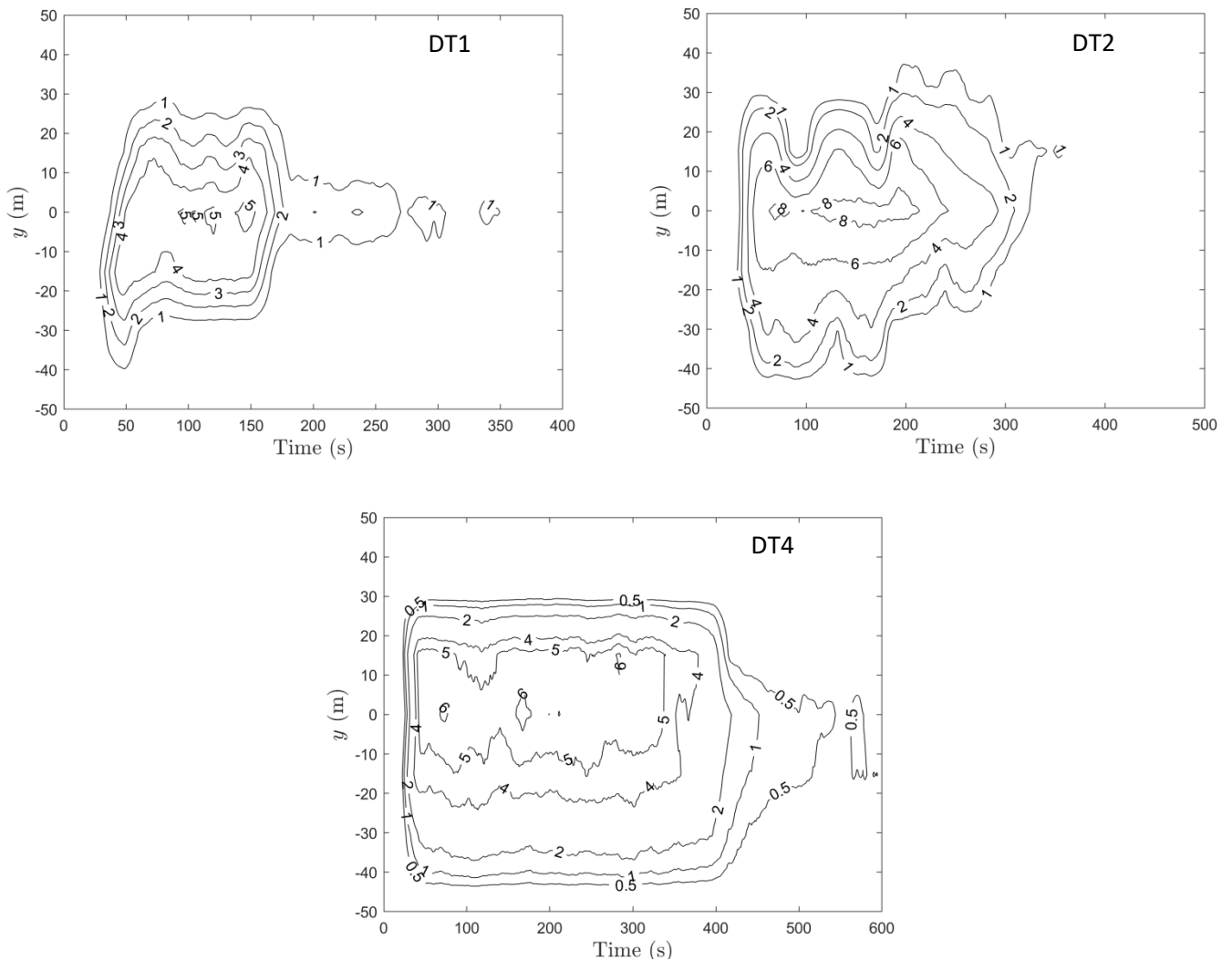


Figure 6 Contours showing the change in ammonia concentration (% v/v) over time at the lowest sensors on the 100 m arc in Desert Tortoise trials 1, 2 and 4.

