APPENDIX A: SENSITIVITY TESTS INPUTS AND SETUP TABLES

This appendix contains two tables for each case and model; the first outlines the assumptions and inputs that were kept constant for each case, and the second provides the inputs varied in the sensitivity. Those parameter values that comprise the base case runs are highlighted in orange.
A.1. Evaporating pools

A.1.1. Direct pool source

Table A.1a: ADMS – Direct pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Duration</td>
<td>Continuous (plume)</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Set source density, heat capacity and molecular mass to be consistent with methane/ammonia</td>
<td>The molecular mass and heat capacity values could be representative of a pool of aqueous ammonia</td>
</tr>
<tr>
<td>Duration</td>
<td>Plume source (continuous)</td>
<td></td>
</tr>
<tr>
<td>Averaging time</td>
<td>10 minutes</td>
<td></td>
</tr>
<tr>
<td>Outputs</td>
<td>Concentrations at ground level, and 1m above ground (not at plume centreline)</td>
<td></td>
</tr>
</tbody>
</table>

Table A.1b: ADMS – Direct pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Area of source</td>
<td>m²</td>
<td>3.1, 19.6, 78.5, 314</td>
<td>Modelled as a square area source. Equivalent diameters: 2, 5, 10, 20 m</td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Emission rate</td>
<td>g/m²/s</td>
<td>25.5, 63.7, 127, 255, 637</td>
<td></td>
</tr>
<tr>
<td>Emission height</td>
<td>m</td>
<td></td>
<td>0, 0.05, 1, 5</td>
<td></td>
</tr>
<tr>
<td>Emission temperature</td>
<td>°C</td>
<td></td>
<td>0, -20, -100</td>
<td>The minimum temperature in ADMS is -100 °C.</td>
</tr>
</tbody>
</table>

Table A.2a DEGADIS – Direct pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>Ground-level, low initial momentum (non-jet) release</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>LNG, chlorine</td>
<td></td>
</tr>
</tbody>
</table>

Table A.2b: DEGADIS – Direct pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>2, 10, 50</td>
<td></td>
</tr>
<tr>
<td>Dimensions of pool</td>
<td>Pool radius</td>
<td>m</td>
<td>1, 5, 10</td>
<td></td>
</tr>
</tbody>
</table>
Table A1.3a DRIFT – Direct pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Averaging times</td>
<td>Short: instantaneous</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Long: 10 minutes</td>
<td></td>
</tr>
<tr>
<td>Duration</td>
<td>Continuous</td>
<td>Using Steady Continuous Release Type</td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (buoyant)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Air (neutrally buoyant)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (dense)</td>
<td></td>
</tr>
<tr>
<td>Release Phase</td>
<td>Gaseous</td>
<td></td>
</tr>
<tr>
<td>Release Temperature</td>
<td>15 °C</td>
<td></td>
</tr>
<tr>
<td>Source Type</td>
<td>Low Momentum Area Source</td>
<td></td>
</tr>
<tr>
<td>Include Dilution Over Source</td>
<td>True</td>
<td></td>
</tr>
<tr>
<td>Atmosphere Inversion Height</td>
<td>Default</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.3b: DRIFT – Direct pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Source Diameter</td>
<td>m</td>
<td>2, 5, 10, 20</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release amount</td>
<td>Release Rate</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table A1.4a: GASTAR – Direct pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release type</td>
<td>‘Continuous’</td>
<td></td>
</tr>
<tr>
<td>Averaging time</td>
<td>10 minutes</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (buoyant)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Ethylene (neutrally buoyant)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (dense)</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.4b: GASTAR – Direct pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Initial plume width</td>
<td>m</td>
<td>2, 5, 10, 20</td>
<td></td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass flux</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td>Emission temperature</td>
<td>K</td>
<td></td>
<td>Methane: 111.7, 116.7, 121.7</td>
<td>Equivalent to: Boiling point (bp), bp + 5, bp + 10</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Ethylene: 169.4, 174.4, 179.4</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Chlorine: 238.7, 243.7, 248.7</td>
<td></td>
</tr>
</tbody>
</table>
### Table A1.5a: SLAB – Direct pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release type</td>
<td>‘Type ‘1’</td>
<td>Evaporating pool release: infinite duration, centre at 0,0,0</td>
</tr>
<tr>
<td>Duration</td>
<td>Continuous (3600 s)</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane, hydrogen cyanide, chlorine</td>
<td></td>
</tr>
<tr>
<td>Averaging time</td>
<td>600 s</td>
<td></td>
</tr>
<tr>
<td>Surface roughness</td>
<td>0.1 m</td>
<td></td>
</tr>
</tbody>
</table>

### Table A1.5b: SLAB – Direct pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Area source</td>
<td>m²</td>
<td>3.1, 19.6, 78.5, 314</td>
<td>Modelled as a square area source. Equivalent diameters: 2, 5, 10, 20m</td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass flux from pool</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td></td>
</tr>
</tbody>
</table>
A.1.2 Bunded pool source

Table A1.6a: ALOHA – Bunded pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pentane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>‘concrete’ option</td>
<td>Note – ALOHA does not have a specific option to specify the presence of a bund – instead simulated by setting a fixed pool diameter</td>
</tr>
<tr>
<td>Outputs</td>
<td>‘Max Average Sustained Release Rate’ (vaporisation rate) Distance to the lower explosive limit (LEL) and 10% LEL values</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.6b: ALOHA – Bunded pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Diameter</td>
<td>m</td>
<td>2, 4, 5, 8, 10 (methane)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>4, 8, 10, 16, 20 (pentane)</td>
<td></td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass flux</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td></td>
<td>-161.6, -162, -165, -170, -180</td>
<td>Varied for methane only For pentane, set to be the same as the base case air and ground temperature (15 °C)</td>
</tr>
<tr>
<td>Air temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
Table A1.7a: GASP/DRIFT – Bunded pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td>Using inbuilt substance properties (SPI files source)</td>
</tr>
<tr>
<td></td>
<td>n-Pentane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>Land</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>Concrete</td>
<td>Using inbuilt substrate properties</td>
</tr>
<tr>
<td>Release type (GASP)</td>
<td>Instantaneous</td>
<td></td>
</tr>
<tr>
<td>Pool geometry</td>
<td>Circular</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Initial pool radius</td>
<td>Set equal to the bund radius</td>
<td></td>
</tr>
<tr>
<td>Initial ground temperature</td>
<td>Equal to the air temperature</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Pool spreading constraints</td>
<td>Bunded</td>
<td></td>
</tr>
<tr>
<td>Pool surface roughness length</td>
<td>0.23 mm</td>
<td>GASP default</td>
</tr>
<tr>
<td>Heat transfer mode</td>
<td>Perfect thermal contact, temperature varying substrate</td>
<td>GASP default</td>
</tr>
<tr>
<td>Thermodynamic options</td>
<td>Calculated pool temperature, 3-dimension conduction from ground (true), convection from atmosphere (true)</td>
<td>GASP defaults</td>
</tr>
<tr>
<td>Additional heat flux into pool</td>
<td>0 kW/m²</td>
<td>GASP default</td>
</tr>
<tr>
<td>Release type (DRIFT)</td>
<td>Time Varying Release</td>
<td>DRIFT default</td>
</tr>
<tr>
<td>Include Dilution Over Pool (DRIFT)</td>
<td>True</td>
<td>DRIFT default</td>
</tr>
</tbody>
</table>

Table A1.7b: GASP - Bunded pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Diameter</td>
<td>m</td>
<td>2, 4, 5, 8, 10, 20</td>
<td></td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td></td>
<td>-162.4, -163, -165, -170, -180 for methane 5, 15, 30 for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td>Air and initial temperature of substrate</td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.8a: HGSYSTEM (LPOOL) – Bunded pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pentane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>‘concrete’ option</td>
<td></td>
</tr>
<tr>
<td>Bund information</td>
<td>‘Dike present’ option</td>
<td>Composition same as substrate (concrete)</td>
</tr>
</tbody>
</table>
### Table A1.8: HGSYSTEM (LPOOL) – Bunded pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Volume flow rate</td>
<td>m³/s</td>
<td>2, 20, 200</td>
<td>Released over one second</td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td>°C</td>
<td></td>
<td>-161, -170, -180</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - pentane</td>
<td>°C</td>
<td></td>
<td>0, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Dimensions of pool</td>
<td>Radius</td>
<td>m</td>
<td>2, 5, 10</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 10, 20</td>
<td>5m/s for DS conditions, 2m/s for F2 conditions</td>
</tr>
</tbody>
</table>

