RESEARCH AND GUIDANCE FROM HSE

Design of the Jack Rabbit III international model inter-comparison exercise on Desert Tortoise and FLADIS

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26th Annual George Mason University Conference on Atmospheric Transport and Dispersion Modeling

July 26-28, 2022

Outline

- Aims
- Methodology
- Participation and benefits
- Modeling
  - Inputs
  - Outputs
- Coordination of the exercise
- Learning points
- Summary

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Aims

- Run a model inter-comparison exercise to evaluate the performance of atmospheric dispersion models using data from previous ammonia release experiments
  - To understand the accuracy of models that may be used to design the Jack Rabbit III trials, e.g. to design the JRIII sensor array
  - To identify important model input parameters that we may need to carefully assess or measure in the trials

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Methodology

- Simulate 3 trials each from the Desert Tortoise and FLADIS pressure-liquefied ammonia field trials
- Desert Tortoise
  - Tests conducted in 1983 at DOE Nevada Test Site
  - Release rates of 81 – 133 kg/s
  - 10 – 41 tonnes of ammonia released
  - Dispersion measurements at 100 m and 800 m
  - Largest tests to date on ammonia
- FLADIS
  - Tests conducted in 1993-4 at Landskrona, Sweden
  - Release rates of 0.25 – 0.55 kg/s
  - Dispersion measurements at 20 m, 70 m and 240 m (transition from dense to passive dispersion)

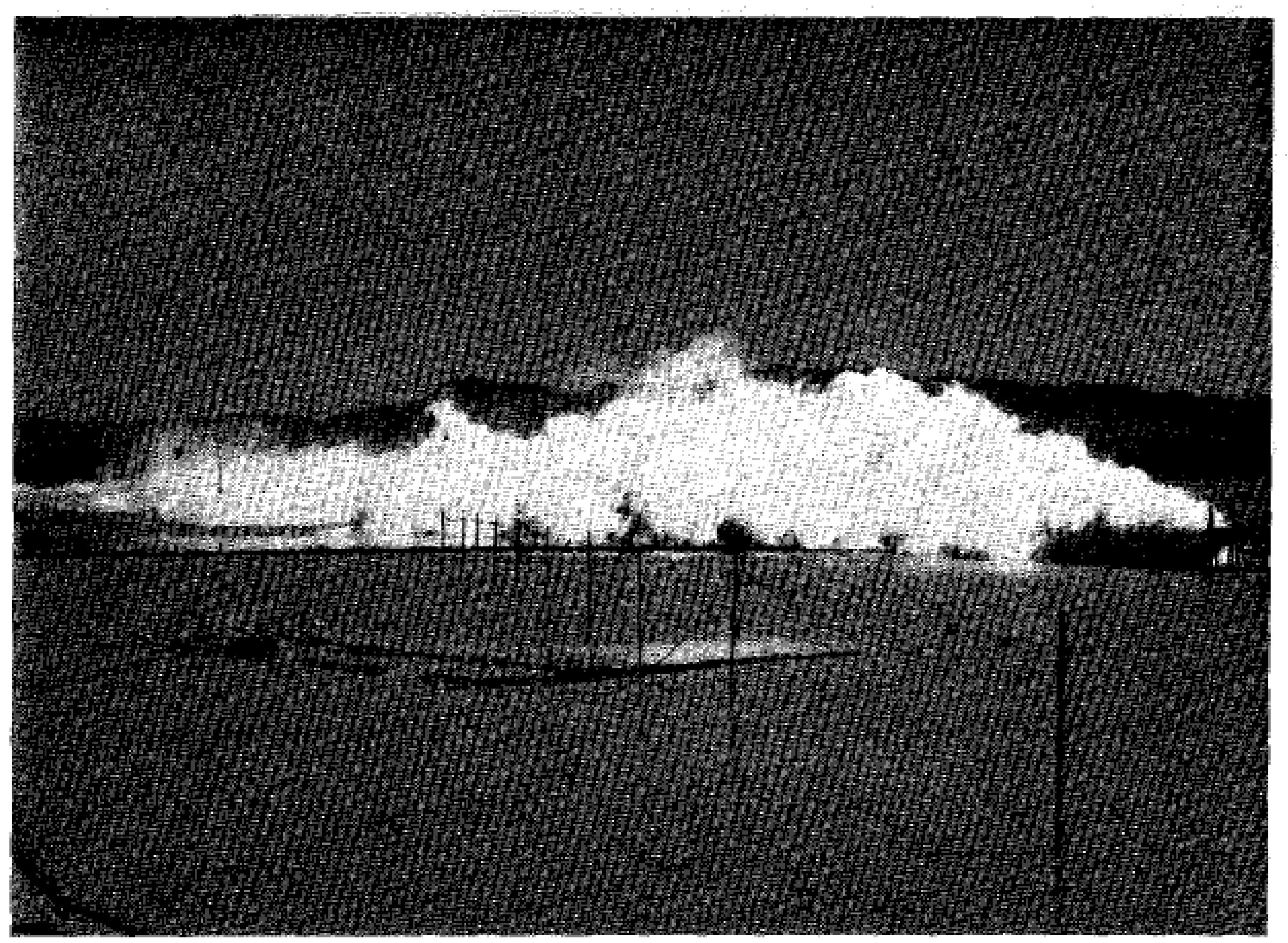

Fig. 15. Desert Tortoise 2 (upwind wide angle camera) Time = 230s. Lawrence Livermore National Laboratory