Cloud Height, σ_z

In the Desert Tortoise trials, sensors were positioned at three heights on each mast (see Table 1). To estimate the cloud height, an exponential function was fitted to the measured concentration data in the form:

$$C(z) = A \exp \left\{ - \left(\frac{z}{a} \right)^s \right\} \quad (4)$$

where A is a constant of proportionality, a is a cloud vertical length scale, and s is a shape parameter. Values of A , a , and s were fitted to the data using the MatLab function “fminsearch” and the cloud height was then calculated from:

$$\sigma_z^2 = \frac{\Gamma\left(\frac{3}{s}\right)}{\Gamma\left(\frac{1}{s}\right)} a^2 \quad (5)$$

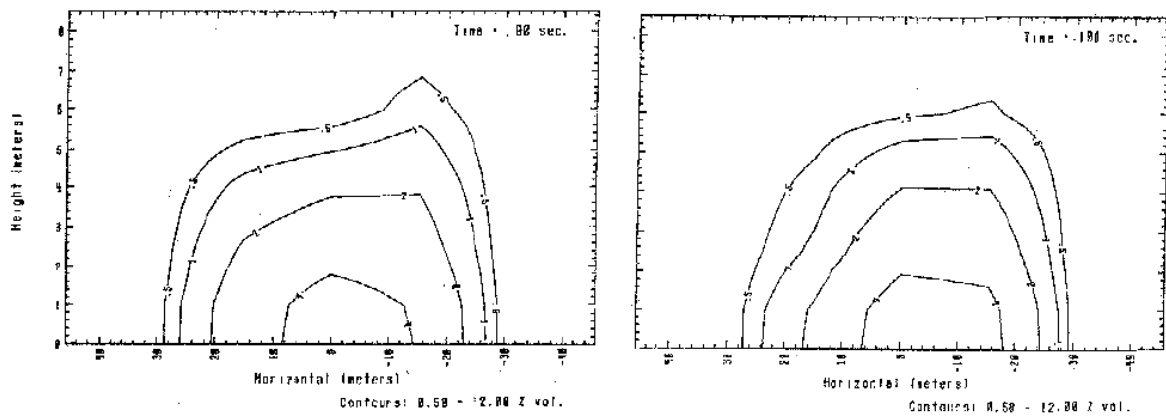
where Γ is the gamma function. The above formula is derived analytically from integration over the vertical profile.

In the Desert Tortoise trials, there were seven sensor masts across the 100 m arc. To improve the robustness of the fit to the data, parameters A , a and s were fitted to the data on each mast and then the final choice of A , a , and s was taken as the median of the values across the arc. The resulting cloud heights at 100 m in Trials DT2 and DT4 were $\sigma_z = 3.7$ m and 3.5 m, respectively.

Cloud Cross-Sectional Shape at 100 m

The report by Goldwire *et al.* (1993) included contour plots of the measured concentration in the vertical the y - z plane at various intervals in time. Some examples are given in Figure 7. To produce these plots, Goldwire *et al.* (1983) interpolated sensor data to ground level using the concentrations measured at the lowest sensors, C_1 , and the mid-height sensors, C_2 . If $C_2 < C_1$, the data was extrapolated to ground level using a quadratic function, assuming that the vertical gradient of concentration at ground level was zero. If $C_2 \geq C_1$, the concentration was extrapolated to ground level assuming a linear change in concentration. Concentrations were also assumed to decay to zero at a height of 12 m.

This same method has been used here to produce plots of the time-averaged concentration on the vertical y - z plane at the 100 m arc in Trials DT2 and DT4, see Figure 8. Contours for DT1 were not generated because of the missing data on the highest sensors. The calculated shape of the cloud as defined by width $2\sigma_y$ and height σ_z have been superimposed onto the plot as a dashed red box to visualize the cloud shape. For both trials the dashed box appears to have a similar aspect ratio to the cloud contour lines. For DT2, the dashed box is closely aligned with the mean concentration contour of 6 % (v/v).