### Table A1.9: LSMS – Bunded pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source configuration</td>
<td>‘Dam break’ (instantaneous)</td>
<td></td>
</tr>
<tr>
<td>Bund information</td>
<td>‘Bund present’ option</td>
<td>Bund height set to be equivalent to a bund capacity that is 25% larger than the liquid volume level</td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) Butane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>‘Homogeneous/impermeable’</td>
<td></td>
</tr>
<tr>
<td>Base case ‘A’ (methane only)</td>
<td>Thermal properties set to represent ‘Standard concrete’ substrate and bund as the base case</td>
<td>Normal situation, to test most parameters</td>
</tr>
<tr>
<td>Base case ‘B’ (methane only)</td>
<td>Set thermal properties of substrate and bund to represent an insulating bund</td>
<td>Set up to isolate and test the effects of solar radiation and wind speed, by switching off the substrate heat flux. Checked that the evaporation rate is (almost) zero when the wind speed is reduced to very low value and insolation set to zero</td>
</tr>
<tr>
<td>General parameter</td>
<td>Model input parameter(s)</td>
<td>Units</td>
</tr>
<tr>
<td>-------------------</td>
<td>--------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>Initial mass in pool – methane (Base Case ‘A’)</td>
<td>Vertical size</td>
<td>m</td>
</tr>
<tr>
<td></td>
<td>Bund depth</td>
<td></td>
</tr>
<tr>
<td>Initial mass in pool- butane (Base Case ‘A’)</td>
<td>Vertical size</td>
<td>m</td>
</tr>
<tr>
<td></td>
<td>Bund depth</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature – methane (Base Case ‘A’)</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>Initial liquid temperature – butane (Base Case ‘A’)</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>Pool and bund radius – methane (Base Case ‘A’)</td>
<td>Pool radius</td>
<td>m</td>
</tr>
<tr>
<td></td>
<td>Liquid depth</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bund depth</td>
<td></td>
</tr>
<tr>
<td>Pool and bund radius – butane</td>
<td>Pool radius</td>
<td>m</td>
</tr>
<tr>
<td></td>
<td>Liquid depth</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bund depth</td>
<td></td>
</tr>
<tr>
<td>Substrate and bund properties (Base Case ‘A’)</td>
<td>‘Standard concrete’, ‘BG1’ concrete, ‘GdF’ concrete</td>
<td></td>
</tr>
<tr>
<td>Substrate temperature (Base Case ‘A’, methane)</td>
<td></td>
<td>K</td>
</tr>
<tr>
<td>Solar flux (Base case ‘B’ only)</td>
<td></td>
<td>kW/m²</td>
</tr>
<tr>
<td>Wind speed (Base cases ‘A’ and ‘B’)</td>
<td></td>
<td>m/s</td>
</tr>
</tbody>
</table>
### Table A1.10a: PHAST – Bunded pool source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) n-Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Inventory type</td>
<td>Atmospheric storage tank</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Catastrophic rupture</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Liquid</td>
<td></td>
</tr>
<tr>
<td>Bund height</td>
<td>5 m</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>User defined (land)</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>10 cm</td>
<td></td>
</tr>
<tr>
<td>Solar radiation flux</td>
<td>0 kW/m(^2)</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>Concrete</td>
<td>Using inbuilt substrate properties</td>
</tr>
</tbody>
</table>

### Table A1.10b: PHAST – Bunded pool source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of bund</td>
<td>Diameter</td>
<td>m</td>
<td>4, 5, 8, 10, 20</td>
<td></td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td></td>
</tr>
<tr>
<td>Storage temperature</td>
<td></td>
<td>°C</td>
<td>-162.4 to -180</td>
<td>for methane 5, 15, 30</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Ground temperature</td>
<td></td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td></td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>m/s</td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
## A.1.3. Instantaneously released pool source on land

### Table A1.11a: HGSYSTEM (LPOOL) – Instantaneously released pool source on land: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release type</td>
<td>Release from reservoir</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td></td>
<td>Pentane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>1 second</td>
<td>To approximate an instantaneous release</td>
</tr>
</tbody>
</table>

### Table A1.11b: HGSYSTEM (LPOOL) – Instantaneously released pool source on land: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow into pool</td>
<td>Volume spill rate</td>
<td>m³/s</td>
<td>2.0, 20.0, 200.0</td>
<td>Varied the orifice diameter to ensure desired volume spill rates using the standard Bernoulli relation option in the model before entering desired flow parameters directly</td>
</tr>
<tr>
<td></td>
<td>Orifice diameter</td>
<td>m</td>
<td>0.309, 0.976, 3.124</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td>°C</td>
<td>-162, -170, -180</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - pentane</td>
<td>°C</td>
<td>0, 15, 30</td>
<td>Reflects the storage temperature, so the ambient temperature also set to the same values</td>
<td></td>
</tr>
<tr>
<td>Ground type</td>
<td>n/a</td>
<td>‘insulated concrete’, ‘wet sand’, ‘dry sand’</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ground temperature</td>
<td>°C</td>
<td>0, 15, 30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Minimum thickness of pool</td>
<td>mm</td>
<td>0.5, 1.0, 2.0</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td>1, 2, 5, 10 , 20</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
LSMS

Table A1.12a: LSMS – Instantaneously released pool source on land: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source configuration</td>
<td>‘Dam break’</td>
<td>instantaneous release</td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Butane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>‘Homogeneous/impermeable’</td>
<td></td>
</tr>
<tr>
<td>Outputs</td>
<td>Vaporisation rate</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Pool duration (methane only)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Maximum pool radius</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.12b: LSMS – Instantaneously released pool source on land: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial mass in</td>
<td>Vertical size</td>
<td>m</td>
<td>0.91, 1.96, 4.2</td>
<td>Keeping aspect ratio constant (height:width of 0.5)</td>
</tr>
<tr>
<td>pool – methane</td>
<td>Initial radius</td>
<td></td>
<td>0.91, 1.96, 4.2</td>
<td>Equivalent to 1, 10, 100 tonnes</td>
</tr>
<tr>
<td>Initial mass in</td>
<td>Vertical size</td>
<td>m</td>
<td>0.82, 1.76, 3.80</td>
<td></td>
</tr>
<tr>
<td>pool – butane</td>
<td>Initial radius</td>
<td></td>
<td>0.82, 1.76, 3.80</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature – methae</td>
<td>K</td>
<td>111.67, 108.15, 93.15</td>
<td>111.67 K is the value obtained when the ‘set to boiling’ option is checked</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature – butane</td>
<td>K</td>
<td>273.12, 288.12, 303.12</td>
<td>The substrate temperature was also set to these values, as this represents an ambient storage temperature</td>
<td></td>
</tr>
<tr>
<td>Initial pool radius - methane</td>
<td>Pool radius</td>
<td>m</td>
<td>0.5, 1.96, 4.0</td>
<td>Keeping the initial height constant at 1.96m (methane) and 1.76 (butane). Also effectively varying the mass</td>
</tr>
<tr>
<td>Initial pool radius - butane</td>
<td></td>
<td>m</td>
<td>0.44, 1.76, 3.53</td>
<td></td>
</tr>
<tr>
<td>Substrate properties</td>
<td>‘Standard concrete’, ‘non-porous sand’, ‘soil’</td>
<td></td>
<td></td>
<td>Set thermal parameters to represent these - (taken from LSMS documentation)</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td>K</td>
<td>283.12, 288.12, 293.12</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Turbulent drag</td>
<td>n/a</td>
<td>0.005, 0.01, 0.02</td>
<td>An advanced option controlling the dynamic spreading of the pool</td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td>1, 2, 5, 10, 20</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
### A.1.4. Continuously released pool source on land

**Table A.1.13a: ALOHA – Continuously released pool source on land: Key fixed parameters and assumptions**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source type</strong></td>
<td>'Tank' option: leak from storage within a spherical tank, 90% full of liquid. Large diameter orifice, located at the bottom of the tank</td>
<td>Did not use the 'Puddle' option, as this does not model spreading effects.</td>
</tr>
<tr>
<td><strong>Substances modelled</strong></td>
<td>Methane (cryogenic) Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td><strong>Release duration</strong></td>
<td>30 minutes</td>
<td></td>
</tr>
<tr>
<td><strong>Orifice</strong></td>
<td>Circular</td>
<td></td>
</tr>
</tbody>
</table>

**Table A.1.13b: ALOHA – Continuously released pool source on land: Parameters varied**

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow into pool</td>
<td>Chemical mass in tank</td>
<td>tonnes</td>
<td>1, 10, 100, 1000</td>
<td>Varied the orifice diameter to ensure that the release duration was constant (30 minutes)</td>
</tr>
<tr>
<td></td>
<td>Tank volume</td>
<td></td>
<td>2.625, 26.25, 262.5, 2625</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Orifice diameter</td>
<td>cm</td>
<td>3.55, 9.7, 24.92, 62</td>
<td>Hole diameter adjusted to give the required duration: 15, 30, 60 minutes</td>
</tr>
<tr>
<td>Duration of release</td>
<td>Orifice diameter</td>
<td>cm</td>
<td>14, 9.7, 6.88</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td>°C</td>
<td></td>
<td>-162, -165, -170, -180</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - pentane</td>
<td>°C</td>
<td></td>
<td>0, 15, 20, 30</td>
<td>Reflects the storage temperature, so the ambient temperature also set to the same values</td>
</tr>
<tr>
<td>Ground type</td>
<td>n/a</td>
<td></td>
<td>'concrete', 'default soil', 'sandy dry soil', 'moist sandy soil'</td>
<td>Tested all of the non-water predefined substrate options</td>
</tr>
<tr>
<td>Ground temperature</td>
<td>°C</td>
<td></td>
<td>10, 15, 20</td>
<td></td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Maximum pool diameter</td>
<td>m</td>
<td>‘unknown’, 12, 11, 10.5</td>
<td>'unknown' is the advised option if there are no barriers to prevent a puddle from spreading</td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
Table A1.14a: GASP/DRIFT – Continuously released pool source on land: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) n-Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties (SPI files source)</td>
</tr>
<tr>
<td>Release type (GASP)</td>
<td>Continuous</td>
<td></td>
</tr>
<tr>
<td>Aperture diameter (GASP)</td>
<td>0.05 m</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>1800 s</td>
<td>The duration of the release into the pool</td>
</tr>
<tr>
<td>Maximum pool age</td>
<td>3600 s</td>
<td>GASP runs until 99% if the spilled substance is vaporised or the maximum pool age is reached.</td>
</tr>
<tr>
<td>Pool geometry</td>
<td>Circular</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Surface type</td>
<td>Land</td>
<td></td>
</tr>
<tr>
<td>Pool spreading constraints</td>
<td>Puddle depth</td>
<td>Only the part of the pool above the puddle depth contributes to the pool spread</td>
</tr>
<tr>
<td>Initial ground temperature</td>
<td>Equal to the air temperature</td>
<td></td>
</tr>
<tr>
<td>Pool surface roughness length</td>
<td>0.23 mm</td>
<td>GASP default</td>
</tr>
<tr>
<td>Heat transfer mode</td>
<td>Perfect thermal contact, temperature varying substrate</td>
<td>GASP default</td>
</tr>
<tr>
<td>Thermodynamic options</td>
<td>Calculated pool temperature, 3-dimension conduction from ground (true), convection from atmosphere (true)</td>
<td>GASP defaults</td>
</tr>
<tr>
<td>Additional heat flux into pool</td>
<td>0 kW/m²</td>
<td>GASP default</td>
</tr>
<tr>
<td>Release type (DRIFT)</td>
<td>Time Varying Release</td>
<td>DRIFT default</td>
</tr>
<tr>
<td>Include Dilution Over Pool (DRIFT)</td>
<td>True</td>
<td>DRIFT default</td>
</tr>
</tbody>
</table>