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Methodology

- Participants provided with specified set of model inputs for Desert Tortoise and FLADIS
- Requested to provide basic set of model outputs (as a minimum)
  - Long time-averaged centerline plume concentrations for each of 6 trials
- Optionally, modelers can provide additional model outputs
  - E.g., predicted plume widths, temperatures, results from sensitivity tests
- Coordinators collated results, cross-plotted predictions against experimental measurements and shared results with participants
- Not a competition but a collaborative effort, with the ultimate goal of improving toxic industrial chemical modeling tools in general
- Timeline
  - Exercise initiated over Winter 2021-2022
  - Results shared with participants in Spring 2022
  - Concluded in Summer 2022 with aim to present findings at GMU conference

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Participation and Benefits

- Work was voluntary, conducted on a “best endeavors” basis
- Participation was welcomed from government agencies, national laboratories, research corporations, universities, oil/gas/chemical industry and engineering consultancies
- All classes of model predictions were welcome
  - Emergency planning and response
  - Regulatory purposes
  - Research
  - e.g., nomograms, integral models, Lagrangian and CFD models
- Opportunity to benchmark models against existing ammonia field trial data, and to share knowledge and experience with other world experts
- Aim to publish the jointly-authored findings in one or more conference papers and in a peer-reviewed journal

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Modeling Inputs and Outputs

- Request for Information (RFI) document provided further details of the exercise

Jack Rabbit III Modelers Working Group

Initial Modeling Exercise (2021-2022)

Version 1.0, 25 October 2021

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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.

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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/).

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Modeling Inputs

		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
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

- All trials involved horizontal releases of pressure-liquefied ammonia over flat, unobstructed terrain
- Data taken primarily from SMEDIS database (https://admlc.com/smedis-dataset)
- Cross-checks carried out with other information sources
  - Modelers Data Archive
  - REDIPHEM
  - Original data reports, e.g. Goldwire *et al*. (1985)
  - Notes provided to explain choice of values

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Modeling and Measurement Uncertainties

- Standing water on the surface of the normally dry lake bed in the Desert Tortoise trials
  - Affected DT1 and DT2 trials, but dried out by the time DT4 test took place
  - Suggested to undertake sensitivity tests with enhanced humidity and/or unstable boundary layer
- Wind speed decreased during the DT4 trial
  - Wind speed also not recorded successfully
  - Largest release and jetting effects may have affected measurements out to 800 m
  - Suggested to undertake sensitivity test with lower wind speed
- Ammonia liquid rainout in DT4
  - "a large pooling on the ground (over 2000 m^2 in extent, and out to 90 m)"
- Pasquill Stability Classes in DT4, FLADIS16 and FLADIS24
  - Conditions on the borderline between Class D-E or C-D
- Wind and turbulence profiles in FLADIS trials
  - Effect of upwind obstacles on dispersion behavior
- Further details given in RFI document