Desert Tortoise 1 8/24/83

100m Row

Fig. 60a. DT1 Vertical Contours at 100 m.

Figure 7 Vertical contours at 100 m in Trial DT1 from Goldwire *et al.* (1983)

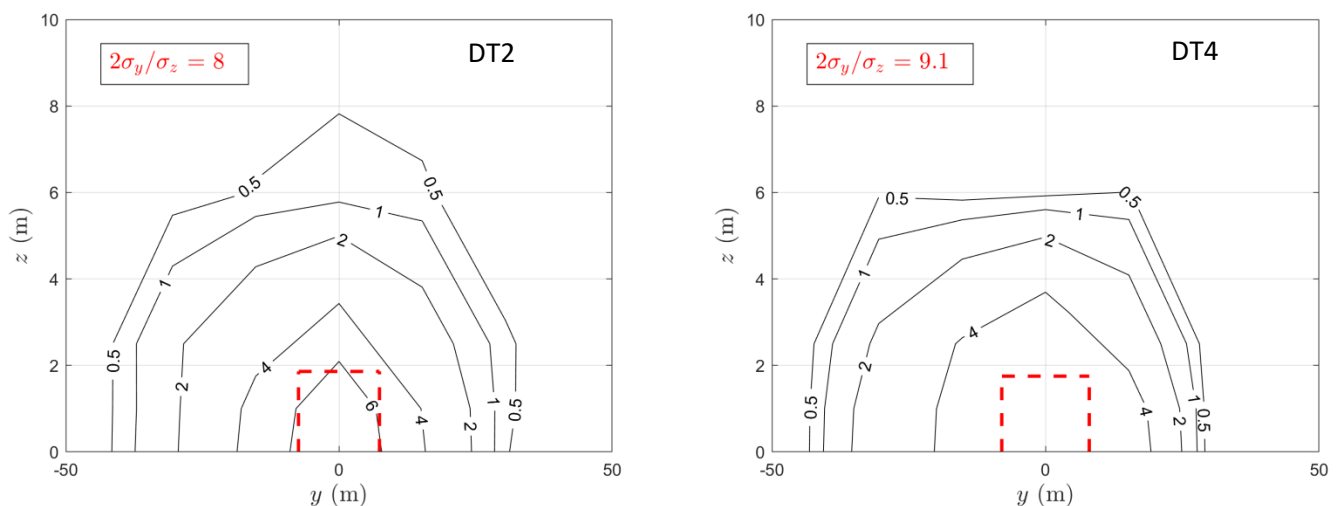


Figure 8 Contours of time-averaged concentration (% v/v) on the y-z plane at x=100 (m) for the Desert Tortoise trials DT2 and DT4. A dashed box is superimposed onto each plot with the mean cloud width and height calculated for each trial

Extrapolation of Cloud Dimensions from 100 m to 50 m

In the preceding analysis, the aspect ratio of the cloud was determined at the first line of sensors, located at a downstream distance of 100 m. The location of the equivalent vapor-only source in Trials 1, 2 and 4 was calculated to be approximately 50 m downwind from the release point (see Table 3). It is therefore necessary to extrapolate the cloud aspect ratio from 100 m to 50 m. To help inform what kind of extrapolation should be used, predicted cloud widths and heights were output from the integral models DRIFT and PHAST. Both of these models account for the transition from jet-dominated flow in the near field to dense gas behavior, and eventually to passive dispersion in the far field. The cloud width output from DRIFT incorporates the effects of plume lateral meander. DRIFT uses the exponential function for the vertical distribution of concentration, as given in Eqn. (4), and the value of cloud height was evaluated from Eqn. (5). For PHAST, the “effective” cloud width and depth were output from the model, which is equivalent to the DRIFT outputs when the profile is Gaussian.