Table A1.14b: GASP/DRIFT – Continuously released pool source on land: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100, 1000</td>
<td>Input as mass release rate in kg/s</td>
</tr>
<tr>
<td>Release duration</td>
<td>Time limited spill</td>
<td>min</td>
<td>15, 30, 60</td>
<td>Input as time limited spill in s</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td>-162.4, -163, -165, -170, -180 for methane 5, 15, 30 for n-pentane</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td></td>
<td></td>
<td>Asphalt, Concrete, Dry Soil, Wet Soil</td>
<td>Inbuilt substrate types</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Puddle depth</td>
<td>mm</td>
<td>2, 5, 10, 20, 50, 100</td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td>Air and initial temperature of substrate</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>m/s</td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>

13
### Table A1.15a: HGSYSTEM (LPOOL) – Continuously released pool source on land: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>Release from reservoir</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane, pentane</td>
<td>Using inbuilt substance properties</td>
</tr>
</tbody>
</table>

### Table A1.15b: HGSYSTEM (LPOOL) – Continuously released pool source on land: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow into pool</td>
<td>Volume spill rate</td>
<td>m3/s</td>
<td>0.002, 0.02, 0.2, 2.0</td>
<td>Varied the orifice diameter to ensure desired volume spill rates using the standard Bernoulli relation option in the model before entering desired flow parameters directly</td>
</tr>
<tr>
<td></td>
<td>Orifice diameter</td>
<td>cm</td>
<td>0.97, 3.1, 9.81, 31.0</td>
<td></td>
</tr>
<tr>
<td>Duration of release</td>
<td>Spill duration</td>
<td>s</td>
<td>900, 1800, 3600</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td>°C</td>
<td></td>
<td>-162, -170, -180</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - pentane</td>
<td>°C</td>
<td></td>
<td>0, 15, 30</td>
<td>Reflects the storage temperature, so the ambient temperature also set to the same values</td>
</tr>
<tr>
<td>Ground type</td>
<td>n/a</td>
<td></td>
<td>‘insulated concrete’, ‘wet sand’, ‘dry sand’</td>
<td></td>
</tr>
<tr>
<td>Ground temperature</td>
<td>°C</td>
<td></td>
<td>0, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Minimum thickness of pool</td>
<td>mm</td>
<td>0.5, 1.0, 2.0</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
### Table A1.16a: LSMS – Continuously released pool source on land: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source configuration</td>
<td>‘Constant inflow’ option, with axisymmetric geometry</td>
<td>Continuous release</td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) Butane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>3600s</td>
<td>The duration of the liquid release into the pool</td>
</tr>
</tbody>
</table>

### Table A1.16b: LSMS - Continuously released pool source on land: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow into pool – methane</td>
<td>Volume flow into pool</td>
<td>m³/s</td>
<td>0.0024, 0.024, 0.24, 2.4</td>
<td>Equivalent to 1, 10, 100, 1000 kg/s</td>
</tr>
<tr>
<td></td>
<td>Source radius</td>
<td>m</td>
<td>0.09, 0.28, 0.86, 2.7</td>
<td>Keeping velocity of liquid flow constant</td>
</tr>
<tr>
<td>Flow into pool – butane</td>
<td>Volume flow into pool</td>
<td>m³/s</td>
<td>0.0017, 0.017, 0.17, 1.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Source radius</td>
<td>m</td>
<td>0.074, 0.23, 0.74, 2.3</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature – methane</td>
<td></td>
<td>K</td>
<td>111.67, 108.15, 93.15</td>
<td>111.67 K is the value obtained when the 'set to boiling' option is checked</td>
</tr>
<tr>
<td>Initial liquid temperature – butane</td>
<td></td>
<td>K</td>
<td>283.12, 288.12, 293.12</td>
<td>The substrate temperature was also set to these values, as this represents an ambient storage temperature</td>
</tr>
<tr>
<td>Substrate properties</td>
<td>n/a</td>
<td></td>
<td>‘Standard concrete’, ‘non-porous sand’, ‘soil’</td>
<td>Set thermal parameters to represent these (taken from LSMS documentation)</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td>K</td>
<td></td>
<td>283.12, 288.12, 293.12</td>
<td></td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Turbulent drag</td>
<td>n/a</td>
<td>0.005, 0.01, 0.02</td>
<td>An advanced option controlling the dynamic spreading of the pool</td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
### Table A1.17a: PHAST – Continuously released pool source on land: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td></td>
<td>n-Pentane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Inventory type</td>
<td>Atmospheric storage tank</td>
<td></td>
</tr>
<tr>
<td>Inventory mass</td>
<td>1000 te</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Continuous spill</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Liquid</td>
<td>User defined spill rate</td>
</tr>
<tr>
<td>Surface type</td>
<td>User defined (land)</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>10 cm</td>
<td></td>
</tr>
<tr>
<td>Solar radiation flux</td>
<td>0 kW/m²</td>
<td></td>
</tr>
</tbody>
</table>

### Table A1.17b: PHAST – Continuously released pool source on land: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100, 1000</td>
<td>Input as mass release rate in kg/s</td>
</tr>
<tr>
<td>Release duration</td>
<td>Time limited spill</td>
<td>min</td>
<td>15, 30, 60</td>
<td>Input as duration of spill in s</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td></td>
<td>-162.4 to -180 for</td>
<td>Asphalt is accustom substrate using the same thermal properties as</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>methane 5, 15, 30</td>
<td>asphalt in GASP, others are using PHAST’s inbuilt substrate types</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td></td>
<td></td>
<td>Asphalt, Concrete,</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Dry Soil, Wet Soil</td>
<td></td>
</tr>
<tr>
<td>Ground temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Minimum pool depth</td>
<td>mm</td>
<td>2, 10, 20, 50, 100</td>
<td>No user specified minimum pool depth for the base case</td>
</tr>
<tr>
<td>Air temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
A.1.5. Instantaneously released pool source on water

Table A1.18a: ALOHA – Instantaneously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>'Puddle' option used</td>
<td>Using the 'Puddle' option means that no spreading is modelled</td>
</tr>
<tr>
<td>Release duration</td>
<td>1 minute</td>
<td>1 minute is the minimum allowed release duration</td>
</tr>
<tr>
<td>Orifice</td>
<td>Circular</td>
<td></td>
</tr>
<tr>
<td>Ground type</td>
<td>'Water'</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.1 cm</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.18b: ALOHA – Instantaneously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill</td>
<td>Pool mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td>Varied the initial pool diameter to ensure that the pool depth was constant (1 cm)</td>
</tr>
<tr>
<td></td>
<td>Diameter</td>
<td>m</td>
<td>17, 55, 174</td>
<td></td>
</tr>
<tr>
<td>Initial diameter</td>
<td>m</td>
<td></td>
<td>50, 54.9, 60, 70</td>
<td>Keeping mass constant, so effectively varying the pool depth</td>
</tr>
<tr>
<td>Convective heat from water</td>
<td>Water temperature</td>
<td>°C</td>
<td>10, 15, 20</td>
<td>Can only vary the temperature (ALOHA calculates the heat flux from this).</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td></td>
<td>-162, -165, -170, -180</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane, hydrogen(cryogenic)</td>
<td></td>
<td></td>
<td>Using inbuilt substance properties</td>
</tr>
</tbody>
</table>
Table A1.19a: GASP/DRIFT – Instantaneously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) n-Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties (SPI files source)</td>
</tr>
<tr>
<td>Release type (GASP)</td>
<td>Instantaneous</td>
<td></td>
</tr>
<tr>
<td>Pool geometry</td>
<td>Circular</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Surface type</td>
<td>Deep water</td>
<td></td>
</tr>
<tr>
<td>Heat transfer coefficient</td>
<td>500 W/m²/K</td>
<td>GASP default for deep water</td>
</tr>
<tr>
<td>Pool spreading constraints</td>
<td>Capillary depth = 0.2 mm</td>
<td>Surface tension provides restoring force for pool spreading on water</td>
</tr>
<tr>
<td>Water temperature</td>
<td>Equal to the air temperature</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Pool surface roughness length</td>
<td>0.23 mm</td>
<td>GASP default</td>
</tr>
<tr>
<td>Thermodynamic options</td>
<td>Calculated pool temperature, convection from atmosphere (true)</td>
<td>GASP defaults</td>
</tr>
<tr>
<td>Additional heat flux into pool</td>
<td>0 kW/m²</td>
<td>GASP default</td>
</tr>
<tr>
<td>Release type (DRIFT)</td>
<td>Time Varying Release</td>
<td>DRIFT default</td>
</tr>
<tr>
<td>Include Dilution Over Pool (DRIFT)</td>
<td>True</td>
<td>DRIFT default</td>
</tr>
</tbody>
</table>

