Jack Rabbit III Modelers Working Group: Initial Model Inter-comparison Exercise for 2021-22

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Outline

- Aims
- Methodology
- Participation
- Benefits
- Modeling
  - Inputs
  - Outputs

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

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)

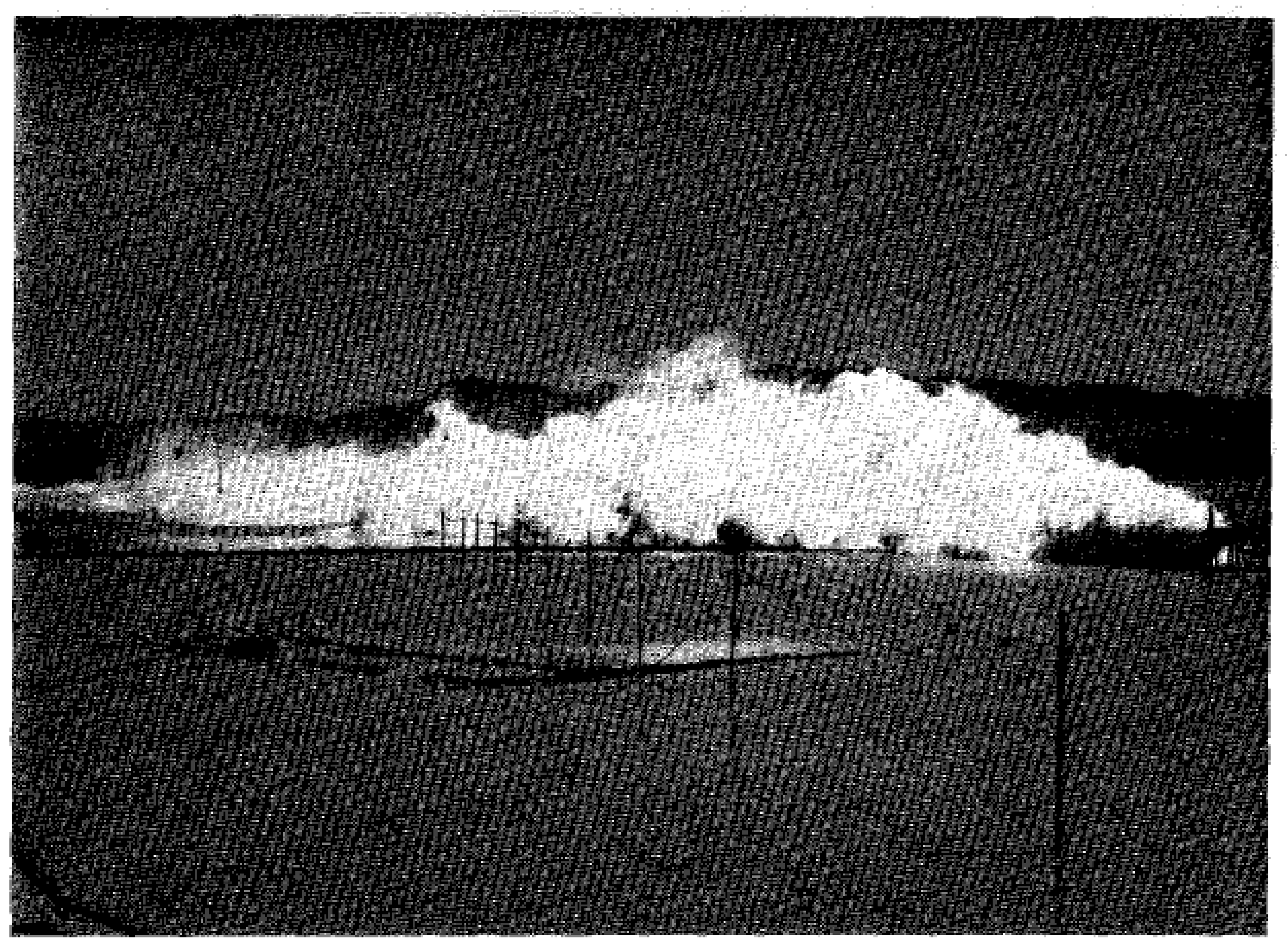

Fig. 15. Desert Tortoise 2 (upwind wide angle camera) Time = 230s. Lawrence Livermore National Laboratory

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 will collate results, cross-plot predictions against experimental measurements and share all results with participants
- This is not a competition but a collaborative effort, with the ultimate goal of improving toxic industrial chemical modeling tools in general
- Timeline
  - Complete modeling work over Winter 2021-2022
  - Share results in Spring 2022
  - Present findings at GMU conference in June 2022

Participation and Benefits

- Work is voluntary, to be conducted on a “best endeavors” basis
- Participation 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
  - 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

Modeling Inputs and Outputs

- Request for Information (RFI) document provides 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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Contents

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.

1

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/).

