DRIFT Dispersion Model Predictions for the Jack Rabbit II Model Inter-Comparison Exercise

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19th conference on "Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes", Bruges, Belgium, 3-6 June 2019
Outline

• Background

• Overview of DRIFT
  – Model capabilities
  – Configuration for JRII model inter-comparison exercise

• Results

• Summary and possible future work

**Aims**
- Conduct large-scale chlorine release experiments
- 10 – 20 ton chlorine releases (inc. road tanker)
- Mock urban array of obstacles
- Different release orientations
- Dispersion measurements to 11 km downwind
- Infiltration into buildings and vehicles
- Measure key source terms parameters
- Study effect of chlorine on emergency responders’ equipment

**Impact**
- Modelling – improve source term, dispersion, deposition, infiltration models
- Resiliency – inform planning, emergency response and policy
- Vulnerability and impact reduction – improve hazard and risk mitigation
Aims of HSE’s involvement in Jack Rabbit II

- Contribute modelling results and help support Jack Rabbit II project
- Validate HSE’s regulatory dispersion model (DRIFT)
- Assess capabilities of other widely-used dispersion models
- Collaborate with experts in the Modelers Working Group and share findings

Benefits of model inter-comparison exercise

- Benchmark models to experimental data using standardized inputs and outputs
- Understand strengths/weaknesses of different modelling approaches
- Collaborate and ultimately help to develop improved models

Aims of this presentation

- Explain DRIFT configuration for model inter-comparison exercise
- Present short summary of results
Previous work: HSL predictions prior to the 2015 trials to help the positioning of sensors

Baseline = 10 ton (9072 kg) release in F2
Background

**Previous work**: CFD simulations to help understand the near-field flow behaviour in the JRII 2015 and 2016 trials
Outline

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• Results

• Summary and possible future work
DRIFT model: capabilities

DRIFT is an integral model

Constant mean wind speed and direction
Meander affects plume width for longer averaging times

Evaporating aerosol of chlorine droplets and condensed water vapour in the dispersing cloud

Vessel

DRIFT does not account for additional turbulence and re-entrainment at impingement

Along-wind diffusion and gravity spreading

Initial gravity spreading and dilution of the source

GASP pool spread and evaporation
Model accounts for heat transfer: conduction from ground (inc. ground cooling effects), air convection and thermal radiation

Two-phase jet

DRIFT may over-predict concentrations for short-duration releases in far-field due to its use of smaller Froude number for gravity spreading derived for continuous releases

DRIFT and GASP are hard-wired to use an atmospheric pressure of 101,325 Pa and cannot use the lower atmospheric pressure measured at Dugway Proving Ground in the Jack Rabbit II trials
Specified input conditions:

Jack Rabbit II Coordinated Model Comparisons to Data
Initial Specification for Modelers

INTRODUCTION

PURPOSE AND OBJECTIVES

The aim of this information note is to specify the model inputs and outputs required to run an inter-model comparison exercise using the Jack Rabbit II data. This note concentrates on three of the nine JRII trials (Trials 1, 6 and 7). The reason for selecting these three trials is that they involved different initial jet directions and/or the presence or absence of the mock urban CONEX grid. Trial 1 involved a downwards directed jet release within the mock-urban CONEX grid, Trial 6 involved the same release orientation but without the mock-urban CONEX grid, and Trial 7 involved a release directed at 45 degrees downwards from the horizontal and azimuthally aligned with the prevailing winds and grid centerline, again without the mock-urban CONEX grid. These initial trials for comparison are further characterized under Release Parameters in Table 1. If there is sufficient interest in this first modeling exercise, other JRII trials may be selected for future model inter-comparisons.