Table A1.19b: GASP/DRIFT – Instantaneously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td>Input as mass with initial pool depth of 1 cm.</td>
</tr>
<tr>
<td>Dimensions of pool</td>
<td>Diameter</td>
<td>m</td>
<td>50, 55, 60, 70</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td></td>
<td>-162.4, -163, -165, -170, -180 for methane 5, 15, 30 for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td></td>
<td>10, 15, 20, 30 for methane 5, 15, 20 for n-pentane</td>
<td>Water and air temperature</td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
Table A1.20a: HGSYSTEM (LPOOL) – Instantaneously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane</td>
<td>Using inbuilt substance properties from DATAPROP</td>
</tr>
<tr>
<td>Release duration</td>
<td>1 second</td>
<td>Approximating an instantaneous release</td>
</tr>
<tr>
<td>Orifice</td>
<td>Circular</td>
<td></td>
</tr>
<tr>
<td>Ground type</td>
<td>‘Water’</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.1 cm</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.20b: HGSYSTEM (LPOOL) – Instantaneously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Volume spill rate</td>
<td>m³/s</td>
<td>2.0, 20.0, 200.0</td>
<td>Varied the orifice diameter to ensure desired volume spill rates using the standard Bernoulli relation option in the model before entering desired flow parameters directly</td>
</tr>
<tr>
<td></td>
<td>Orifice diameter</td>
<td>cm</td>
<td>0.309, 0.976, 3.124</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td>°C</td>
<td></td>
<td>-162, -170, -180</td>
<td></td>
</tr>
<tr>
<td>Substrate temperature</td>
<td>°C</td>
<td></td>
<td>0, 15, 30</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.21a: LSMS – Instantaneously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source configuration</td>
<td>‘Dam break’</td>
<td></td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) Butane (non-cryogenic)</td>
<td></td>
</tr>
<tr>
<td>Substrate</td>
<td>‘Water’</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>‘Set to boiling’</td>
<td>111.67</td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.001 m</td>
<td></td>
</tr>
</tbody>
</table>
Table A1.21b: LSMS – Instantaneously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill – methane</td>
<td>Vertical size</td>
<td>m</td>
<td>0.91, 1.96, 4.2</td>
<td>Keeping aspect ratio constant (height:width of 0.5)</td>
</tr>
<tr>
<td></td>
<td>Initial radius</td>
<td></td>
<td>0.91, 1.96, 4.2</td>
<td>Equivalent to 1, 10, 100 tonnes</td>
</tr>
<tr>
<td>Initial mass in pool – hydrogen</td>
<td>Vertical size</td>
<td>m</td>
<td>1.6, 3.6, 7.7</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Initial radius</td>
<td></td>
<td>1.6, 3.6, 7.7</td>
<td></td>
</tr>
<tr>
<td>Initial pool radius - methane</td>
<td>m</td>
<td></td>
<td>0.5, 1.96, 4.0</td>
<td>Keeping the initial height constant. \ Also effectively varying the mass</td>
</tr>
<tr>
<td>Initial pool radius - hydrogen</td>
<td>m</td>
<td></td>
<td>0.9, 3.6, 7.0</td>
<td></td>
</tr>
<tr>
<td>Convective heat flux from water</td>
<td>Initial heat flux</td>
<td>kW/m²</td>
<td>5, 50, 500</td>
<td></td>
</tr>
<tr>
<td>Roughness length</td>
<td>m</td>
<td></td>
<td>0.0001, 0.001, 0.1</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.22a: PHAST – Instantaneously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) / n-Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Inventory type</td>
<td>Atmospheric storage tank</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Catastrophic rupture</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Liquid</td>
<td></td>
</tr>
<tr>
<td>Release temperature</td>
<td>-162.4 °C for methane / 15 °C for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>Deep water or channel</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>1 mm</td>
<td></td>
</tr>
<tr>
<td>Solar radiation flux</td>
<td>0 kW/m²</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>15 °C</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.22b: PHAST – Instantaneously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td>Input as inventory mass</td>
</tr>
<tr>
<td>Water temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
### A.1.6. Continuously released pool source on water

#### Table A1.23a: ALOHA – Continuously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>‘Tank’ source type: leak from storage within a spherical tank, 90% full of liquid. Large diameter orifice, located at the bottom of the tank</td>
<td>Did not use the ‘Puddle’ option, as this does not model spreading effects.</td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Release duration</td>
<td>30 minutes</td>
<td></td>
</tr>
<tr>
<td>Orifice</td>
<td>Circular hole in vessel wall (not short pipe)</td>
<td></td>
</tr>
<tr>
<td>Ground type</td>
<td>‘Water’</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.1 cm</td>
<td></td>
</tr>
</tbody>
</table>

#### Table A1.23b: ALOHA - Continuously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow into pool</td>
<td>Chemical mass in tank</td>
<td>tonnes</td>
<td>1, 10, 100, 1000</td>
<td>Varied the orifice diameter to ensure that the release duration was constant (30 minutes)</td>
</tr>
<tr>
<td></td>
<td>Tank volume</td>
<td></td>
<td>2.625, 26.25, 262.5, 2625</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Orifice diameter</td>
<td>cm</td>
<td>3.55, 9.7, 24.92, 62</td>
<td>Hole diameter adjusted to give the required duration: 15, 30, 60 minutes</td>
</tr>
<tr>
<td>Duration of release</td>
<td>Orifice diameter</td>
<td>cm</td>
<td>14, 9.7, 6.88</td>
<td>Hole diameter adjusted to give the required duration: 15, 30, 60 minutes</td>
</tr>
<tr>
<td>Convective heat from water</td>
<td>Water temperature</td>
<td>°C</td>
<td>10, 15, 20</td>
<td>Can only vary the temperature (ALOHA calculates the heat flux from this).</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td></td>
<td>-162, -165, -170, -180</td>
<td></td>
</tr>
</tbody>
</table>
Table A1.24a: GASP/DRIFT – Continuously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) n-Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties (SPI files source)</td>
</tr>
<tr>
<td>Release type (GASP)</td>
<td>Continuous</td>
<td></td>
</tr>
<tr>
<td>Aperture diameter (GASP)</td>
<td>0.05 m</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>1800 s</td>
<td>The duration of the release into the pool</td>
</tr>
<tr>
<td>Maximum pool age</td>
<td>3600 s</td>
<td>GASP runs until 99% if the spilled substance is vaporised or the maximum pool age is reached.</td>
</tr>
<tr>
<td>Pool geometry</td>
<td>Circular</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>Deep water</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Heat transfer coefficient</td>
<td>500 W/m²/K</td>
<td>GASP default for deep water</td>
</tr>
<tr>
<td>Pool spreading constraints</td>
<td>Capillary depth = 0.2 mm</td>
<td>Surface tension provides restoring force for pool spreading on water</td>
</tr>
<tr>
<td>Water temperature</td>
<td>Equal to the air temperature</td>
<td>Inbuilt assumption in GASP</td>
</tr>
<tr>
<td>Pool surface roughness length</td>
<td>0.23 mm</td>
<td></td>
</tr>
<tr>
<td>Thermodynamic options</td>
<td>Calculated pool temperature, convection from atmosphere (true)</td>
<td>GASP defaults</td>
</tr>
<tr>
<td>Additional heat flux into pool</td>
<td>0 kW/m²</td>
<td>GASP default</td>
</tr>
<tr>
<td>Release type (DRIFT)</td>
<td>Time Varying Release</td>
<td>DRIFT default</td>
</tr>
<tr>
<td>Include Dilution Over Pool (DRIFT)</td>
<td>True</td>
<td>DRIFT default</td>
</tr>
</tbody>
</table>

Table A1.24b: GASP/DRIFT – Continuously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100, 1000</td>
<td>Input as mass release rate in kg/s</td>
</tr>
<tr>
<td>Release duration</td>
<td>Time limited spill</td>
<td>min</td>
<td>15, 30, 60</td>
<td>Input as time limited spill in s</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>°C</td>
<td>-162.4, -163, -165, -170, -180 for methane</td>
<td>5, 15, 30 for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td>Water and air temperature</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table A1.25a: HGSYSTEM (LPOOL) – Continuously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td>Using inbuilt substance properties from DATAPROP</td>
</tr>
<tr>
<td>Ground type</td>
<td>‘Water’</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.1 cm</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.25b: HGSYSTEM (LPOOL) – Continuously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s) varied</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow into pool</td>
<td>Volume spill rate</td>
<td>m³/s</td>
<td>0.0024, 0.024, 0.24, 2.4</td>
<td>Varied the orifice diameter to ensure desired volume spill rates using the standard Bernoulli relation option in the model before entering desired flow parameters directly</td>
</tr>
<tr>
<td></td>
<td>Orifice diameter</td>
<td>cm</td>
<td>0.309, 0.976, 3.124</td>
<td></td>
</tr>
<tr>
<td>Duration of release</td>
<td>Spill duration</td>
<td>s</td>
<td>900, 1800, 3600</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td>°C</td>
<td></td>
<td>-162, -170, -180</td>
<td></td>
</tr>
<tr>
<td>Water temperature</td>
<td>°C</td>
<td></td>
<td>0, 15, 30</td>
<td></td>
</tr>
</tbody>
</table>