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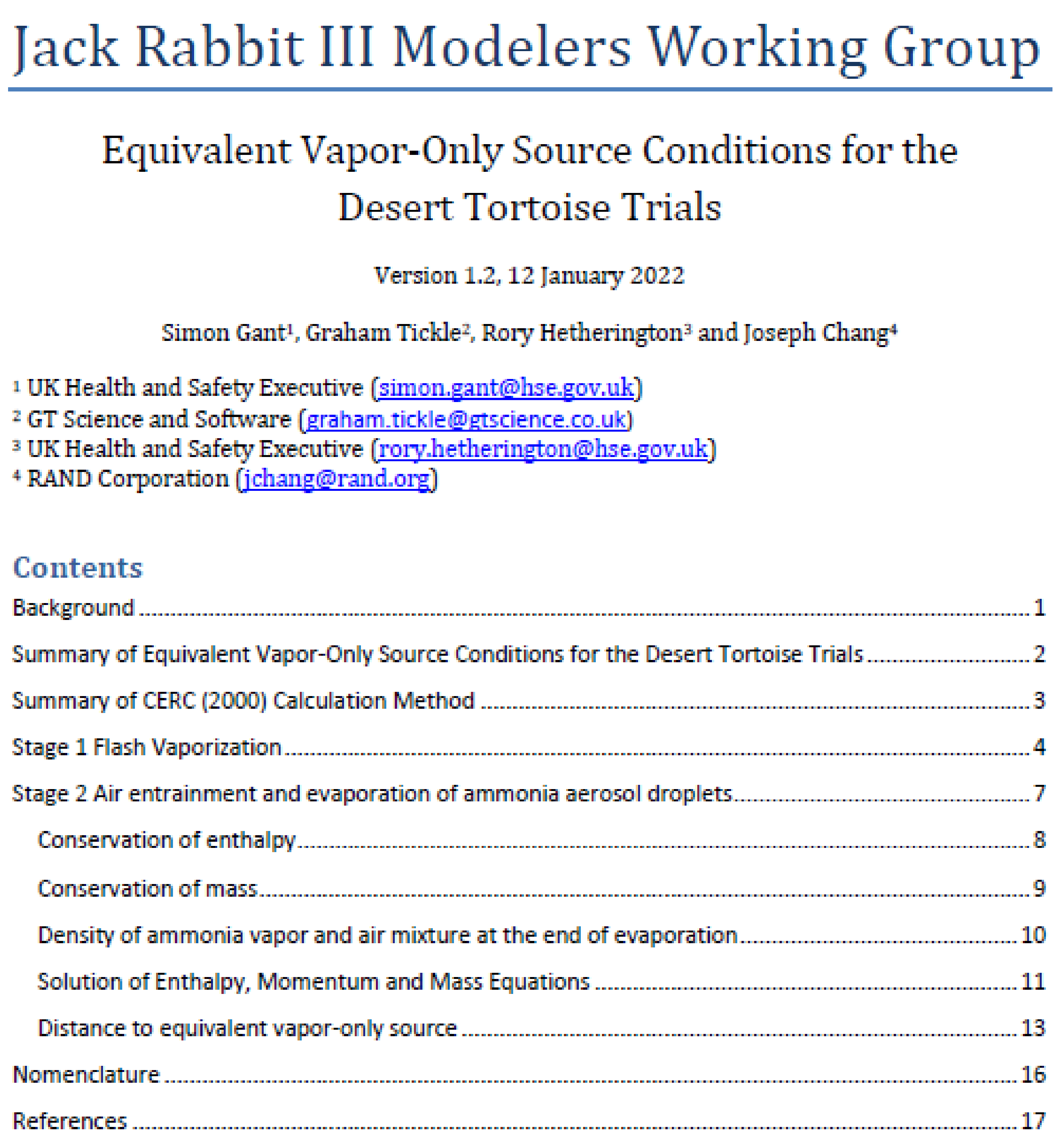
Equivalent Vapor-Only Source Terms

- Several modeling groups required equivalent vapor-only source conditions
- None available in SMEDIS for DT4 and so CERC method was coded up independently to provide DT4 conditions for modelers



Jack Rabbit III Modelers Working Group

Equivalent Vapor-Only Source Conditions for the Desert Tortoise Trials

Version 1.2, 12 January 2022

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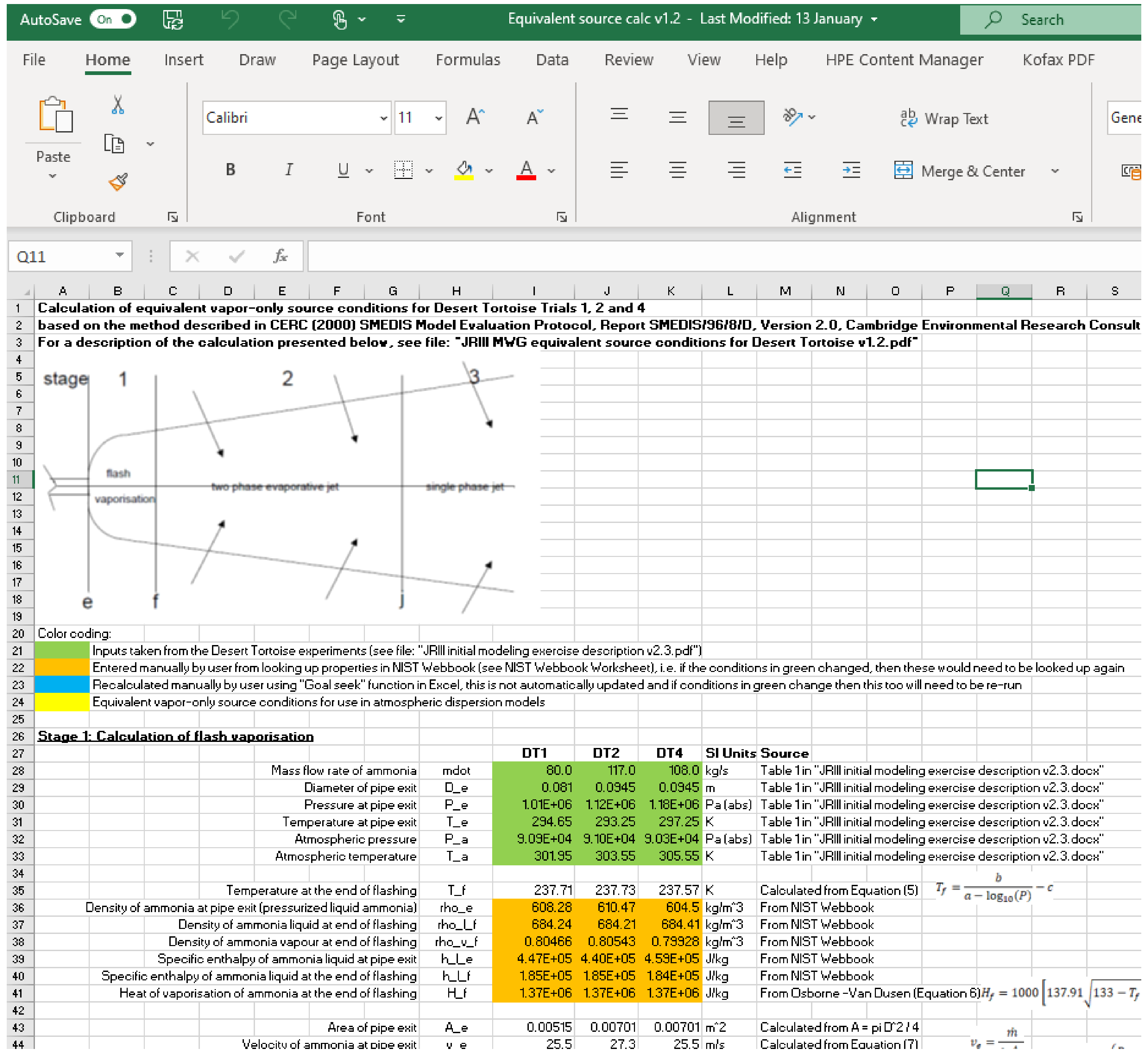
JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf



		DT1	DT2	DT4	SI Units	Source
Mass flow rate of ammonia	mdot	80.0	117.0	108.0	kg/s	Table 1 in "JRIII initial modeling exercise description v2.3.docx"
Diameter of pipe exit	D_e	0.081	0.0945	0.0945	m	Table 1 in "JRIII initial modeling exercise description v2.3.docx"
Pressure at pipe exit	P_e	1.01E+06	1.12E+06	1.18E+06	Pa (abs)	Table 1 in "JRIII initial modeling exercise description v2.3.docx"
Temperature at pipe exit	T_e	294.65	293.25	297.25	K	Table 1 in "JRIII initial modeling exercise description v2.3.docx"
Atmospheric pressure	P_a	9.09E+04	9.10E+04	9.03E+04	Pa (abs)	Table 1 in "JRIII initial modeling exercise description v2.3.docx"
Atmospheric temperature	T_a	301.95	303.55	305.55	K	Table 1 in "JRIII initial modeling exercise description v2.3.docx"
Temperature at the end of flashing	T_f	237.71	237.73	237.57	K	Calculated from Equation (5) $T_f = \frac{b}{a-\log_{10}(P)} - c$
Density of ammonia at pipe exit (pressurized liquid ammonia)	rho_e	608.28	610.47	604.5	kg/m^3	From NIST Webbook
Density of ammonia liquid at end of flashing	rho_L_f	684.24	684.21	684.41	kg/m^3	From NIST Webbook
Density of ammonia vapour at end of flashing	rho_v_f	0.80466	0.80543	0.79928	kg/m^3	From NIST Webbook
Specific enthalpy of ammonia liquid at pipe exit	h_L_e	4.47E+05	4.40E+05	4.59E+05	J/kg	From NIST Webbook
Specific enthalpy of ammonia liquid at the end of flashing	h_L_f	1.85E+05	1.85E+05	1.84E+05	J/kg	From NIST Webbook
Heat of vaporisation of ammonia at the end of flashing	H_f	1.37E+06	1.37E+06	1.37E+06	J/kg	From Osborne -Van Dusen (Equation 6) $H_f = 1000\,[137.91\sqrt{133 - T_f}$
Area of pipe exit	A_e	0.00515	0.00701	0.00701	m^2	Calculated from A = pi D^2 / 4
Velocity of ammonia at pipe exit	v_e	25.5	27.3	25.5	m/s	Calculated from Equation (7)

Equivalent source calc v1.2.xlsx

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Equivalent Vapor-Only Source Terms

Desert Tortoise

Table 1 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 (%)	Temperature (K)	Half-width[a] (m)
DT1[b]	51.0	7.5	13	205	6.40
DT2[b]	48.3	6.0	13	205	8.40
DT4[c]	49.5	8.59	14.3	205	6.99