Figure 9 compares the measured and the predicted cloud aspect ratios for the Desert Tortoise trials. From a distance of around 50 m to 200 m, the two dispersion models predict roughly a linear increase in aspect ratio with distance. Extrapolating linearly from the experimental data at 100 m to 50 m gives an aspect ratio of approximately $AR = 2\sigma_y/\sigma_z = 5$. There is some uncertainty in adopting this value for all of the Desert Tortoise trials. The aspect ratio at 100 m was slightly different in DT2 and DT4 ($AR = 8.0$ and 9.1 , respectively) and both of these trials involved larger release rates of ammonia than DT1 ($10.3 \text{ m}^3/\text{min}$ and $9.5 \text{ m}^3/\text{min}$, versus $7.0 \text{ m}^3/\text{min}$ in DT1). The assumed linear increase AR with distance is also only based on model predictions. For these reasons, it would be useful if time allows for modelers to undertake sensitivity tests using higher and lower values of AR . Given that the SMEDIS project assumed $AR = 2$, this seems like a suitable lower bounding value for model sensitivity tests, to enable like-for-like comparison to previous SMEDIS results. As an upper bound, it is proposed to use a value of $AR = 8$, based on the results shown in Figure 9.

Table 3 Recommended equivalent vapor-only source conditions for the Desert Tortoise trials for the Jack Rabbit III modeling exercise, from “Equivalent Vapor-Only Source Conditions for the Desert Tortoise Trials” (File: JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf)

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Temperature (K)
DT1	51.0	7.5	13	205
DT2	48.3	6.0	13	205
DT4	49.5	8.59	14.3	205