Table A1.26a: LSMS – Continuously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source configuration</td>
<td>‘Constant inflow’ option, with axisymmetric geometry</td>
<td>Continuous release</td>
</tr>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Release type</td>
<td>‘Constant inflow’</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>3600 s</td>
<td>The duration of the liquid release into the pool</td>
</tr>
<tr>
<td>Substrate</td>
<td>‘Water’</td>
<td></td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>‘Set to boiling’</td>
<td>111.67</td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.001 m</td>
<td></td>
</tr>
</tbody>
</table>
### Table A1.26: LSMS – Continuously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flow into pool</td>
<td>Volume flow into pool</td>
<td>m³/s</td>
<td>0.0024, 0.024, 0.24, 2.4</td>
<td>Equivalent to 1, 10, 100, 1000 kg/s Keeping velocity of liquid flow constant</td>
</tr>
<tr>
<td></td>
<td>(initial) source radius</td>
<td>m</td>
<td>0.09, 0.28, 0.86, 2.7</td>
<td></td>
</tr>
<tr>
<td>Convective heat flux from water</td>
<td>Initial heat flux</td>
<td>kW/m²</td>
<td>5, 50, 500</td>
<td></td>
</tr>
</tbody>
</table>

### Table A1.27a: PHAST – Continuously released pool source on water: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Methane (cryogenic) n-Pentane (non-cryogenic)</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Inventory type</td>
<td>Atmospheric storage tank</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Liquid spill</td>
<td>Specified rate for a given duration</td>
</tr>
<tr>
<td>Release phase</td>
<td>Liquid</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>Deep water or channel</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>1 mm</td>
<td></td>
</tr>
<tr>
<td>Solar radiation flux</td>
<td>0 kW/m²</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>15 °C</td>
<td></td>
</tr>
</tbody>
</table>

### Table A1.27b: PHAST – Continuously released pool source on water: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td>Input as inventory mass</td>
</tr>
<tr>
<td>Release duration</td>
<td>Time limited spill</td>
<td>min</td>
<td>15, 30, 60</td>
<td>Input as duration of spill in s</td>
</tr>
<tr>
<td>Release temperature</td>
<td>°C</td>
<td></td>
<td>-162.4 to -180 for methane 5, 15, 30 for n-pentane</td>
<td></td>
</tr>
<tr>
<td>Water temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td></td>
<td>1, 2, 5, 7, 10, 20</td>
<td></td>
</tr>
</tbody>
</table>
A.2. Pressurised catastrophic failure (flashing)

A.2.1 Direct source

Table A2.1a: ALOHA – Pressurised catastrophic failure (flashing): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance modelled</td>
<td>Chlorine</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>‘Direct source’</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Superheated Liquid/Two-Phase</td>
<td>1 minute is the minimum allowed release duration in ALOHA, and is the default for instantaneous sources</td>
</tr>
<tr>
<td>Release duration</td>
<td>Instantaneous (1 minute)</td>
<td>The source height cannot be varied for dense gas releases, when using the ‘direct source’ release type. Releases are always modelled at ground level.</td>
</tr>
<tr>
<td>Source height</td>
<td>0m</td>
<td></td>
</tr>
</tbody>
</table>

Table A2.1b: ALOHA – Pressurised catastrophic failure (flashing): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>kg</td>
<td>100, 1000, 10000, 100000, 1000000</td>
<td></td>
</tr>
</tbody>
</table>

Table A2.2a: GASTAR – Pressurised catastrophic failure (flashing): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance modelled</td>
<td>Chlorine</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>‘Instantaneous’</td>
<td>Taken from GASTAR’s flash calculation utility, based on storage temperature of 15 °C and atmospheric pressure of 1013mb</td>
</tr>
<tr>
<td>Release phase</td>
<td>Superheated Liquid/Two-Phase</td>
<td></td>
</tr>
<tr>
<td>Release temperature</td>
<td>238.7 K</td>
<td>Fraction of initial release that is hazardous (determines the initial quantity of air in the instantaneous cloud)</td>
</tr>
<tr>
<td>Hazardous fraction</td>
<td>1000000 ppm</td>
<td></td>
</tr>
<tr>
<td>Initial cloud radius</td>
<td>Based on jet output parameter values extracted from ACE model runs</td>
<td></td>
</tr>
<tr>
<td>Momentum initially well mixed option</td>
<td>Selected</td>
<td>This should only be deselected if the release has zero ambient velocity</td>
</tr>
<tr>
<td>General parameter</td>
<td>Model input parameter(s)</td>
<td>Units</td>
</tr>
<tr>
<td>-------------------</td>
<td>--------------------------</td>
<td>-------</td>
</tr>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>kg</td>
</tr>
<tr>
<td>Initial liquid fraction</td>
<td></td>
<td>kg/kg</td>
</tr>
<tr>
<td>Aspect ratio</td>
<td>Diameter</td>
<td>m</td>
</tr>
<tr>
<td>Mass of entrained air</td>
<td></td>
<td>kg</td>
</tr>
</tbody>
</table>

Table A2.3a: HGSYSTEM (HEGABOX) – Pressurised catastrophic failure (flashing): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance modelled</td>
<td>Chlorine</td>
<td>Used the ‘INICONC’ parameter to simulate the catastrophic failure. “Useful for very ‘violent’ releases where at the start of the HEGABOX simulation significant entrainment already has occurred.”</td>
</tr>
<tr>
<td>Release type</td>
<td>Release in HEGABOX</td>
<td>Used the ‘INICONC’ parameter to simulate the catastrophic failure. “Useful for very ‘violent’ releases where at the start of the HEGABOX simulation significant entrainment already has occurred.”</td>
</tr>
<tr>
<td>Initial air entrainment</td>
<td>0.33 mole pollutant/mole total mixture.</td>
<td>Used the ‘INICONC’ parameter to simulate the catastrophic failure. “Useful for very ‘violent’ releases where at the start of the HEGABOX simulation significant entrainment already has occurred.”</td>
</tr>
</tbody>
</table>

Table A2.3b: HGSYSTEM (HEGABOX) – Pressurised catastrophic failure (flashing): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>kg</td>
<td>1000, 10000, 100000</td>
<td>Wet pollutant</td>
</tr>
<tr>
<td>Aspect ratio</td>
<td>Initial cloud radius</td>
<td>m</td>
<td>24.0, 35.0, 52.0</td>
<td>Equivalent aspect ratios: 1, 0.33, 0.1</td>
</tr>
<tr>
<td>Initial air entrainment</td>
<td>0.064, 0.32</td>
<td>mole pollutant/mole total mixture</td>
<td>Used the ‘INICONC’ parameter to simulate the catastrophic failure. “Useful for very ‘violent’ releases where at the start of the HEGABOX simulation significant entrainment already has occurred.”</td>
<td></td>
</tr>
</tbody>
</table>
### A.2.2 Catastrophic failure source term models

#### Table A2.4a: ACE/DRIFT – Pressurised catastrophic failure (flashing): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance modelled</td>
<td>Chlorine</td>
<td></td>
</tr>
<tr>
<td>Release type (DRIFT)</td>
<td>Instantaneous</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Superheated Liquid/Two-Phase</td>
<td></td>
</tr>
<tr>
<td>Release temperature</td>
<td>From ACE output</td>
<td>Airborne fraction in liquid phase</td>
</tr>
<tr>
<td>Liquid fraction</td>
<td>From ACE output</td>
<td>Total mass of contaminant in instantaneous cloud</td>
</tr>
<tr>
<td>Contaminant mass</td>
<td>Form ACE output</td>
<td></td>
</tr>
<tr>
<td>Contaminant fraction</td>
<td>From ACE output</td>
<td>Fraction of airborne cloud that determines the initial quantity of air in the instantaneous cloud</td>
</tr>
<tr>
<td>Initial cloud radius</td>
<td>From ACE output</td>
<td></td>
</tr>
</tbody>
</table>

#### Table A2.4b: ACE/DRIFT – Pressurised catastrophic failure (flashing): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>1, 10, 100</td>
<td></td>
</tr>
<tr>
<td>Storage temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pad pressure</td>
<td>barg</td>
<td>0, 1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td></td>
<td>Down, Omni</td>
<td></td>
</tr>
<tr>
<td>Include pool (DRIFT)</td>
<td></td>
<td>No, Yes</td>
<td></td>
<td>No: vaporisation from pool ignored Yes: pool vaporisation calculated by GASP and incorporated.</td>
</tr>
<tr>
<td>Dilution at source (DRIFT)</td>
<td></td>
<td>Yes, No</td>
<td></td>
<td>Yes: dilution calculated by ACE No: flashing release directly input to DRIFT with no initial dilution</td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
<td>Water and air temperature</td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>D5, F2</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

#### Table A2.5a: PHAST – Pressurised catastrophic failure (flashing): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance modelled</td>
<td>Chlorine</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Inventory type</td>
<td>Pressure vessel</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Catastrophic rupture</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>User defined (land)</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>10 cm</td>
<td></td>
</tr>
<tr>
<td>Solar radiation flux</td>
<td>0 kW/m²</td>
<td></td>
</tr>
</tbody>
</table>
Table A2.5b: PHAST—Pressurised catastrophic failure (flashing): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Mass</td>
<td>tonnes</td>
<td>10, 100, 1000</td>
<td>Input as inventory mass</td>
</tr>
<tr>
<td>Storage temperature</td>
<td>°C</td>
<td></td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Storage pressure</td>
<td>barg</td>
<td>Saturated vapour pressure (svp), svp+1, svp+2, svp+3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td>2, 5, 10</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Relative humidity</td>
<td>%</td>
<td>0, 50, 70, 95</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
A.3. Jet releases