The objectives of the intended inter-model comparison exercise are:

- More broadly disseminate a best understanding of the Jack Rabbit II data base
- Provide for a consistent comparison of models to data; as many models as possible; to inform the community and provide a basis for model improvement where needed
- Provide a forum for technology transfer to the chlorine industry concerned with risk management
- Encourage collaboration among modelers, which should lead to improved models all-around

File “JRII Model Comparison Specifications_REVISED 17May18b.docx”
in email from Tom Mazzola, 17 May 2018
## DRIFT model: setup for JRII simulations

<table>
<thead>
<tr>
<th></th>
<th>Trial 1</th>
<th>Trial 6</th>
<th>Trial 7</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Primary release</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Discharge rate (kg/s)</td>
<td>224.</td>
<td>260</td>
<td>259</td>
</tr>
<tr>
<td>Discharge period (s)</td>
<td>20.3</td>
<td>32.2</td>
<td>33.3</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>-37.3</td>
<td>-37.4</td>
<td>-37.4</td>
</tr>
<tr>
<td>Vapor fraction (ignoring KE effects)</td>
<td>0.171</td>
<td>0.172</td>
<td>0.172</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>18.3</td>
<td>18.2</td>
<td>18.1</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>50.8</td>
<td>44.2</td>
<td>44.2</td>
</tr>
<tr>
<td>Area (m²)</td>
<td>0.241</td>
<td>0.324</td>
<td>0.323</td>
</tr>
<tr>
<td><strong>Primary release modified for rainout</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Discharge rate (kg/s)</td>
<td>145</td>
<td>168</td>
<td>162</td>
</tr>
<tr>
<td>Discharge period (s)</td>
<td>20.4</td>
<td>32.4</td>
<td>33.6</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>-37.3</td>
<td>-37.4</td>
<td>-37.4</td>
</tr>
<tr>
<td>Vapor fraction (ignoring KE effects)</td>
<td>0.264</td>
<td>0.266</td>
<td>0.274</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>11.9</td>
<td>11.8</td>
<td>11.4</td>
</tr>
<tr>
<td>Velocity (m/s)</td>
<td>50.8</td>
<td>44.2</td>
<td>44.2</td>
</tr>
<tr>
<td>Area (m²)</td>
<td>0.240</td>
<td>0.323</td>
<td>0.322</td>
</tr>
<tr>
<td><strong>Evaporated rainout</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Discharge rate (kg/s)</td>
<td>43.2</td>
<td>34.0</td>
<td>34.0</td>
</tr>
<tr>
<td>Discharge period (s)</td>
<td>36.8</td>
<td>86.4</td>
<td>93.4</td>
</tr>
<tr>
<td>Temperature (°C)</td>
<td>-37.3</td>
<td>-37.4</td>
<td>-37.4</td>
</tr>
<tr>
<td>Vapor fraction</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>3.16</td>
<td>3.15</td>
<td>3.14</td>
</tr>
<tr>
<td>Area (m²)</td>
<td>491</td>
<td>491</td>
<td>491</td>
</tr>
</tbody>
</table>

- **Blue** = DRIFT input
- **Red** = DRIFT uses a different value
- **Green** = Calculated internally by DRIFT (not prescribed)
- **Black** = Not used

DRIFT uses -33.7 °C at standard atmospheric pressure of 101,325 Pa

From file: “JRII Model Comparison Specifications_REVISED 17May18b.docx “
DRIFT model: setup for JRII simulations

Two-stage modelling process:

1.) Two-phase jet

Jet entrains air and droplets evaporate until it impinges

Source conditions taken from: “Primary release” specified conditions

Conditions when jet hits ground used to calculate area source for Stage 2

2.) Dispersion

Area source (two-phase) from jet in Stage 1

Evaporating pool source from: “Evaporated rainout” specified conditions
DRIFT model: setup for JRII simulations

Two-stage modelling process:

1.) Two-phase jet

Source conditions taken from:
“Primary release” discharge rate = 224 kg/s for Trial 1

Rainout mass rate = (“Primary release” discharge rate) - (“Primary release modified for rainout” discharge rate) = 224 - 145 = 79 kg/s for Trial 1

i.e. the rainout mass fraction = 79/224 = 35% for Trial 1

Diameter of jet at impingement, \( D \)

DRIFT grows this diameter \( D \) using its model for upwind spreading at the source (due to gravity spreading only)

2.) Dispersion

Area source (two-phase) from jet in Stage 1

- Dispersed liquid droplet mass fraction accounts for rainout in impinging jet
- Condensed liquid water phase accounts for water lost in rainout
- Entrained air in impinging jet from Stage 1 is retained in area source for Stage 2

Evaporating pool source from:
“Evaporated rainout” release rate = 43.2 kg/s for Trial 1

Source diameter = \( D \) (from jet impingement)
### DRIFT model: setup for JRII simulations