JRIII MWG equivalent source conditions for Desert Tortoise v1.2.pdf

FLADIS

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

JRIII initial modeling exercise description v2.3.pdf

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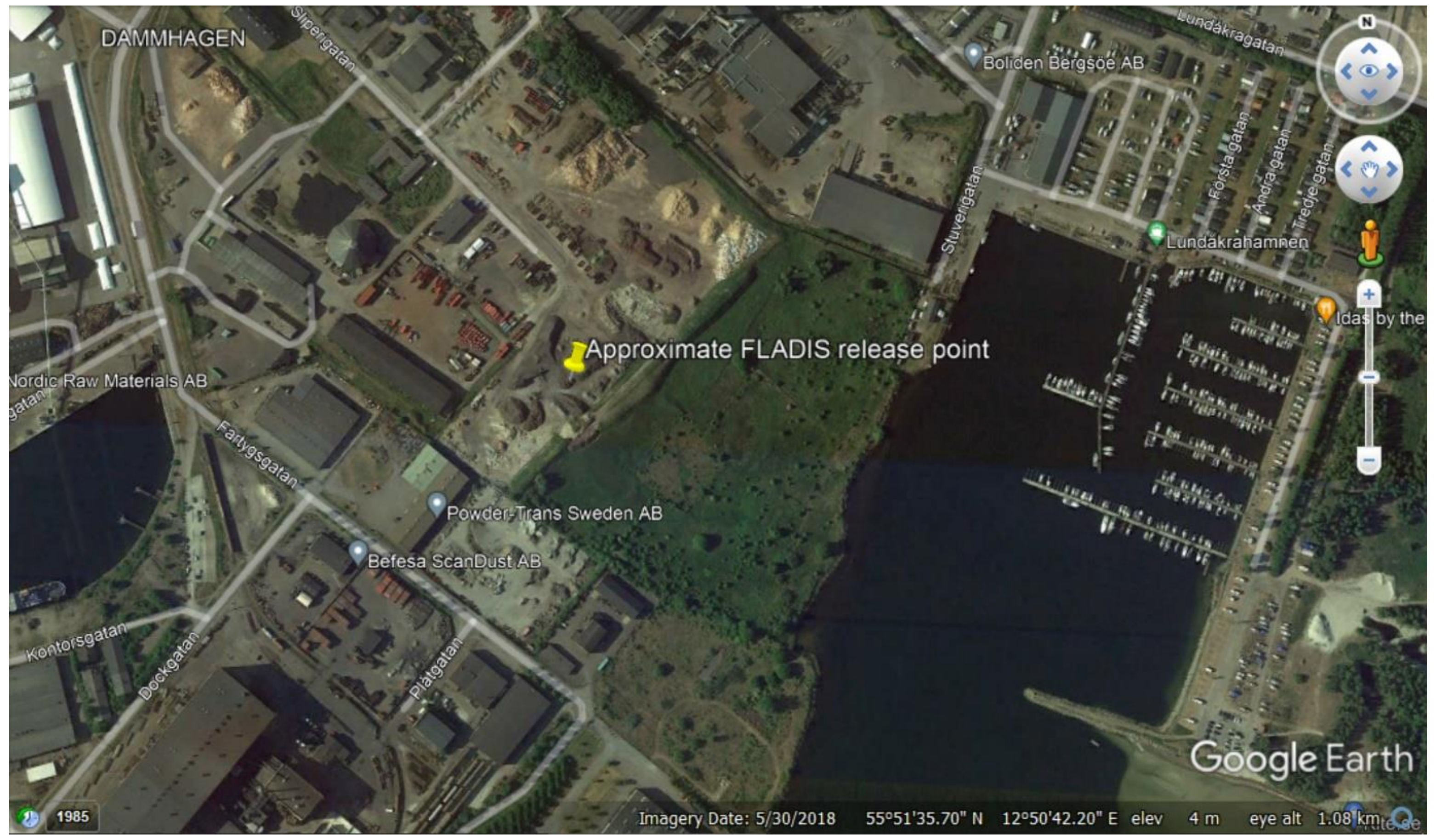
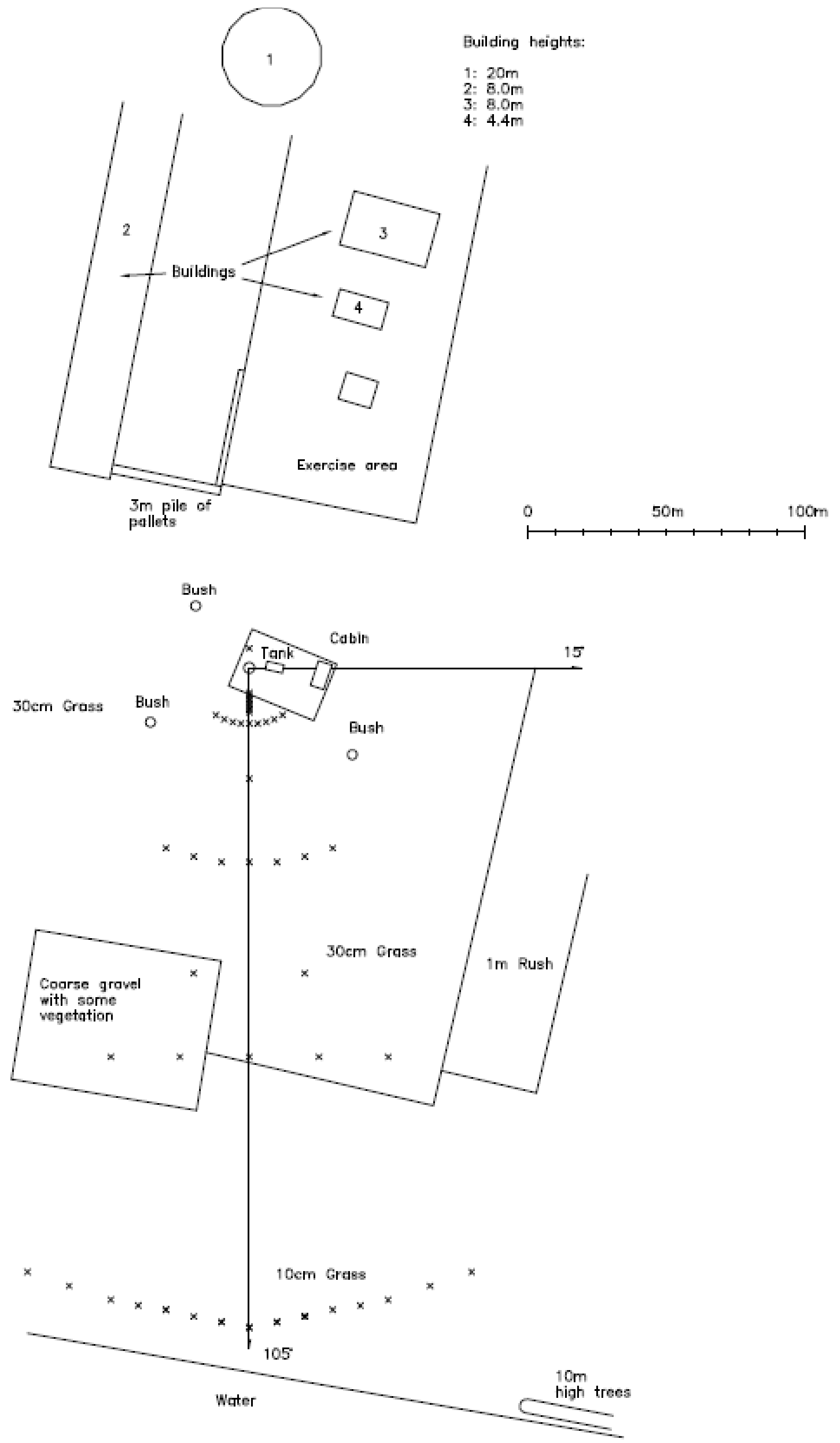
CFD Geometry for FLADIS

