DRIFT Results for the Jack Rabbit II Coordinated Model Inter-Comparison Exercise

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Graham Tickle (GT Science & Software)
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- Ronald Meris (DTRA)
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- Steven Herring (DSTL)
- Andy Byrnes (UVU)

DISCLAIMER:
- 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 contribution made to this paper by the HSE authors was funded solely by HSE. The contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy.
Outline

• Aims

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

• Preliminary model results
  – Maximum arc-wise concentration versus downwind distance
  – Maximum concentration across the azimuth angle of the arcs
  – Contour plots

• Sensitivity analysis
  – Dry deposition velocity set to zero
  – Increased roughness for urban array in Trial 1

• Conclusions and Future Directions
Aims

Aims of HSE’s involvement in Jack Rabbit II:

• To contribute DRIFT model results to the model inter-comparison exercise

• To volunteer and provide help (if needed) to the coordinators:
  – Support Graham Tickle’s source modelling efforts
  – Provide quality assurance checks on the experimental data
  – Volunteer to cross-plot other model results and compare to the data

• To work with DNV GL on the PHAST model results (later...)

• To collaborate with other experts in the Modelers’ Working Group and share findings
**DRIFT model: capabilities**

**DRIFT is an integral model**

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

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

- **Initial gravity spreading and dilution of the source**

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

- **Vessel**

- **Two-phase jet**

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

- **Along-wind diffusion and gravity spreading**

- **Flat terrain with uniform aerodynamic roughness and specified dry deposition velocity**

**DRIFT may over-predict concentrations for short-duration releases in far-field due to use of smaller Froude number for gravity spreading derived for continuous releases**
## JRII Coordinated Model Inter-Comparison Exercise: Source Conditions

Source conditions provided by Tom Spicer and Graham Tickle:

<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>18.32</td>
<td>18.15</td>
<td>18.12</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>11.89</td>
<td>11.79</td>
<td>11.41</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>3.160</td>
<td>3.152</td>
<td>3.144</td>
</tr>
<tr>
<td>Area (m²)</td>
<td>491</td>
<td>491</td>
<td>491</td>
</tr>
</tbody>
</table>

Data source: JRII Model Comparison Specifications_REVISED 17May18b.docx
Meteorological conditions provided by Steve Hanna:

<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 (°C) 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), H(_s), (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>

Dry deposition velocity, \(v_d = 0.04\) cm/s

Data source: 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: Spicer and Tickle “Primary release modified for rainout”

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: Spicer and Tickle “Evaporated rainout”
DRIFT model: setup for JRII simulations

Other DRIFT model inputs:

• Ground surface roughness, $z_0 = 0.5$ mm
  – No account taken of mock urban array in Trial 1
  – Sensitivity tests performed to investigate this matter

• Dry deposition velocity, $v_d = 0.04$ cm/s
  – Previous work has shown results are very sensitive to the deposition velocity, but this is a low value
  – Sensitivity tests performed with $v_d = 0$ cm/s

• Fixed wind speeds and atmospheric stability for the duration of each trial
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  – Maximum concentration across the azimuth angle of the arc
  – Contour plots

• Sensitivity analysis
  – Dry deposition velocity set to zero
  – Increased roughness for urban array in Trial 1

• Conclusions and Future Directions
JR II: Wind Conditions and Mass Released

Analysis by Steve Hanna for meteorology and Tom Spicer for chlorine mass

Data sources: “P190 JR II Recommended met for modelers 14 March 2018.xlsx” for meteorology
“GCPS-sp-2017-JR2-source+release-rate-PSP-final-JR2-rates-rev02.docx” for chlorine mass released
**JRII: Selected trials for current exercise**

Analysis by Steve Hanna for meteorology and Tom Spicer for chlorine mass

Data sources:
- "P190 JR II Recommended met for modelers 14 March 2018.xlsx" for meteorology
- “GCPS-sp-2017-JR2-source+release-rate-PSP-final-JR2-rates-rev02.docx” for chlorine mass released
Max Arc-Wise Concentration vs. Distance

Key to plots shown on subsequent slides

Example plot:

Colors show three different averaging times
DRIFT used averaging time = 2 s, 20 s, 1 min
Sensor raw data was between 1 s and 3 s
Joe Chang sensor averages for 20 s and 1 min