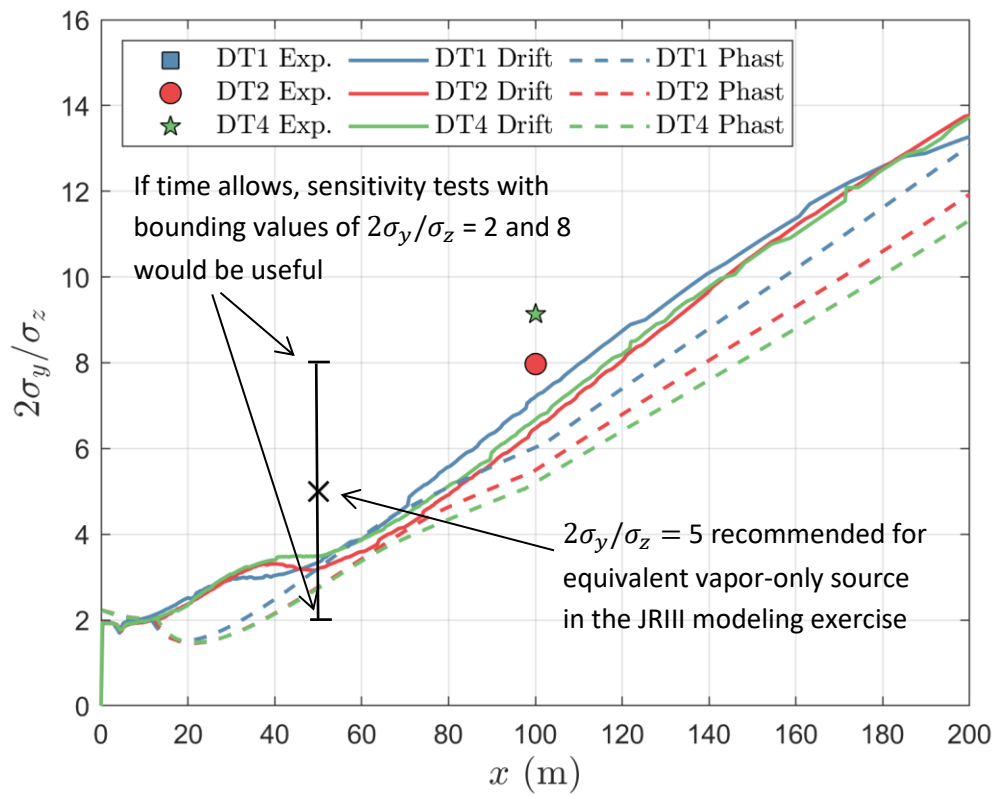


Figure 9 Aspect ratio of the Desert Tortoise clouds as a function of downstream position. Circle and star symbols show the values determined from the DT2 and DT4 experimental data at 100 m. Colored lines show model predictions from DRIFT and PHAST. Black cross indicates the value recommended for the JRIII modeling exercise, i.e., an aspect ratio of $2\sigma_y/\sigma_z = 5$.

Summary of Equivalent Vapor-Only Source Conditions

A summary of the recommended vapor-only source conditions for DT1, DT2, and DT4 is given in Table 4. Values of the downstream distance, velocity, molar concentration and temperature are identical to the values distributed previously in file “JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf”. Three new columns are present in this version of the table: density, cloud width and cloud height.

The density column has been added since models such as the Britter and McQuaid (1988) workbook require a cloud density as a model input. The values given here were calculated from the molar concentration and temperature using the following expression:

$$\rho_j = \frac{\alpha_{gj}M_g + (1 - \alpha_{gj})M_a}{\frac{\alpha_{gj}M_g}{\rho_{gj}} + \frac{(1 - \alpha_{gj})M_a}{\rho_{aj}}} \quad (6)$$

where α is the mole fraction, M is the relative molecular mass and ρ the density. Subscripts g and a refer to ammonia and air, respectively, and subscript j refers to the vapor-only jet conditions (see “JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf” for further details).

The final additional two columns in Table 4 of cloud width and height were calculated based on the aspect ratio of $AR = 2\sigma_y/\sigma_z = 5$. These values supersede the previous values given in “JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf”, which assumed an aspect ratio of $AR = 2$. The cross-sectional areas of the source are unchanged from values given previously, but the aspect ratio has been changed to $AR = 5$.

These are the source conditions that should be used by default by modelers participating in the JRIII modeling exercise, if their model does not have the ability to simulate two-phase source conditions. If time allows, it would be useful for modelers to assess the impact of varying the source aspect ratio between limits of $AR = 2$ and 8 (whilst keeping the source area the same).

Table 4 Recommended equivalent vapor-only source conditions for the Desert Tortoise trials for the Jack Rabbit III modeling exercise

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Density ^d (kg/m ³)	Temperature (K)	Full-Width, $2\sigma_y$ (m) ^a	Height, σ_z (m) ^a
DT1 ^b	51.0	7.5	13	1.46	205	20.2	4.0
DT2 ^b	48.3	6.0	13	1.46	205	26.6	5.3
DT4 ^c	49.5	8.59	14.3	1.44	205	22.1	4.4

Notes:

^a The source size has been specified as a rectangular window of with aspect ratio $2\sigma_y/\sigma_z = 5$.

^b These conditions come from the SMEDIS database, <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”.

^c The calculation method used to find these values was described in values calculated here using the method described in “Equivalent Vapor-Only Source Conditions for the Desert Tortoise Trials” [File: JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf]

^d Cloud densities were calculated from the ammonia concentration and temperature, using ideal gas law.

Nomenclature

Roman

a	Shape parameter
A	Constant of proportionality
b	Shape parameter
C	Time-averaged concentration
C'	Instantaneous concentration
C_m	Centerline concentration
M	Relative molecular mass
x	Distance downwind
y	Lateral direction
z	Vertical direction

Greek

α	Mole fraction
ρ	Density
σ_y	Cloud half-width
σ_z	Cloud height

Symbols

$\langle \rangle$	Time averaging
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Subscripts

a	Air
g	Ammonia
j	Vapor-only jet conditions

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