A.3.1. Direct source

Table A3.1a: ADMS – Direct jet source (no expansion): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance modelled</td>
<td>Methane, air</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>‘jet’ source type</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Gaseous</td>
<td></td>
</tr>
<tr>
<td>Release temperature</td>
<td>15 °C</td>
<td></td>
</tr>
<tr>
<td>Release heat capacity</td>
<td>Methane: 2220 J/°C/kg</td>
<td>Air: 1012 J/°C/kg</td>
</tr>
<tr>
<td>Release molecular mass</td>
<td>Methane: 16</td>
<td>Air: 28.97</td>
</tr>
</tbody>
</table>

Table A3.1b: ADMS – Direct jet source (no expansion): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pseudo diameter - methane</td>
<td></td>
<td>m</td>
<td>0.01, 0.05, <strong>0.1199</strong>, 0.2, 0.5</td>
<td>Keeping velocity value constant (at 652 m/s for methane and 479 m/s for air). Effectively varying volume (and mass) flow rates</td>
</tr>
<tr>
<td>Pseudo diameter - air</td>
<td></td>
<td>m</td>
<td>0.01, 0.05, <strong>0.1199</strong>, 0.2, 0.5</td>
<td></td>
</tr>
<tr>
<td>Mass flow-methane</td>
<td>velocity</td>
<td>m/s</td>
<td>130, 261, <strong>652</strong>, 977</td>
<td>Keeping pseudo diameter constant</td>
</tr>
<tr>
<td>Mass flow-air</td>
<td>velocity</td>
<td>m/s</td>
<td>95.7, 192, <strong>479</strong>, 719, 957</td>
<td></td>
</tr>
<tr>
<td>Release height</td>
<td></td>
<td>m</td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td></td>
<td><strong>Horizontal</strong>, vertical</td>
<td>Downwind for horizontal, Upwards for vertical</td>
</tr>
<tr>
<td>Duration</td>
<td></td>
<td>s</td>
<td><strong>Continuous</strong>, 1800, 180, 18</td>
<td>Plume run for continuous, puff run otherwise</td>
</tr>
<tr>
<td>Averaging time</td>
<td></td>
<td>s</td>
<td>600, 1</td>
<td></td>
</tr>
</tbody>
</table>
Table A3.2a: DRIFT – Direct jet source (no expansion): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled (Source density)</td>
<td>Methane (buoyant gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Air (neutrally buoyant gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (dense gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (two-phase flashing)</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Finite duration, Steady continuous (for infinite duration)</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Gaseous</td>
<td>Inbuilt jet expansion model circumvented for gas jets by defining composition using User defined multi-component mixture with v. small amount of water liquid.</td>
</tr>
<tr>
<td></td>
<td>Superheated Liquid/Two-phase</td>
<td>Inbuilt jet expansion model circumvented for superheated jets by specifying two-phase release with at normal boiling temperature (i.e. no superheat)</td>
</tr>
<tr>
<td>Source type</td>
<td>Momentum jet</td>
<td></td>
</tr>
<tr>
<td>Release temperature</td>
<td>15 °C for gaseous</td>
<td>Corresponds to storage temperature for gaseous, exit plane temperature for two-phase</td>
</tr>
<tr>
<td></td>
<td>Normal boiling point for two-phase</td>
<td></td>
</tr>
<tr>
<td>Release pressure</td>
<td>101325 Pa</td>
<td>Ambient pressure</td>
</tr>
<tr>
<td>Liquid fraction</td>
<td>0.0 for gaseous</td>
<td>Fixed flash fraction assumed for direct two-phase source</td>
</tr>
<tr>
<td></td>
<td>0.8 for two-phase</td>
<td></td>
</tr>
<tr>
<td>Rainout fraction</td>
<td>0.0</td>
<td>No rainout included</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.8 (gaseous)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1 (two-phase)</td>
<td></td>
</tr>
</tbody>
</table>

Table A3.2b: DRIFT – Direct jet source (no expansion): Parameters varied

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release rate</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>s</td>
<td>18, 180, 1800, infinite</td>
<td></td>
</tr>
<tr>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.05, 0.1, 0.5</td>
<td></td>
</tr>
<tr>
<td>Release height</td>
<td>m</td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td>Horizontal, vertical</td>
<td>Downwind for horizontal</td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>D5, F2</td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td>0, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Relative humidity</td>
<td>%</td>
<td>0, 50, 70, 100</td>
<td></td>
</tr>
<tr>
<td>Inversion height</td>
<td>m</td>
<td>50, 100, 200</td>
<td>For F2 conditions only</td>
</tr>
</tbody>
</table>
### Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Chlorine (dense gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Methane (buoyant gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (two-phase flashing)</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Gaseous</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Superheated Liquid</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>‘Gas or liquid jet’ release</td>
<td></td>
</tr>
<tr>
<td></td>
<td>‘Thermal release’ for gaseous releases</td>
<td></td>
</tr>
<tr>
<td></td>
<td>‘Aerosol release’ for two-phase releases</td>
<td></td>
</tr>
<tr>
<td>Release temperature</td>
<td>288 K for gaseous releases</td>
<td>Set to be the same as the ambient temperature, for gaseous releases</td>
</tr>
<tr>
<td></td>
<td>238.7 K for two-phase releases</td>
<td>238.7 K is the boiling point of chlorine (taken from GASTAR’s chemical database)</td>
</tr>
<tr>
<td>Hazardous fraction</td>
<td>1000000 ppm</td>
<td></td>
</tr>
<tr>
<td>Outputs</td>
<td>Near field concentrations</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Far field concentrations</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Jet parameters: Jet edge and centre</td>
<td></td>
</tr>
<tr>
<td></td>
<td>touchdown distance</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Jet transition point</td>
<td>The transition point is the distance downwind where the jet model</td>
</tr>
<tr>
<td></td>
<td></td>
<td>calculations stop and the dense gas model calculations begin — when</td>
</tr>
<tr>
<td></td>
<td></td>
<td>the jet velocity reduces to a specific level and the jet has touched</td>
</tr>
<tr>
<td></td>
<td></td>
<td>down.</td>
</tr>
</tbody>
</table>

### Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pseudo diameter: gaseous chlorine</td>
<td>m</td>
<td></td>
<td>0.01, 0.05, 0.084, 0.1, 0.5</td>
<td>Keeping mass flow rate constant. Base case values based on output from DRIFT</td>
</tr>
<tr>
<td>Pseudo diameter: gaseous methane</td>
<td>m</td>
<td></td>
<td>0.01, 0.05, 0.120, 0.2, 0.5</td>
<td></td>
</tr>
<tr>
<td>Pseudo diameter: two-phase chlorine</td>
<td>m</td>
<td></td>
<td>0.01, 0.05, 0.113, 0.1, 0.5</td>
<td></td>
</tr>
<tr>
<td>Release rate</td>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td>Keeping diameter constant</td>
</tr>
<tr>
<td>Diameter and release rate</td>
<td>Diameter</td>
<td>m</td>
<td>0.084, 0.115, 0.160, 0.250</td>
<td>Varying both parameters simultaneously. Based on output from DRIFT, where hole diameter is kept constant (equivalent to varying the storage pressure)</td>
</tr>
<tr>
<td></td>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td>Release height</td>
<td>m</td>
<td></td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td></td>
<td>Horizontal, vertical</td>
<td>Downwind for horizontal</td>
</tr>
<tr>
<td>Aerosol liquid fraction (two-phase chlorine only)</td>
<td></td>
<td></td>
<td>0.7, 0.8, 0.9</td>
<td></td>
</tr>
<tr>
<td>Averaging time</td>
<td>s</td>
<td></td>
<td>600, 1</td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td></td>
<td>D5, F2</td>
<td></td>
</tr>
</tbody>
</table>
### Table A3.4a: SLAB – Direct jet source (no expansion): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spill type</td>
<td>Type ‘2’ (for base case)</td>
<td>horizontal jet release: area with plane perpendicular to ambient wind direction, velocity pointing downwind</td>
</tr>
<tr>
<td>Substances modelled (Source density)</td>
<td>Methane (buoyant gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (dense gas)</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Gaseous</td>
<td></td>
</tr>
</tbody>
</table>

### Table A3.4b: SLAB – Direct jet source (no expansion): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release rate</td>
<td></td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td>Jet radius - methane</td>
<td></td>
<td>m</td>
<td>0.005, 0.025, 0.060, 0.1, 0.25</td>
<td></td>
</tr>
<tr>
<td>Jet radius - chlorine</td>
<td></td>
<td>m</td>
<td>0.005, 0.025, 0.042, 0.05, 0.25</td>
<td></td>
</tr>
<tr>
<td>Jet radius and release rate - methane</td>
<td>Radius</td>
<td>m</td>
<td>0.060, 0.084, 0.117, 0.185</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>5, 10, 20, 50</td>
<td>Downwind for horizontal</td>
</tr>
<tr>
<td>Jet radius and release rate - chlorine</td>
<td>Radius</td>
<td>m</td>
<td>0.084, 0.115, 0.160, 0.25</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Mass flow rate</td>
<td>kg/s</td>
<td>5, 10, 20, 50</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td></td>
<td>Horizontal, vertical</td>
<td></td>
</tr>
<tr>
<td>Release height</td>
<td></td>
<td>m</td>
<td>1, 10</td>
<td></td>
</tr>
</tbody>
</table>
A.3.2. Source term jet models

