Integral model predictions of chlorine dispersion for the proposed Jack Rabbit II experiments in 2016

HSL: Bryan McKenna*, Simon Gant, Maria Garcia, Rachel Batt
HSE: Harvey Tucker
DNV-GL: Henk Witlox, Jan Stene
GT Science & Software: Graham Tickle
Contents

• Objectives
• Jack Rabbit II experiments
• PHAST and DRIFT models
• Discharge
• Dispersion
• Conclusions
Objectives

- To provide dispersion model predictions prior to Jack Rabbit II experiments to help position sensors
- Main question: will sensors reach saturation (maximum) concentration and not record useful data?

Sensor locations:

Sensor saturation concentrations:
- Jaz = 100,000 ppmv
- Canary = 10,000 ppmv
- MiniRAE = 2,000 ppmv
- ToxiRAE = 50 ppmv

For context: IDLH = 10 ppmv

- Modelling methodology: predict reasonably conservative estimates and run sensitivity tests
Jack Rabbit II Experiments

Chlorine Release
Mass = 10 tons (US) [9,072kg]
Tank temperature = 20°C
Tank pressure = saturation (5.9barg)
Hole diameter = 6inch
Different types of release

Terrain
Surface roughness $z_0 = 1$mm

Weather
Wind speed = 2m/s @ height = 10m (but could be up to 6m/s)
Atmospheric pressure = 0.8525atm
Temperature = 20°C
Humidity = 40% RH
Time of release = 7:00am (stable atmosphere: base case = F2 weather)
2015 Experiments

• Vertical release (downwards)
• Model uncertainties
  – Flashing in the orifice?
  – Rainout?
• 2015 tests proved that
  – There is flashing
    • Experimental release rates lower than predicted for metastable liquid
  – There is rainout
# Tests modelled (2016)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Test 1</th>
<th>Test 2</th>
<th>Test 3</th>
<th>Test 4</th>
<th>Test 5</th>
<th>Test 6</th>
<th>Test 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release type</td>
<td>Vertical downwards</td>
<td>-45deg</td>
<td>Horizontal</td>
<td></td>
<td></td>
<td>Vertical upwards</td>
<td></td>
</tr>
<tr>
<td>Phase</td>
<td>Liquid*</td>
<td>Liquid*</td>
<td>Liquid*</td>
<td>Liquid*</td>
<td>Liquid*</td>
<td><strong>2-phase</strong></td>
<td>Vapour</td>
</tr>
<tr>
<td>Flashing</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>Yes</td>
<td>No</td>
</tr>
<tr>
<td><strong>Rainout</strong></td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>Release height from vessel bottom</td>
<td>0m</td>
<td>0m</td>
<td>0m</td>
<td>0.2m</td>
<td>0.7m</td>
<td>0.99m (below liquid level)</td>
<td>1.37m</td>
</tr>
<tr>
<td>Weather</td>
<td>F2</td>
<td>D6</td>
<td>F2</td>
<td>F2</td>
<td>F2</td>
<td>F2</td>
<td>F2</td>
</tr>
<tr>
<td>Roughness length</td>
<td>1mm</td>
<td>1mm</td>
<td><strong>5mm</strong></td>
<td>1mm</td>
<td>1mm</td>
<td>1mm</td>
<td>1mm</td>
</tr>
</tbody>
</table>

* Metastable liquid (agreed by the MWG)
** Models are conservative if assuming no rainout
PHAST Model

• Model used: Time-varying release
  – Absence of along-wind diffusion: conservative predictions in the far field
  – Is it adequate for a release from top of the vessel?
    • It does not account for liquid swell
    • It takes into account the liquid level in the tank
    • Leak and Finite duration scenarios were also considered
    • Time-varying model used for consistency purposes
DRIFT model

• Constant release rate
  – HSE Stream release rate calculation
• DRIFT finite-duration dispersion model accounts for:
  – Additional gravity spreading and dilution over the source
  – Along-wind diffusion
  – Along-wind gravity spreading
  – Limitations: 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
Discharge Predictions

Release duration 229 sec
Phast. Vertical upwards, aligned in the wind direction (azimuth of 345 degrees)
Drift. Vertical upwards, aligned in the wind direction (azimuth of 345 degrees)
Phast. Centreline concentration, aligned in the wind direction (azimuth of 345 degrees)
Phast Results Summary

Jaz sensors may saturate

Canary sensors may saturate

Maximum concentration at each sensor arc

Use Jaz sensors

Use Canary sensors

Use MiniRAE sensors

100,000 ppm (Jaz)

10,000 ppm (Canary)

2,000 ppm (MiniRAE)

50 ppm (ToxiRAE)
Drift. Centreline concentration, aligned in the wind direction (azimuth of 345 degrees)
Drift. Centreline concentration, aligned in the wind direction (azimuth of 345 degrees)
**Drift Results Summary**

- **Jaz sensors may saturate**
  - Use Jaz sensors at distances:
    - 120m: 100,000 ppm (Jaz)
    - 200m: 100,000 ppm (Jaz)
    - 500m: 10,000 ppm (Canary)
    - 1km: 2,000 ppm (MiniRAE)
    - 2km: 50 ppm (ToxiRAE)

- **Canary sensors may saturate**
  - Use Canary sensors at distances:
    - 500m: 100,000 ppm (Jaz)
    - 1km: 10,000 ppm (Canary)
    - 2km: 2,000 ppm (MiniRAE)
    - 5km: 50 ppm (ToxiRAE)

- **Use MiniRAE sensors** at 5km: 50 ppm (ToxiRAE)

- **Use ToxiRAE sensors** at 11km: 50 ppm (ToxiRAE)

---

© British Crown Copyright
Conclusions

• Provided model predictions of 2016 Jack Rabbit II experiments using two different integral dispersion models: PHAST and DRIFT
• Performed model sensitivity tests:
  – Downwards: D6 weather, 5mm roughness
  – Upwards: 2-phase release vs. gas release
• Provided helpful information (hopefully) for positioning of sensors in Jack Rabbit II experiments
Disclaimer

• The contribution made to this paper by HSL was funded by the Health and Safety Executive (HSE). The contents, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy.

