JACK RABBIT II 2015 CHLORINE RELEASE EXPERIMENTS:
SIMULATIONS OF THE TRIALS USING DRIFT AND PHAST

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Bryan McKenna, Maria Garcia, Simon Gant, Adrian Kelsey, Alison McGillivray, James Stewart, Rachel Batt, Mike Wardman, Harvey Tucker (HSE)

Graham Tickle (GT Science & Software)

Henk Witlox (DNV GL)
Jack Rabbit II Phase 1 (2015)

- Chlorine releases of 4.5 to 8 tonnes
- Release from a pressure vessel through a 6 inch diameter hole, 1 m above ground level
  - Release orientation directly downwards
  - Mock urban array of obstacles
- Dispersion measurements up to 11 km downwind
- Infiltration measurements into buildings and vehicles
- Measurements of source terms and weather conditions
## Release conditions

<table>
<thead>
<tr>
<th>Trial</th>
<th>Mass of Chlorine (kg)</th>
<th>Initial Tank Pressure (kPa)</th>
<th>Wind Direction relative to urban grid (degrees)</th>
<th>Wind Speed at 2 m reference height (m s(^{-1}))</th>
<th>Atmospheric Temperature (K)</th>
<th>Relative Humidity (%)</th>
<th>Atmospheric Pressure (kPa)</th>
<th>Pasquill Stability Class*</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>4509</td>
<td>738</td>
<td>-18</td>
<td>2.0</td>
<td>290.9</td>
<td>39.2</td>
<td>87</td>
<td>F</td>
</tr>
<tr>
<td>2</td>
<td>8151</td>
<td>693</td>
<td>-7</td>
<td>4.2</td>
<td>295.9</td>
<td>33.6</td>
<td>88</td>
<td>C</td>
</tr>
<tr>
<td>3</td>
<td>4512</td>
<td>658</td>
<td>+4</td>
<td>3.9</td>
<td>295.7</td>
<td>30.3</td>
<td>87</td>
<td>D</td>
</tr>
<tr>
<td>4</td>
<td>6970</td>
<td>602</td>
<td>+18</td>
<td>2.3</td>
<td>295.7</td>
<td>26.9</td>
<td>87</td>
<td>D</td>
</tr>
<tr>
<td>5</td>
<td>8303</td>
<td>674</td>
<td>+17</td>
<td>2.7</td>
<td>295.4</td>
<td>26.5</td>
<td>87</td>
<td>D</td>
</tr>
</tbody>
</table>

*Stability classes were provided by Dugway, except for Trial 1 which was estimated by HSE*
Modelling methodology

- Meta-stable liquid flow through orifice (sensitivity with flashing)
- Surface roughness 0.4 m for urban grid / 1 mm for desert
- Two simulations run and blended together 100 m downwind
- Base case with no rainout, and sensitivity with full rainout
- Used source and weather data from experiments
- Short averaging times used to predict peak concentrations
- Described by McKenna et al. (2016, 2017)
Drift 3.7.2 (ESR Technology)

- STREAM (HSE discharge model) was used to model the release rate
- Drift’s two-phase jet model was used to predict conditions at impact point with the ground
- Drift’s low momentum area source model was used with the finite duration model
- GASP (ESR Technology) was used for pool evaporation and combined with Drift for rainout cases
- Drift accounts for along-wind diffusion and along-wind gravity spreading
Phast 7.11 (DNV GL)

- Time-varying leak model was used in Phast
- Source modelled as a number of time steps, each with a corresponding dispersion calculation
- Release was angled -90° from the horizontal
- For the rainout cases, Phast uses the default pool evaporation model and accounts for the addition of chlorine vapour from the pool back into the dispersing cloud
- The time-varying model does not account for along-wind diffusion or along-wind gravity spreading. Phast 8.0 will include these effects and is scheduled to be released end of October
Comparison of concentration data

- **Trial 1**
  - DRIFT baseline without rainout
  - DRIFT with rainout
  - Measured max arc-wise concentration
  - Canary sensor data: only 3 sensors
  - MiniRAE saturated/exceeded calibration
  - ToxiRAE saturated
  - Narrow plume passed between sensors
  - Plume passed beyond edge of arc