Meteorological conditions:

<table>
<thead>
<tr>
<th>Weather/Environment</th>
<th>Trial 1</th>
<th>Trial 6</th>
<th>Trial 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atmospheric pressure (mbar)</td>
<td>873.7</td>
<td>871.1</td>
<td>868.5</td>
</tr>
<tr>
<td>Initial wind speed(^2) (m/s) at z = 2 m</td>
<td>1.45</td>
<td>2.42</td>
<td>3.98</td>
</tr>
<tr>
<td>Initial wind direction(^2) at z = 2 m</td>
<td>147.4</td>
<td>146.9</td>
<td>149.6</td>
</tr>
<tr>
<td>Initial temperature (ºC) at z = 2 m</td>
<td>17.5</td>
<td>22.3</td>
<td>18.7</td>
</tr>
<tr>
<td>Surface roughness (mm)</td>
<td>0.5</td>
<td>0.5</td>
<td>0.5</td>
</tr>
<tr>
<td>Friction velocity(^3), u* (m/s)</td>
<td>0.108</td>
<td>0.093</td>
<td>0.210</td>
</tr>
<tr>
<td>Sensible heat flux(^3), Hs, (K-m/s)</td>
<td>-0.012</td>
<td>-0.0034</td>
<td>-0.0160</td>
</tr>
<tr>
<td>Vertical profiles of wind speed and direction and temperature(^4)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inverse Monin-Obukhov length (m(^{-1}))</td>
<td>0.124</td>
<td>0.056</td>
<td>0.0229</td>
</tr>
<tr>
<td>Pasquill Class(^5)</td>
<td>E/F</td>
<td>E</td>
<td>D/E</td>
</tr>
</tbody>
</table>

From file: “JRII Model Comparison Specifications_REVISED 17May18b.docx “

**DRIFT standard atmospheric pressure of 101,325 Pa**

**Blue** = DRIFT input

**Red** = DRIFT uses a different value

**Black** = Not used
DRIFT model: setup for JRII simulations

DRIFT uses a standard log-law velocity profile with modifications for atmospheric stability in the surface layer from Businger (1973)
DRIFT model: setup for JRII simulations

Three sets of DRIFT results submitted to the model inter-comparison exercise:

1. **DRIFT1** = Baseline case: atmospheric wind profile based on the specified value of “Initial wind speed at $z = 2\text{m}$”

2. **DRIFT2** = Atmospheric wind profile based on the specified “Friction velocity ($u^*$)”, instead of the initial wind speed at $z = 2\text{m}$

3. **DRIFT3** = Same as DRIFT1 baseline case but with dry deposition switched off, by changing the deposition velocity from $v_d = 0.04 \text{ cm/s (in DRIFT1 and DRIFT2)}$ to $v_d = 0.0 \text{ cm/s (in DRIFT3)}$. 
Other DRIFT model inputs:

• Ground surface roughness, $z_0 = 0.5$ mm
  – No account taken of mock urban array in Trial 1
  – Sensitivity tests could be performed to investigate this matter later
  – Previous DRIFT results presented at GMU conference and Harmo-18 used a high roughness length of $z_0 = 0.4$ m in first 100 m downwind of release point to account for presence of mock urban array (increased mixing and dilution)

• Fixed wind speeds and atmospheric stability for the duration of each trial, not changing over time like in the experiments
Wind direction is given relative to sensor axis of 345° i.e. angle = 0° is along centerline of sensor array.

Wind measurements taken by PWIDS 19, located 100 m upwind of release point.

- Trial 1
- Trial 6
- Trial 7

- Wind speed
- Wind direction

Arrival time of max concentration at 500 m arc
Arrival time of max concentration at 11 km arc
Outline

- Background
- Overview of DRIFT
  - Model capabilities
  - Configuration for JR II model inter-comparison exercise
- Results
  - Quick review of experimental data
  - Maximum arc-wise concentrations
  - Contour plots
- Summary and possible future work
NB. Trial 6 and 7 MiniRAE data not scaled in response to pre/post calibration tests
Trial 1

ToxiRAE sensor saturated at 50 ppm

Trial 6

ToxiRAE sensor saturated at 50 ppm

Trial 7

MiniRAE saturated at 2000 ppm

NB. Trial 6 and 7 MiniRAE data not scaled in response to pre/post calibration tests

Canary upper calibration limit of 15,000 ppm

Bifurcated cloud in near-field?