Lines show DRIFT base case results

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

Both x and y axes are log scales
Max Arc-Wise Concentration vs. Distance

**Trial 1**
- Concentration (ppm)
- Downwind distance (km)
- 2s (Raw), 20s, 1min

**Trial 6**
- Concentration (ppm)
- Downwind distance (km)
- 2s (Raw), 20s, 1min

**Trial 7**
- Concentration (ppm)
- Downwind distance (km)
- 2s (Raw), 20s, 1min

---

Mock urban array
1.5 m/s
-18°
Vertically down release

Vertically down release

Open terrain
8,391 kg
Vertically down release

Open terrain
9,072 kg
45-deg down release

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Max Arc-Wise Concentration vs. Distance

Does DRIFT over-predict concentration in Trial 1 because it does not account for the mock urban array? See later sensitivity tests...
Max Concentration vs. Azimuth Angle

Key to plots shown on subsequent slides

Example plot:

- Colors show three different averaging times:
  - DRIFT used averaging time = 2 s, 20 s, 1 min
  - Sensor raw data was between 1 s and 3 s
  - Joe Chang sensor averages for 20 s and 1 min

- Lines show DRIFT base case results

- Symbols show measurements:
  - 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
- Assessed by visual inspection of graphs of time-series concentration at each sensor

Both x and y axes are linear scales

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Max Concentration vs. Azimuth Angle

Trial 1: 4,545 kg vertically down release, mock urban array, wind speed 1.5 m/s

DRIFT’s over-prediction of concentration looks larger here since the vertical scale is linear.
Max Concentration vs. Azimuth Angle

**Trial 6:** 8,391 kg vertically down release, open terrain, wind speed 2.4 m/s
Max Concentration vs. Azimuth Angle

Trial 7: 9,072 kg 45-deg down release, open terrain, wind speed 4.0 m/s

Recall that triangles indicate saturated sensors: actual concentrations may have been higher
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

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Concentration Contours

Trial 1: Near 30s
- 1.5 m/s -18°
- Mock urban array
- Vertically down release
- 4,545 kg

Trial 6: Near 30s
- 2.4 m/s -18°
- Open terrain
- Vertically down release
- 8,391 kg

Trial 7: Near 30s
- 4.0 m/s -15°
- Open terrain
- 45-deg down release
- 9,072 kg
Concentration Contours

Trial 1: Near 60s
- Eastings (km): -0.5 to 0.5
- Northing (km): -0.4 to 0.6
- Concentration: Vertically down release
- Mass: 4,545 kg
- Wind Speed: 1.5 m/s
- Wind Direction: -18°

Trial 6: Near 60s
- Eastings (km): -0.5 to 0.5
- Northing (km): -0.4 to 0.6
- Concentration: Vertically down release
- Mass: 8,391 kg
- Wind Speed: 2.4 m/s
- Wind Direction: -18°

Trial 7: Near 60s
- Eastings (km): -0.5 to 0.5
- Northing (km): -0.4 to 0.6
- Concentration: Vertically down release
- Mass: 9,072 kg
- Wind Speed: 4.0 m/s
- Wind Direction: -15°
Concentration Contours

Trial 1: Near 120s
- 1.5 m/s
- -18°
- Vertically down release
- 4,545 kg

Trial 6: Near 120s
- 2.4 m/s
- -18°
- Vertically down release
- 8,391 kg

Trial 7: Near 120s
- 4.0 m/s
- -15°
- 45-deg down release
- 9,072 kg

Mock urban array
Open terrain
Open terrain

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Concentration Contours

Mock urban array

Vertically down release

Open terrain

Vertically down release

Open terrain

45-deg down release

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Concentration Contours

Mock urban array

Vertically down release

Open terrain

Vertically down release

Open terrain

45-deg down release

1.5 m/s -18°

2.4 m/s -18°

4.0 m/s -15°
Concentration Contours

**Trial 1: Mid 120s**
- Eastings (km): 
- Northings (km): 
- Mock urban array: 4,545 kg
- Vertically down release: 1.5 m/s -18°

**Trial 6: Mid 120s**
- Eastings (km): 
- Northings (km): 
- Open terrain: 8,391 kg
- Vertically down release: 2.4 m/s -18°