- For the FLADIS trials: details of Landskrona test site geometry provided to help setup CFD model geometry



https://xnet.hsl.gov.uk/fileshare/public/3385/approximate-fladis-release-point.kmz



Jack Rabbit III Modelers Working Group

FLADIS Geometry and Wind Directions

Version 1.0, 7 December 2021

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Background

At the Jack Rabbit III Modelers Working Group meeting on 3 December 2021, several CFD modeling teams said that they would like to construct a three-dimensional geometry of the FLADIS test site to model the wake effects from buildings located upwind of the release location.

The purpose of this document is to summarize the information available on the FLADIS site geometry and wind directions in Trials 9, 16 and 24.

Maps and location of the FLADIS test site

The FLADIS experiments took place at the test site of Hydro-Care in Landskrona, Sweden.

Maps of the FLADIS test site are given in Figures 1 and 2 below, showing the location of buildings, the release point and the sensor array. The heights of buildings and other obstacles are given in these two figures. Photos of the FLADIS experiments that were distributed with the FLADIS dataset are also shown in Figure 3.

Morten Nielsen (Danish Technical University) kindly provided a KMZ file with the approximate location of the release point, which can be downloaded from the following link:

FLADIS test site geometry and wind directions v1.pdf

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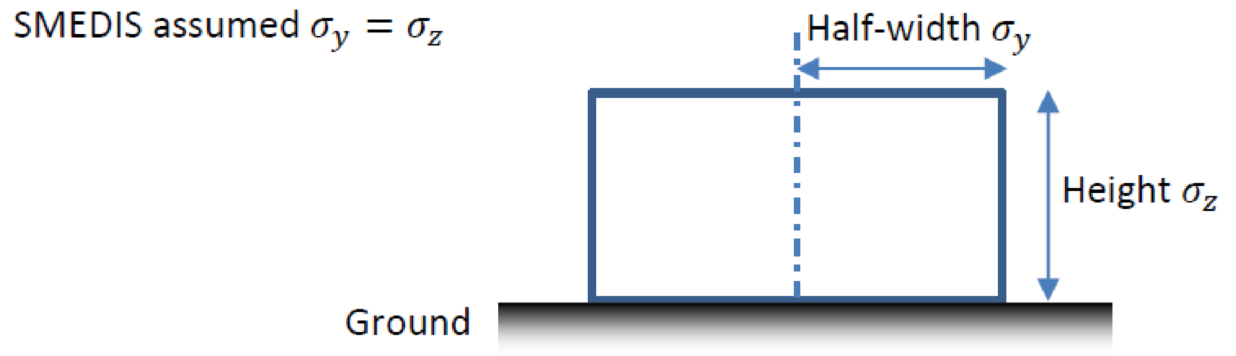
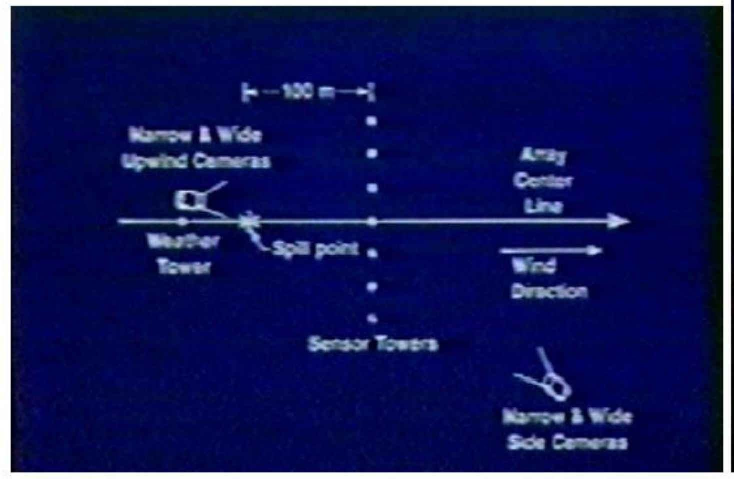
Desert Tortoise Cloud Aspect Ratio