- **Trial 2**
  - PHAST baseline without rainout
  - PHAST with rainout

- **Trial 3**
  - PHAST baseline without rainout
  - PHAST with rainout

- **Trial 4**
  - DRIFT baseline without rainout
  - DRIFT with rainout
  - Measured max arc-wise concentration
  - Canary sensor data: only 3 sensors
  - MiniRAE saturated/exceeded calibration
  - ToxiRAE saturated
  - Narrow plume passed between sensors
  - Plume passed beyond edge of arc

- **Trial 5**
  - PHAST baseline without rainout
  - PHAST with rainout
Comparison of Toxic Load data

SLOT/SLOD values available from http://www.hse.gov.uk/chemicals/haztox.htm
Global Sensitivity Analysis using Drift

- Vary all parameters simultaneously

- Benefits
  - Results do not depend on choice of baseline
  - Information provided on interactions between inputs
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>
<th>Wind Speed at 2m reference height (m s⁻¹)</th>
<th>Temperature (K)</th>
<th>1/Monin-Obukhov Length (m⁻¹)</th>
<th>Vapour Deposition Velocity (cm s⁻¹)</th>
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<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>
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- Flashing or metastable release

- Model output: Distance to 100 ppm concentration
Global Sensitivity Analysis method

- Gaussian Emulation Machine (GEM) software
  - [https://www.tonyohagan.co.uk/academic/GEM/](https://www.tonyohagan.co.uk/academic/GEM/)

- Emulator constructed from 127 Drift simulations
  - Sobol’ sequence sampling method
    - 64 with metastable release
    - 63 with flashing release

- Cross-validation checks performed to ensure emulator produces a good fit to the Drift results

- Sensitivity analysis results:
  - Which inputs affect the outputs? (Variance: main and total effects)
  - How do the inputs affect the outputs? (Mean-based analysis)
Drift results used to build emulator

Sensitivity analysis based on predicted distance to 100 ppm concentration
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:
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<td>0.08</td>
<td>5/0.05</td>
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- 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
Discussion

• Deposition velocity
  – 5 cm s\(^{-1}\) chosen from max value in literature (Hanna and Chang, 2008)
    • Deposition velocity dominated the dispersion behaviour
  – 0.05 cm s\(^{-1}\) more realistic for Dugway (lab exps by Hearn et al., 2012)
    • Atmospheric stability dominated the dispersion behaviour
  – Conclusion: Great care is needed in selecting the deposition velocity
  – Simplified deposition model in Drift does not account for saturation or other complex effects (e.g. response of vegetation)
  – Models tuned to field trial experiments with inherent deposition effects?
    • Avoid double accounting for the phenomenon
    • Need to validate deposition models
Discussion

• Inventory probably had little effect here because:
  – 6-inch hole diameter was used in all cases
  – Maximum flow rate remained almost constant (the release duration changed as the inventory changed)
    • Could look at a range of hole sizes to examine any effects of different flow rates

• Catastrophic releases may exhibit different behaviour

• Results from global sensitivity analysis depend on:
  – Defined ranges of the input parameters
  – Choice of model output (in this case, downwind distance to 100 ppm)
Summary

• Drift and Phast models in best agreement with the experimental data when they accounted for rainout, but tended to over-predict concentrations to a greater extent when rainout was ignored.

• Global sensitivity analysis using Drift showed that dry deposition could have a dominating effect on the predicted concentrations of these trials if a high deposition velocity of 5 cm s⁻¹ was assumed.

• However, 5 cm s⁻¹ is probably far too high a value for Dugway and further analysis using a lower dry deposition value of 0.05 cm s⁻¹ showed that atmospheric stability (Inverse Monin-Obukhov length) had a dominating effect in that case, with deposition having practically no effect.

• Further work on dry deposition is required to understand reasonable modelling assumptions and inputs for chlorine releases.
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Disclaimer

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