Table A3.5a: ALOHA – Jet source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>Chlorine (dense gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Methane (buoyant gas)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (two-phase flashing)</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Gaseous</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Superheated Liquid</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>‘Tank’ source type: leak from a very</td>
<td></td>
</tr>
<tr>
<td></td>
<td>large vessel to give constant outflow.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>‘Tank contains gas only’ specified</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>Continuous</td>
<td>ALOHA limits release times to 1 hour</td>
</tr>
<tr>
<td>Orifice</td>
<td>Circular hole in vessel wall (not short</td>
<td></td>
</tr>
<tr>
<td></td>
<td>pipe)</td>
<td></td>
</tr>
</tbody>
</table>

Table A3.5b: ALOHA – Jet source: Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orifice diameter: gaseous</td>
<td></td>
<td>m</td>
<td>0.001, 0.01, 0.05, 0.1, 0.5</td>
<td>Keeping storage pressure constant (at 2.78 atm)</td>
</tr>
<tr>
<td>chlorine</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Orifice diameter: gaseous</td>
<td></td>
<td>m</td>
<td>0.001, 0.01, 0.05, 0.1, 0.5</td>
<td>Keeping storage pressure constant (at 23.3 atm)</td>
</tr>
<tr>
<td>methane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Orifice diameter: two-phase</td>
<td></td>
<td>m</td>
<td>0.001, 0.01, 0.05, 0.1, 0.5</td>
<td></td>
</tr>
<tr>
<td>chlorine</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release rate – gaseous</td>
<td></td>
<td>atm</td>
<td>1.29, 2.78, 5.48</td>
<td>Equivalent to 2, 5 and 10 kg/s release rate</td>
</tr>
<tr>
<td>chlorine</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release rate – gaseous</td>
<td></td>
<td>atm</td>
<td>9.45, 23.3, 45.7, 88.0, 220.5</td>
<td>Equivalent to 2, 5, 10, 20 and 50 kg/s release rate</td>
</tr>
<tr>
<td>methane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Storage temperature – two-phase chlorine</td>
<td></td>
<td>°C</td>
<td>0, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Orifice type</td>
<td></td>
<td></td>
<td>Circular hole / Pipe or valve</td>
<td></td>
</tr>
<tr>
<td>Parameter</td>
<td>Values used</td>
<td>Notes</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----------------------------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-----------------------------------------------------------------------------------------</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Substances modelled</strong></td>
<td>Methane (buoyant gas)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>(Source density)</td>
<td>Air (neutrally buoyant gas)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (dense gas)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Chlorine (two-phase flashing)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Release type</strong></td>
<td>Finite duration</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Steady continuous (for infinite duration)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Release phase</strong></td>
<td>Gaseous</td>
<td>Using inbuilt jet expansion model</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Superheated Liquid/Two-phase</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Source type</strong></td>
<td>Momentum jet</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Release rate</strong></td>
<td>User specified or Calculated</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>User specified fixed flow rates. Calculated flow rates based upon the following flow rate models: Isentropic gas flow, metastable liquid flow, two-phase homogeneous equilibrium flow (using ‘omega’ method)</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Release temperature</strong></td>
<td>15 °C</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Release pressure</strong></td>
<td>101325 Pa for metastable liquid</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Choke pressure for choked two-phase flow</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Calculated by DRIFT for gaseous discharge.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Release pressure = exit pressure for superheated/two-phase releases. Exit pressure set equal to choke pressure for two-phase flow calculated using ‘omega’ discharge model.</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Liquid fraction</strong></td>
<td>0.0 for gaseous</td>
<td>Liquid fraction for choked two-phase flow calculated using ‘Omega’ discharge model.</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1.0 for metastable liquid</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Calculated liquid fraction at exit for choked two-phase flow</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Rainout fraction</strong></td>
<td>0.0</td>
<td>No rainout included</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Table A3.6b: DRIF – Jet source (with expansion): Parameters varied**

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.05, 0.1, 0.5</td>
<td>Varied for fixed orifice diameter or varied with orifice diameter based upon flow rate model (gaseous, liquid, two-phase)</td>
</tr>
<tr>
<td>Release rate</td>
<td>kg/s</td>
<td>2, 5, 10, 20, 50, Calculated</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>s</td>
<td>18, 180, 1800, infinite</td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D5, F2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td>15, 30</td>
<td></td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td></td>
<td>0.6 (liquid), 0.8 (gaseous), 1.0</td>
<td></td>
</tr>
</tbody>
</table>
### Table A3.7a: HGSYSTEM (AEROPLUME) – Jet source (with expansion): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
</table>
| Substances modelled (Source density) | Methane (buoyant gas)  
Chlorine (dense gas)  
Chlorine (two-phase flashing) |                                                                       |
| Release phase                      | Gaseous  
Two-phase                                             |                                                                       |
| Source type                        | Jet                                                       |                                                                       |

### Table A3.7b: HGSYSTEM (AEROPLUME) – Jet source (with expansion): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orifice diameter - methane</td>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.02, 0.05, 0.1</td>
<td></td>
</tr>
<tr>
<td>Mass flow rate</td>
<td></td>
<td>kg/s</td>
<td>0.003, 0.32, 1.3, 8.0, 32.1</td>
<td></td>
</tr>
<tr>
<td>Orifice diameter - chlorine</td>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.02, 0.05, 0.1</td>
<td></td>
</tr>
<tr>
<td>Mass flow rate</td>
<td></td>
<td>kg/s</td>
<td>0.0008, 0.008, 0.32, 2.0, 8.1</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td></td>
<td>s</td>
<td>18, 180, 1800, infinite</td>
<td></td>
</tr>
<tr>
<td>Vapour discharge coefficient</td>
<td></td>
<td></td>
<td>0.6, 0.8, 1.0</td>
<td>Two phase release only</td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td></td>
<td>Horizontal, vertical (up)</td>
<td></td>
</tr>
<tr>
<td>Release height</td>
<td></td>
<td></td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Storage pressure - methane</td>
<td></td>
<td>atm</td>
<td>9.5, 23.3, 45.7, 88, 200</td>
<td></td>
</tr>
<tr>
<td>Storage pressure - chlorine</td>
<td></td>
<td></td>
<td>1.3, 2.8, 5.5, 88, 200</td>
<td></td>
</tr>
<tr>
<td>Storage temperature</td>
<td></td>
<td></td>
<td>0, 15, 30</td>
<td>Two phase release only</td>
</tr>
</tbody>
</table>

### Table A3.8a: PHAST – Jet source (with expansion): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
</table>
| Substances modelled                | Methane (buoyant gas)  
Air (neutrally buoyant gas)  
Chlorine (dense gas)  
Chlorine (two-phase) | Using inbuilt substance properties                  |
| Inventory type                     | Pressure Vessel                                           |                                            |
| Inventory mass                     | 1000 te                                                   |                                            |
| Storage Phase                      | Vapour: methane, air, chlorine gas  
Liquid: chlorine |                                            |
| Surface type                       | User defined (land)                                        |                                            |
| Solar radiation flux               | 0 kW/m²                                                   |                                            |
Table A3.8b: PHAST – Jet source (with expansion): Parameters varied

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Storage pressure</td>
<td>barg</td>
<td>Methane gas: 200, 17 Air: 12.3 Chlorine: Saturated vapour pressure (svp), svp+1, svp+2, svp+3</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td></td>
<td>Vapour, metastable liquid, two-phase</td>
<td></td>
</tr>
<tr>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.05, 0.1</td>
<td></td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td></td>
<td>0.6, 0.8, 1</td>
<td></td>
</tr>
<tr>
<td>Release elevation</td>
<td>m</td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td>Horizontal, up, down, impinged</td>
<td>Impinged is equivalent to some momentum being lost from the jet</td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>D2, D5, D10, F2</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>m</td>
<td>0.001, 0.01, 0.1, 0.1</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
</tr>
<tr>
<td>Relative humidity</td>
<td>%</td>
<td>0, 50, 70, 95</td>
<td></td>
</tr>
</tbody>
</table>
## A.4. Spray releases

### Table A4.1a: DRIFT – Spray source: Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>m-xylene, water</td>
<td></td>
</tr>
<tr>
<td>Release type</td>
<td>Finite duration</td>
<td></td>
</tr>
<tr>
<td>Release duration</td>
<td>1800 s</td>
<td></td>
</tr>
<tr>
<td>Release phase</td>
<td>Superheated Liquid/Two-phase</td>
<td></td>
</tr>
<tr>
<td>Source type</td>
<td>Momentum jet</td>
<td></td>
</tr>
<tr>
<td>Release pressure</td>
<td>101325 Pa</td>
<td>Exit pressure for un-choked liquid release is atmospheric</td>
</tr>
<tr>
<td>Liquid fraction</td>
<td>1.0</td>
<td>Pure liquid release</td>
</tr>
<tr>
<td>Rainout fraction</td>
<td>0.0</td>
<td>No rainout at source included</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.6</td>
<td></td>
</tr>
</tbody>
</table>

### Table A4.1b: DRIFT – Spray source: Parameters varied

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.1</td>
<td></td>
</tr>
<tr>
<td>Release rate</td>
<td>kg/s</td>
<td>From PHAST</td>
<td>Corresponding to storage pressures of 5, 10, 20, 50 and 100 barg</td>
</tr>
<tr>
<td>Release temperature</td>
<td>°C</td>
<td>15, 30, 100</td>
<td></td>
</tr>
<tr>
<td>Liquid deposition options</td>
<td></td>
<td>Deposition, No deposition</td>
<td>As determined by PHAST for the specified release conditions</td>
</tr>
<tr>
<td>Initial droplet diameter</td>
<td>m</td>
<td>From PHAST</td>
<td></td>
</tr>
<tr>
<td>Release elevation</td>
<td>m</td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td>Horizontal, vertical</td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>D5, F2</td>
<td></td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>°C</td>
<td>5, 15, 30</td>
<td></td>
</tr>
</tbody>
</table>