**Trial 7: Mid 120s**
- Eastings (km): 
- Northings (km): 
- Open terrain: 9,072 kg
- 45-deg down release: 4.0 m/s -15°
Concentration Contours

Trial 1: Mid 300s

Trial 6: Mid 300s

Trial 7: Mid 300s

Mock urban array

Vertically down release

Open terrain

Vertically down release

Open terrain

Vertically down release

1.5 m/s -18°

2.4 m/s -18°

4.0 m/s -15°

4,545 kg

8,391 kg

9,072 kg

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Concentration Contours

Trial 1: Mid 600s
- Eastings (km): -1 to 1
- Northing (km): -1 to 2.5
- Concentration: 4,545 kg, 1.5 m/s, -18°

Trial 6: Mid 600s
- Eastings (km): -1 to 1
- Northing (km): -1 to 2.5
- Concentration: 8,391 kg, 2.4 m/s, -18°

Trial 7: Mid 600s
- Eastings (km): -1 to 1
- Northing (km): -1 to 2.5
- Concentration: 9,072 kg, 4.0 m/s, -15°

Mock urban array
Vertically down release

Open terrain
Vertically down release

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Concentration Contours

Trial 1: Mid 1200s
- Northings (km)
- Eastings (km)
- Concentration (ppm)

Trial 6: Mid 1200s
- Northings (km)
- Eastings (km)
- Concentration (ppm)

Trial 7: Mid 1200s
- Northings (km)
- Eastings (km)
- Concentration (ppm)

Mock urban array
- 4,545 kg
- Vertically down release

Open terrain
- 8,391 kg
- Vertically down release

Open terrain
- 9,072 kg
- 45-deg down release

1.5 m/s
-18°

2.4 m/s
-18°

4.0 m/s
-15°

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Concentration Contours

Trial 1: Far 600s
- 1.5 m/s
- -18°
- Vertically down release
- Mock urban array
- 4,545 kg

Trial 6: Far 600s
- 2.4 m/s
- -18°
- Vertically down release
- Open terrain
- 8,391 kg

Trial 7: Far 600s
- 4.0 m/s
- -15°
- Vertically down release
- Open terrain
- 9,072 kg
- 45-deg down release
Concentration Contours

Trial 1: Far 1200s
Mock urban array
Vertically down release
4,545 kg
1.5 m/s -18°

Trial 6: Far 1200s
Open terrain
Vertically down release
8,391 kg
2.4 m/s -18°

Trial 7: Far 1200s
Open terrain
45-deg down release
9,072 kg
4.0 m/s -15°

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Concentration Contours

Trial 1: Far 1800s
- Northing: 10 km
- Easting: -10 to 5 km
- Release: 4,545 kg
- Velocity: 1.5 m/s
- Angle: -18°
- Terrain: Vertically down release
- Schematic: Mock urban array

Trial 6: Far 1800s
- Northing: 10 km
- Easting: -10 to 5 km
- Release: 8,391 kg
- Velocity: 2.4 m/s
- Angle: -18°
- Terrain: Vertically down release
- Schematic: Open terrain

Trial 7: Far 1800s
- Northing: 10 km
- Easting: -10 to 5 km
- Release: 9,072 kg
- Velocity: 4.0 m/s
- Angle: 45-deg down release
- Terrain: Open terrain

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Concentration Contours

**Trial 1: Far 2700s**
- Mock urban array 4,545 kg
- Vertically down release 1.5 m/s -18°

**Trial 6: Far 2700s**
- Open terrain 8,391 kg
- Vertically down release 2.4 m/s -18°

**Trial 7: Far 2700s**
- Open terrain 9,072 kg
- 45-deg down release 4.0 m/s -15°
Concentration Contours

Trial 1: Far 3600s
- Northing: 4,545 kg
- Easting: 1.5 m/s -18°
- Vertically down release

Trial 6: Far 3600s
- Northing: 8,391 kg
- Easting: 2.4 m/s -18°
- Vertically down release

Trial 7: Far 3600s
- Northing: 9,072 kg
- Easting: 4.0 m/s -15°
- 45-deg down release

Mock urban array

Open terrain
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• Sensitivity analysis
  – Dry deposition velocity set to zero
  – Increased roughness for urban array in Trial 1