Sparse array of sensors at some positions

500 m MiniRAE saturated at 2,000 ppm
Maximum Arc-Wise Concentration

- **Trial 1**: Wind speed 1.5 m/s, Chlorine mass released 4.5 t, Mock urban array vertically-down release.
- **Trial 6**: Wind speed 2.4 m/s, Chlorine mass released 8.4 t, Unobstructed vertically-down release.
- **Trial 7**: Wind speed 4.0 m/s, Chlorine mass released 8.6 t, Unobstructed 45-deg down release.
Concentration Contours

Key to plots shown on subsequent slides

Example plot:

Contours show predicted concentration at the specified time (t = 120 s in this case)

Predicted concentrations above upper scale limit (100,000 ppm here) are shown as red

Symbols show maximum measured concentration over all time at that location (not at the specified time). Symbol color scale matches the contours

- Triangles indicate sensor saturated (concentration may be higher than indicated)
- Circles indicate sensor did not saturate

Any sensors that measured noise (not signal) have been set to zero concentration

Black contour lines highlight the 5 set levels: 1000, 3000, 10000 etc.

Color scale is logarithmic, not linear

Predicted concentrations below lower scale limit (1,000 ppm here) are not shown, i.e. contour limits are clipped to this lower bound so that background appears white, not blue
Near-field: time = 30 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Near-field: time = 60 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Near-field: time = 120 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Near-field: time = 300 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Near-field: time = 600 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Mid-field
Mid-field: time = 300 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Mid-field: time = 600 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height

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Mid-field: time = 1200 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Mid-field: time = 1800 s

Trial 1

Trial 6

Trial 7

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Far-field
Far-field: time = 1200 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height.
Far-field: time = 1800 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Far-field: time = 2700 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Far-field: time = 3600 s

All results are for the DRIFT1 model using the specified reference velocity at 2 m height
Maximum concentrations over all time
Summary

• Details have been provided of the DRIFT model configuration

• Baseline DRIFT1 using reference wind speed predicted:
  – Around 60% of the maximum arc-wise concentrations within a factor of two of the measurements
  – Trend to over-prediction, but several measurements may have under-reported the actual concentrations

• Sensitivity tests
  – DRIFT2: using $U^*$ instead of $U_{ref}$ affects Trial 1 results
  – DRIFT3: Switching deposition off had minor effect in Trial 1

• Need to be careful not to over-interpret DRIFT results in Trial 1 due to presence of mock urban array
Possible Future Work

• Further analysis of Jack Rabbit II Trial 1, 6 and 7
  – Comparisons of cloud width and height
  – Time-varying concentrations and toxic load
  – Statistical Performance Measures (SPMs): FAC2, VG, MG etc.

• Assess impact of sensors saturating or cloud missing sensors
  – Calculate second set of SPMs using subset of data unaffected by these issues?

• Examine the other Jack Rabbit II trials?

• Validate pool evaporation models with Trial 7 and 8 liquid dump data

• Update HSE model evaluation protocol for DRIFT

• Revisit simulations from 2008 of chlorine railcar incidents (Graniteville, Festus and Macdona) using learning gained from Jack Rabbit II
Acknowledgements

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- Ronald Meris (DTRA)
- Thomas Mazzola, John Magerko (Engility/SAIC)
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- Joseph Chang (RAND)
- Andy Byrnes (UVU)
- Thomas Spicer (Arkansas University)
- Richard Babarsky (US Army)
- Nathan Platt, Jeffry Urban and Kevin Luong (IDA)
- Jeffrey Weil (NCAR)
- Luca delle Monache (NCAR/UCSD)
- John Boyd (ARA)
- Steven Herring and Joel Howard (DSTL)

Co-authors:

- Graham Tickle (GT Science and Software)
- Adrian Kelsey and Harvey Tucker (HSE)

GT Science & Software contributed towards the work on DRIFT, but the DRIFT simulations presented in this paper were performed by HSE and have not been independently checked by the software developer. The work presented here was funded by HSE. The contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy.
Extra material
Summary of differences between runs DRIFT1, DRIFT2 and DRIFT3