2

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 involve 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

Modeling Inputs

- Equivalent source conditions from SMEDIS database: either after flashing phase or at a location where all of the ammonia liquid has vaporized

Desert Tortoise

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

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

Rectangular source window

DT4 not analysed in SMEDIS project

FLADIS

Trial	Flash Fraction	Density (kg/m³)	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

Circular source window

1. Conditions at end of flashing phase

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

2. Conditions at location where all the ammonia liquid has vaporized

Modeling and Measurement Uncertainties

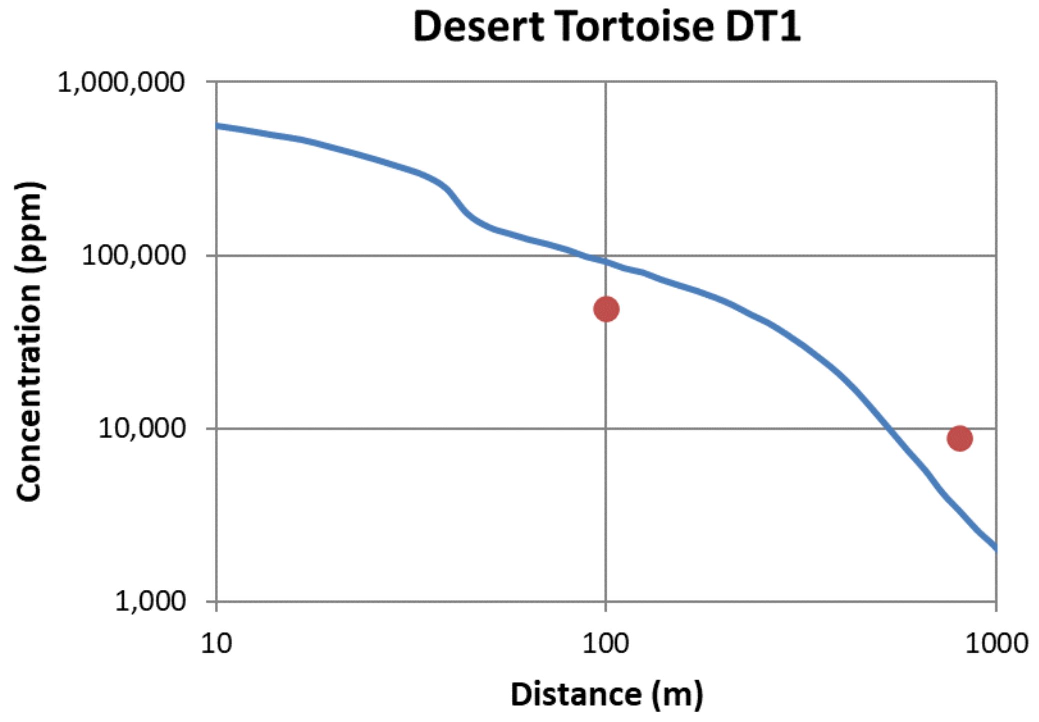
- Standing water on the surface of the normally dry lake bed in the Desert Tortoise trials
  - Affected DT1 and DT2 trials, but dried out by the time DT4 test took place
  - Suggested to undertake sensitivity tests with enhanced humidity and/or unstable boundary layer
- Decrease in wind speed during 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

Basic Set of Modeling Outputs

- Long time-averaged plume centerline concentration vs distance
  - Plume centerline = arc-max concentration (i.e., max concentration at any height or radial position at the given downwind distance)
  - If concentrations can only be output at a defined height, the sensor heights could be used (details given in the RFI document)
  - Note: averaging time for each trial is different (see table on Slide 8)
  - Desert Tortoise concentrations measured at 100 m using heated sensor that evaporated ammonia droplets (i.e., it measured total liquid plus vapor concentration). Ideally, output this quantity.
- Requested format: CSV or Excel file with two columns
  - Distance from actual source (m)
  - Predicted concentration (ppm by volume)
- Sufficient number of data points to plot a smooth curve from source to maximum downwind distances of:
  - 1000 m for Desert Tortoise
  - 250 m for FLADIS trials

	A	B
1	Distance (m)	Concentration (ppmv)
2	0.4	654655
3	1.6	701347
4	2.9	706457
5	4.3	686570
6	5.9	651095
7	7.6	608689
8	9.5	569924
9	11.6	532655
10	13.9	495754
11	16.5	466084
12	19.4	425720
13	22.5	388857
14	26.0	354318
15	29.9	321769
16	34.1	289853

Table continued to distance of 1000 m for Desert Tortoise



Basic Set of Modeling Outputs

- Short description of modeling approach
  - Name and version of model
  - Description of any deviations from the prescribed model input conditions
    - 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 centerline values
    - e.g., vapor concentrations output at height of X m that do not take into account the aerosol concentration
  - Requested in Word, Powerpoint or plain text file

Optional Extra Modeling Outputs

- Predicted plume widths using the long averaging time
- Predicted mean temperatures on the plume centerline
- For Desert Tortoise only
  - Plume centerline concentrations using a short averaging time of 1 s
- For FLADIS only
  - Plume centerline concentrations and plume widths using a moving frame of reference that follows the center of the plume, i.e., without lateral meandering effects (all other model outputs should be for a stationary reference frame)
- Results from model sensitivity tests

- Above results requested in CSV or Excel files with similar format to basic set of outputs

	A	B
1	Distance (m)	Concentration (ppmv)
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3	1.6	701347
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Table continued to distance of
1000 m for Desert Tortoise
250 m for FLADIS

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- For further details of this model inter-comparison exercise, please contact:

  - Joe Chang (jchang@rand.org)
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Thank you

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