• Conclusions and Future Directions
Dry Deposition Sensitivity Test

- Base case with dry deposition velocity $v_d = 0.04 \text{ cm/s}$
- Dry deposition velocity set to zero (no deposition)

Trial 1
- Concentration (ppm) vs. Downwind distance (km)
- Mock urban array
- Vertically down release
- 1.5 m/s -18°
- 4,545 kg

Trial 6
- Concentration (ppm) vs. Downwind distance (km)
- Open terrain
- Vertically down release
- 2.4 m/s -18°
- 8,391 kg

Trial 7
- Concentration (ppm) vs. Downwind distance (km)
- Open terrain
- Vertically down release
- 4.0 m/s -15°
- 9,072 kg

All results are for 2 s (raw) averaging times
Dry Deposition Sensitivity Test

- Base case with dry deposition velocity $v_d = 0.04 \text{ cm/s}$
- Dry deposition velocity set to zero (no deposition)

Trial 1

- Logarithmic scale: the difference is roughly 20 ppm versus 30 ppm at 11 km

Enlarged image for Trial 1

All results are for 2 s (raw) averaging times
Mock Urban Array Sensitivity Test

- There is no obstacle-resolving model in DRIFT, only a uniform surface roughness can be used
- Approach: run two simulations with different roughness lengths: a.) $z_0 = 0.4$ m, b.) $z_0 = 0.5$ mm
- Blend the two simulations together at the downwind edge of the mock urban array (approx. 100 m)
- Displace the centerline concentration profile of the $z_0 = 0.5$ mm result to match the $z_0 = 0.4$ m result
- This approach was taken in HSL’s previous DRIFT and PHAST simulations for JRII at GMU last year

All results are for 2 s (raw) averaging times
Conclusions and Future Directions

• DRIFT results for model inter-comparison exercise
  – Reasonably good predictions for Trials 6 and 7
  – Over-prediction in Trial 1: Effect of mock urban array? Wind speed profile?
  – Dry deposition velocity of 0.04 cm/s has a small effect (e.g. 20 ppm to 30 ppm at 11 km)

• Effect of averaging times
  – Small difference in using raw, 20 s or 1 minute averaging times

• Future DRIFT work
  – Investigate further the cloud speed in Trials 1 and 6, and over-prediction in Trial 1
  – Toxic load: calculate from time-varying concentrations and compare to IDA data
  – Source terms: sensitivity test using standard risk assessment approach for modelling Trials 1, 6 and 7 using DRIFT source models
  – Sensitivity tests to investigate other uncertainties: e.g. changing meteorology and dry deposition
Conclusions and Future Directions

- Future work on model inter-comparison exercise
  - Work with DNV GL on PHAST simulations
  - Help to cross-plot results from other models

- Chlorine incident analysis
  - Re-examine model predictions for three chlorine incidents (Festus, Macdona, Graniteville) using PHAST and DRIFT
  - Do we understand yet why the six models over-predicted the number of casualties in the original Hanna et al. (2008) study?

Comparison of Six Widely-Used Dense Gas Dispersion Models for Three Recent Chlorine Railcar Accidents

Steven Hanna, Seshu Dharmanuram, John Zhang, Ian Sykes, Henk Witlox, Shah Khajehnejad, and Kay Koslen

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Comparison of Six Widely-Used Dense Gas Dispersion Models for Three Recent Chlorine Railcar Accidents

Steven Hanna, Seshu Dhamavaram, John Zhang, Ian Sykes, Henk Witlox, Shah Khajehnejad, and Kay Kolen
Thank you

Questions?
Modified $u^*$ to match reference wind speed

Trial 1

- T3 PWIDS avg 1340 and 1350
- DRIFT $u^*=0.108 \text{m/s}; l=0.124 \text{m}; z_0=0.5 \text{mm}$
- DRIFT $u^*=0.0537 \text{m/s}; l=0.124 \text{m}; z_0=0.5 \text{mm}$

Trial 7

- T3 PWIDS avg 1400 and 1410
- DRIFT $u^*=0.21 \text{m/s}; l=0.0229 \text{m}; z_0=0.5 \text{mm}$
- DRIFT $u^*=0.164 \text{m/s}; l=0.0229 \text{m}; z_0=0.5 \text{mm}$
Modified $u^*$ to match reference wind speed