<table>
<thead>
<tr>
<th></th>
<th>Trial 1</th>
<th></th>
<th>Trial 6</th>
<th></th>
<th>Trial 7</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>DRIFT1</td>
<td>DRIFT2</td>
<td>DRIFT3</td>
<td>DRIFT1</td>
<td>DRIFT2</td>
<td>DRIFT3</td>
</tr>
<tr>
<td>Initial wind speed (m/s) at z = 2 m</td>
<td>1.45</td>
<td>2.92</td>
<td>1.45</td>
<td>2.42</td>
<td>2.34</td>
<td>2.42</td>
</tr>
<tr>
<td>Friction velocity, u* (m/s)</td>
<td>0.054</td>
<td>0.108</td>
<td>0.054</td>
<td>0.096</td>
<td>0.093</td>
<td>0.096</td>
</tr>
<tr>
<td>Deposition velocity, v_d (cm/s)</td>
<td>0.04</td>
<td>0.04</td>
<td>0.0</td>
<td>0.04</td>
<td>0.04</td>
<td>0.0</td>
</tr>
</tbody>
</table>
Further plots of the JRII experimental data

• To show behaviour of some ToxiRAE and MiniRAE sensors that saturated and recorded a plateau in the recorded concentration over time
• Time-varying concentrations for Canary sensors to show that they recorded useful data even when above their calibration limit
Trial 6

Time-Series Concentrations at Selected Sensors

Corrections applied later from pre/post calibration tests, which raise 1K-20 max conc from 1,910 ppm to 3,053 ppm

ToxiRAE sensor saturated at 50 ppm

MiniRAE sensor saturated at 2000 ppm

Canary calibrated to 15,000 ppm
Extra slide with plots of the maximum arc-wise concentrations for different averaging times, showing that it has relatively little effect on the data
Extra slides taken from Harmo-18 presentation H18-134:

“Jack Rabbit II 2015 chlorine release experiments: simulations of the trials using DRIFT and PHAST”
by Bryan McKenna, Maria Garcia, Simon Gant, Adrian Kelsey, Alison McGillivray, James Stewart, Rachel Batt, Mike Wardman, Harvey Tucker, Graham Tickle and Henk Witlox

To demonstrate that dispersion model predictions can be very sensitive to the deposition rate – it can have a greater effect than wind speed or atmospheric stability in some cases
Range of model inputs and outputs

• Model inputs:
  – Chosen based on Jack Rabbit II experimental ranges and uncertainties:
    – Flashing or metastable release

<table>
<thead>
<tr>
<th>Inventory (kg)</th>
<th>DRIFT Rainout Fraction</th>
<th>Wind Speed at 2m reference height (m s(^{-1}))</th>
<th>Temperature (K)</th>
<th>(1/\text{Monin-Obukhov Length} \text{ (m}^{-1}))</th>
<th>Vapour Deposition Velocity (cm s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>4000</td>
<td>0</td>
<td>1.5</td>
<td>288</td>
<td>-0.12</td>
<td>0</td>
</tr>
<tr>
<td>9000</td>
<td>1</td>
<td>5</td>
<td>303</td>
<td>0.08</td>
<td>5</td>
</tr>
</tbody>
</table>

5 cm s\(^{-1}\) chosen as highest value of deposition rate found in the literature (upper bounding case)
Not representative of Dugway salt playa
Main and total effects on Lowry Plot

Deposition velocity has the strongest effect on the results
Surface plot showing physical effects

Distance to 100 ppm concentration (m)

Largest dispersion distance with high wind speed and low deposition velocity

Wind speed (m s$^{-1}$)  Deposition velocity (cm s$^{-1}$)
Range of model inputs and outputs

• Model inputs:
  – Chosen based on Jack Rabbit II experimental ranges and uncertainties:

<table>
<thead>
<tr>
<th>Inventory (kg)</th>
<th>DRIFT Rainout Fraction</th>
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<td>5</td>
<td>303</td>
<td>0.08</td>
<td>5</td>
</tr>
</tbody>
</table>
  – Flashing or metastable release

• Model output: Distance to 100 ppm concentration
Deposition velocity range: 0 – 0.05 cm s^{-1}

Atmospheric stability has the strongest effect on the results