- Aspect ratio of Desert Tortoise cloud for modelers using equivalent vapour-only source conditions: independent assessment for DT trials based on analysis of experimental data





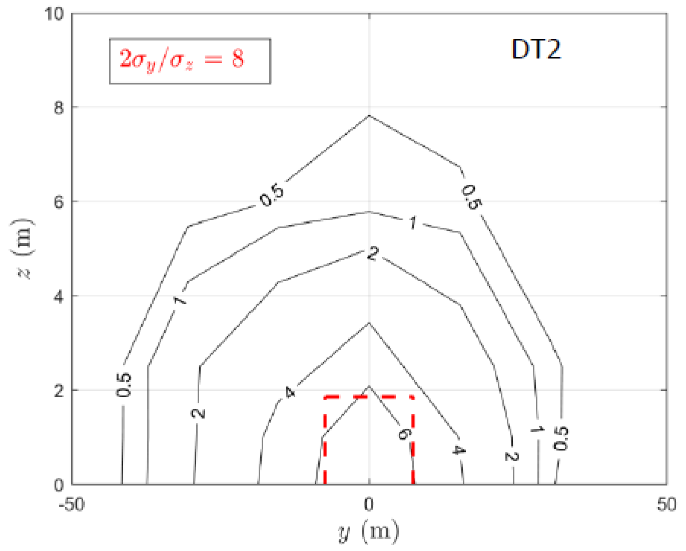


Table 4 Recommended equivalent vapor-only source conditions for the Desert Tortoise trials for the Jack Rabbit III modeling exercise

Trial	Downstream Distance (m)	Velocity (m/s)	Molar Conc (%)	Density[d] (kg/m³)	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

Revised aspect ratio of $2\sigma_y/\sigma_z = 5$.

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

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JRIII MWG Aspect Ratio for Desert Tortoise v1.1.pdf

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Coordination of JRIII Modeling Exercise

- 2 Nov 2021: GMU conference briefing
- 27 Jan 2022: Meeting with participants to discuss exercise with Q&A session
- 28 Feb 2022: Deadline for submission of initial results
- 25 March 2022: Meeting with participants to review of initial results from 16 groups
- 16 May 2022: Meeting with Phast modelers (HSE, DNV, Syngenta, DGA)
- 25 May 2022: Meeting with CFD modelers (Gexcon, DGA, INERIS)
- 17 June 2022: Meeting with participants to review all results from 19 groups
- 26-28 June 2022: GMU conference presentations
- 27-30 Sept 2022: Harmo conference presentations (Portugal)