• DNV-GL have provided guidance on the appropriate methodology to use with PHAST, but the PHAST simulations presented here were performed by HSL and have not been independently checked by DNV-GL.

• GT Science & Software have provided guidance on the appropriate methodology to use with Drift, but the Drift simulations presented here were performed by HSL and have not been independently checked by GT Science & Software.
Thanks for contributions from:

• Simon Gant, Maria Garcia, Rachel Batt (HSL)
• Henk Witlox, Jan Stene (DNV-GL)
• Graham Tickle (GT Science & Software)
• Jack Rabbit II Modelling Working Group

Any questions?
Introduction to HSL

• Multi-disciplinary:
  – Fire and process safety
  – Computational modelling
  – Exposure control
  – Toxicology etc.

• Approx. 400 staff
• 550 acre test site
• Fire galleries and burn hall
• Impact track
• Anechoic chamber
• Thermal test chamber
• Imaging/sampling from UAV
Introduction to HSL

Buncefield Incident Investigation

CO₂ two-phase jets

Emulators for global sensitivity analysis

Concentration fluctuations: flammable/toxic

© C. Fukushima, J. Westerweel, TU Delft
Phast. Vertical downwards
Phast. Vertical downwards (Test 1)

Contours at ground level
Drift. Vertical downwards

Vertical downwards

- Test 1. Base Case
- Test 2. D6 weather
- Test 3. 5mm roughness

Centrefile concentration / ppm

Downwind distance / m

© British Crown Copyright
Drift. Vertical downwards (Test 1)

Contours at ground level

- Outdoor Conc Criteria 1: 100,000 ppmv
- Outdoor Conc Criteria 2: 10,000 ppmv
- Outdoor Conc Criteria 3: 2,000 ppmv
- Outdoor Conc Criteria 4: 50 ppmv
Main question: will sensors reach saturation (maximum) concentration and not record useful data?

![Downwind distance to sensor threshold concentration chart]

- Test 1. Downwards
- Test 4. -45deg from horizontal
- Test 5. Horizontal
- Test 6. Upwards. 2-phase
- Test 7. Upwards. Gas
Drift Results Summary

- Main question: will sensors reach saturation (maximum) concentration and not record useful data?

### Downwind distance to sensor threshold concentration

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>100,000 ppm (Jaz)</td>
<td>100</td>
<td>1,000</td>
<td>10</td>
<td>10</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>10,000 ppm (Canary)</td>
<td>1,000</td>
<td>1,000</td>
<td>100</td>
<td>100</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>2,000 ppm (MiniRAE)</td>
<td>10,000</td>
<td>10,000</td>
<td>1,000</td>
<td>1,000</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>50 ppm (ToxiRAE)</td>
<td>10,000</td>
<td>10,000</td>
<td>10,000</td>
<td>10,000</td>
<td>1,000</td>
<td>1,000</td>
</tr>
</tbody>
</table>
PHAST Model

- **Equation-of-state**
  - **Default PHAST EOS** since it provides more accurate liquid density for chlorine from DIPPR than SRK or Peng-Robinson EOS

- **Orifice flow**
  - **Meta-stable liquid** since it gives higher mass flow rate than flashing in the orifice
  - **Compressible flow** since it gives slightly higher mass flow rate than Bernoulli

- **Jet expansion to atmospheric pressure**
  - **Conservation of Momentum** model: more accurate velocity than isentropic model

- **Droplet Size Model**
  - **DNV Phase III JIP model**: appropriate for use with Conservation of Momentum jet expansion model (choice has no effect on dispersion results)

- **Averaging time**
  - **18.75 s**: i.e. no time averaging in PHAST, in order to match short averaging time of sensors and predict peak concentrations
DRIFT Finite-Duration Model

Centreline Concentration

Cloud Shape

\[ f(t) \times b(t) \times f(t) \]

distance

concentration

continuous

finite

\[ x_b(t) \quad x_f(t) \]
DRIFT Time-Varying Model

• Split into finite-duration segments
• Add concentrations

Combined = #1 + #2
DRIFT Modelling Assumptions (1)

• Aerosol modelling
  – Flash expansion of superheated liquid in jet phase
  – Vaporisation based upon homogeneous equilibrium
  – Liquid chlorine assumed to form ideal solution with condensed water

• Low-momentum area source
  – Neglects jet entrainment after impingement, but accounts for gravity spreading (and gravity driven edge entrainment)

• Finite-duration dispersion model includes
  – Along-wind and across-wind spreading of the cloud (gravity and passive)
  – Shear leaning of the cloud when passive
DRIFT Modelling Assumptions (2)

• Terrain
  – Horizontal flat ground

• Other
  – Constant meteorological conditions
  – Short time averaging
  – Heat transfer from ground to cloud neglected