Timeline of roughly 6 months from start to end of exercise

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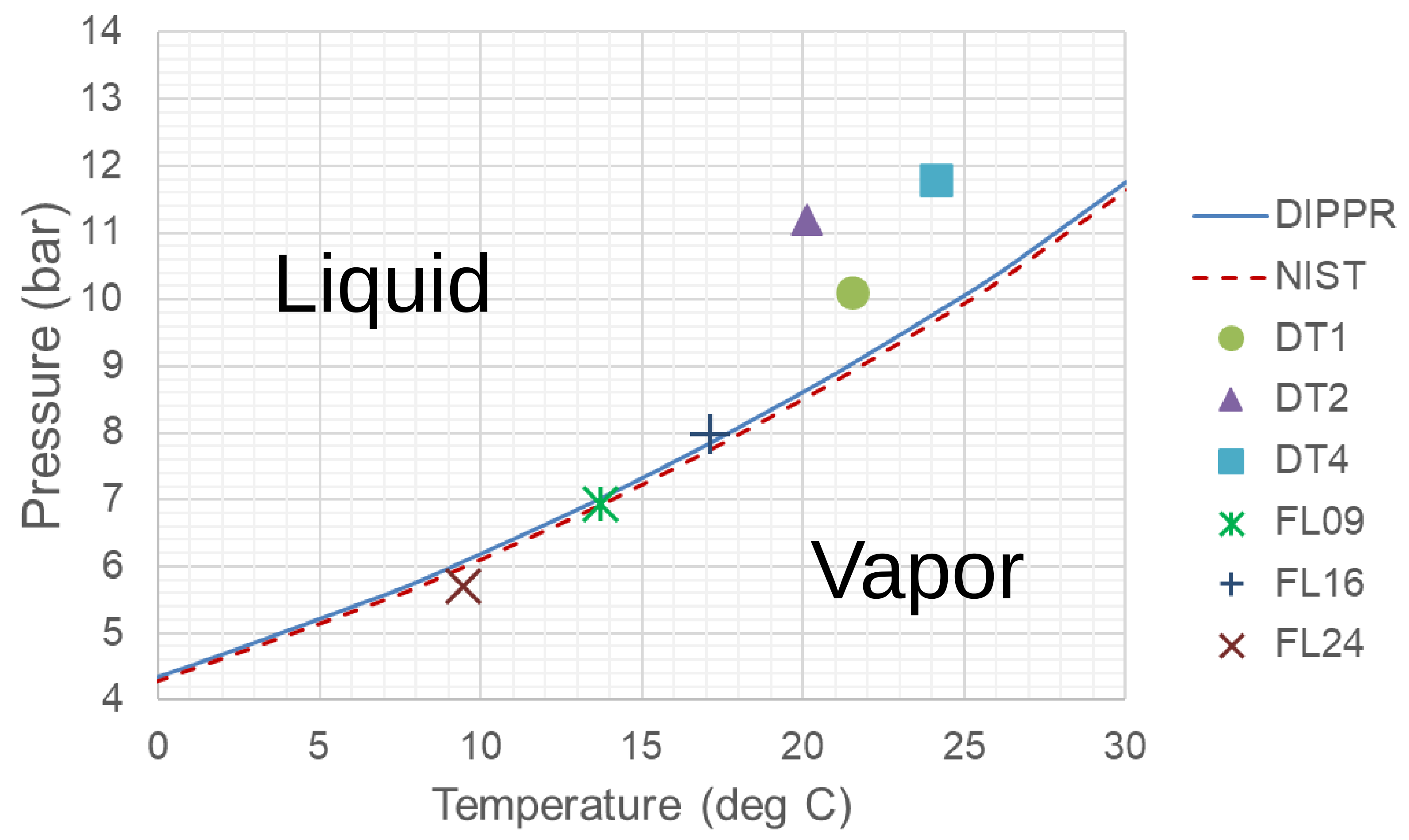
Learning Points as a Coordinator

- Need to take into account that different models have different requirements (e.g., Lat-Long for HPAC, geometry for CFD modelers) when drawing up specification documents
- Need clear definition for parameters like cloud width, σ_y
- Should have highlighted that specified exit pressures and temperatures for some FLADIS trials were "vapor" according to phase diagram, despite release consisting of practically 100% liquid fraction
- Four detailed specification documents (65 pages in total) were produced as the work progressed
  - Better to produce complete specification up-front with a concise summary?



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Summary

- Widespread support from the atmospheric dispersion modeling community: 26 sets of dispersion model predictions from 21 groups (USA, UK, Europe)
- Useful open discussions in main MWG meetings and in smaller sub-groups
- Insight into performance of models and their sensitivity to inputs
- Improved understanding of how best to run certain models
- Appreciation for some important parameters to measure or assess
- Networking between different groups (e.g., users of same model)
- Good preparation for next steps:
  - Modeling of previous large-scale ammonia incident(s)
  - Preparation for future JRIII trials, e.g., sensor arrays placement

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- Sincere thanks to all participants for making this work so successful

Joseph Chang[1], Sun McMasters[3], Ray Jablonski[3], Helen Mearns[3], Shannon Fox[3], Ron Meris[4], Scott Bradley[4], Sean Miner[4], Matthew King[4], Steven Hanna[5], Thomas Mazzola[6], Tom Spicer[7], Rory Hetherington[1], Alison McGillivray[1], Adrian Kelsey[1], April Lockhart[1], Harvey Tucker[1], Graham Tickle[8], Oscar Björnham[9], Bertrand Carissimo[10], Luciano Fabbri[11], Maureen Wood[11], Karim Habib[12], Mike Harper[13], Frank Hart[13]Thomas Vik[14], Anders Helgeland[14], Joel Howard[15], Veronica Bowman[15], Daniel Silk[15], Lorenzo Mauri[16], Shona Mackie[16], Andreas Mack[16], Jean-Marc Lacome[17], Stephen Puttick[18], Adeel Ibrahim[18], Derek Miller[19], Seshu Dharmavaram[19], Amy Shen[19], Alyssa Cunningham[20], Desiree Beverley[20], Matthew O'Neal[20], Laurent Verdier[21], Stéphane Burkhart[21], Chris Dixon[22], Sandra Nilsen[23]

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