### Table A4.2a: PHAST – Jet source (with expansion): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substances modelled</td>
<td>m-xylene, water</td>
<td>Using inbuilt substance properties</td>
</tr>
<tr>
<td>Inventory type</td>
<td>Pressure Vessel</td>
<td></td>
</tr>
<tr>
<td>Inventory mass</td>
<td>1000 te</td>
<td></td>
</tr>
<tr>
<td>Storage and release phase</td>
<td>Liquid</td>
<td></td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.6</td>
<td></td>
</tr>
<tr>
<td>Surface type</td>
<td>User defined (land)</td>
<td></td>
</tr>
<tr>
<td>Surface roughness length</td>
<td>0.1 m</td>
<td></td>
</tr>
<tr>
<td>Solar radiation flux</td>
<td>0 kW/m²</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>15°C</td>
<td></td>
</tr>
<tr>
<td>Relative humidity</td>
<td>70%</td>
<td></td>
</tr>
</tbody>
</table>
### Table A4.2b: PHAST – Jet source (with expansion): Parameters varied

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Storage temperature</td>
<td>°C</td>
<td>15, 30, 100</td>
<td></td>
</tr>
<tr>
<td>Storage pressure</td>
<td>barg</td>
<td>5, 10, 20, 50, 100</td>
<td></td>
</tr>
<tr>
<td>Orifice diameter</td>
<td>m</td>
<td>0.001, 0.01, 0.1</td>
<td></td>
</tr>
<tr>
<td>Release elevation</td>
<td>m</td>
<td>1, 10</td>
<td></td>
</tr>
<tr>
<td>Release direction</td>
<td></td>
<td>Horizontal, up</td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>D2, D5, D10, F2</td>
<td></td>
</tr>
</tbody>
</table>
A.5. Fire plume (warehouse)

Table A5.1a: ADMS – Warehouse fire: Key fixed parameters and assumptions for both enclosed warehouse cases

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>Point source(s)</td>
<td></td>
</tr>
<tr>
<td>Pollutants modelled</td>
<td>Gaseous, particulate</td>
<td>Particulates included to test effect on deposition output</td>
</tr>
<tr>
<td>Pollutant emission rate</td>
<td>100g/s</td>
<td></td>
</tr>
<tr>
<td>Source height</td>
<td>10m</td>
<td></td>
</tr>
<tr>
<td>Efflux type</td>
<td>‘Exit velocity’</td>
<td></td>
</tr>
<tr>
<td>Cases</td>
<td>‘High temperature case’</td>
<td></td>
</tr>
<tr>
<td></td>
<td>‘Low temperature case’</td>
<td></td>
</tr>
<tr>
<td>Outputs</td>
<td>Maximum plume height,</td>
<td>Maximum plume height output where possible/relevant, for high</td>
</tr>
<tr>
<td></td>
<td>ground level concentrations</td>
<td>temperature case only</td>
</tr>
</tbody>
</table>

Table A5.1b: ADMS – Warehouse fire case: Parameters varied for both enclosed warehouse cases

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (high temperature case)</td>
<td>°C</td>
<td>50, 100, 300, 400, 600</td>
<td></td>
</tr>
<tr>
<td>Temperature (low temperature case)</td>
<td>°C</td>
<td>15, 30, 50, 100</td>
<td></td>
</tr>
<tr>
<td>Velocity (high temperature case)</td>
<td>m/s</td>
<td>5, 10, 20, 30</td>
<td></td>
</tr>
<tr>
<td>Velocity (low temperature case)</td>
<td>m/s</td>
<td>0.2, 2, 5, 10</td>
<td></td>
</tr>
<tr>
<td>Source diameter</td>
<td>m</td>
<td>0.5, 2, 4, 10</td>
<td>The single source was located in the centre of the warehouse roof.</td>
</tr>
<tr>
<td>No of openings (sources)</td>
<td></td>
<td>1, 2, 5, 10</td>
<td>Multiple sources located at regular intervals along building centreline</td>
</tr>
<tr>
<td>Building downwash</td>
<td></td>
<td>Modelled, not modelled</td>
<td>Building of 10m height, 30m width and 100m length</td>
</tr>
<tr>
<td>Building alignment</td>
<td></td>
<td>Aligned with wind, perpendicularly to wind</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>m/s</td>
<td>1, 2, 5, 10</td>
<td>Affects dry deposition of particulates only</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>m</td>
<td>$1 \times 10^6$, $1 \times 10^5$</td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>D5, F2, D15</td>
<td></td>
</tr>
</tbody>
</table>
### Table A5.2a: HOTSPOT – Warehouse fire: Key fixed parameters and assumptions for cases (a) and (b)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>‘General fire’</td>
<td></td>
</tr>
<tr>
<td>Radionuclide</td>
<td>Am-241</td>
<td></td>
</tr>
<tr>
<td>‘Material at risk’</td>
<td>50 curies</td>
<td>Total activity of the nuclide involved in the fire</td>
</tr>
<tr>
<td>Damage ratio</td>
<td>1</td>
<td>Default value – This is the fraction of the ‘material at risk’ actually impacted in the release scenario</td>
</tr>
<tr>
<td>Airborne fraction</td>
<td>0.01</td>
<td>Fraction of the ‘material at risk’ that is released to the atmosphere</td>
</tr>
<tr>
<td>Respirable fraction</td>
<td>0.05</td>
<td></td>
</tr>
<tr>
<td>Deposition velocity</td>
<td>0.3 cm/sec</td>
<td></td>
</tr>
<tr>
<td>Height - case (b) only</td>
<td>0m</td>
<td>Only fixed in case (b) (varied in case (a))</td>
</tr>
<tr>
<td>Air temperature - case (b) only</td>
<td>15 °C</td>
<td>Not required for case (a)</td>
</tr>
</tbody>
</table>

### Table A5.2b: HOTSPOT – Warehouse fire cases a) Entering height, radius and cloud top, and b) Entering heat emission rate: Parameters varied

<table>
<thead>
<tr>
<th>Case</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>Height</td>
<td>m</td>
<td>0, 5, 10</td>
<td>This is the ‘elevation of burning debris’</td>
</tr>
<tr>
<td></td>
<td>Radius</td>
<td>m</td>
<td>10, 20, 50, 100</td>
<td>This is the effective radius of the fire</td>
</tr>
<tr>
<td></td>
<td>Cloud top</td>
<td>m</td>
<td>10, 20, 50</td>
<td>This is the cloud top of the plume</td>
</tr>
<tr>
<td>b</td>
<td>Heat emission rate</td>
<td>cal/g</td>
<td>4.78 x 10^6, 9.56 x 10^6, 1.91 x 10^7</td>
<td>Equivalent to 20, 40 and 80 MW</td>
</tr>
</tbody>
</table>
### A.6. Fire plume (outside burning pool)

#### Table A6.1a: ADMS – Fire plume (outside burning pool): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of sources</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Pollutants modelled</td>
<td>Gaseous, particulate</td>
<td>Particulates included to test effect on deposition output</td>
</tr>
<tr>
<td>Pollutant emission rate</td>
<td>100g/s</td>
<td></td>
</tr>
<tr>
<td>Efflux type</td>
<td>'Exit velocity'</td>
<td></td>
</tr>
<tr>
<td>Building downwash effects</td>
<td>Not modelled</td>
<td></td>
</tr>
<tr>
<td>Deposition velocity</td>
<td>0.3 cm/sec</td>
<td></td>
</tr>
<tr>
<td>Outputs</td>
<td>Maximum plume height, ground level</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>°C</td>
<td>100, 200, 300, 400, 500</td>
<td></td>
</tr>
<tr>
<td>Velocity</td>
<td>m/s</td>
<td>5, 10, 20, 30</td>
<td>Equivalent areas: 3, 79, 707, 1963 m²</td>
</tr>
<tr>
<td>Source diameter</td>
<td>m</td>
<td>2, 10, 30, 50</td>
<td></td>
</tr>
<tr>
<td>Source height</td>
<td>m</td>
<td>0, 2, 5, 10, 20</td>
<td></td>
</tr>
<tr>
<td>Source type</td>
<td></td>
<td>Point source, area source</td>
<td></td>
</tr>
</tbody>
</table>

#### Table A6.1b: ADMS– Fire plume (outside burning pool): Parameters varied

| Temperature              | °C    | 100, 200, 300, 400, 500 |       |
| Velocity                 | m/s   | 5, 10, 20, 30 | Equivalent areas: 3, 79, 707, 1963 m² |
| Source diameter          | m     | 2, 10, 30, 50 |       |
| Source height            | m     | 0, 2, 5, 10, 20 |       |
| Source type              |       | Point source, area source |       |

#### Table A6.2a: ALOHA – Fire plume (outside burning pool): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>'Burning puddle (pool fire)' source</td>
<td></td>
</tr>
<tr>
<td>Fuels modelled</td>
<td>Methane</td>
<td></td>
</tr>
<tr>
<td>Outputs</td>
<td>Flame length, burn duration, burn rate, total amount burned</td>
<td></td>
</tr>
</tbody>
</table>

#### Table A6.2b: ALOHA – Fire plume (outside burning pool): Parameters varied

<table>
<thead>
<tr>
<th>General parameter</th>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pool size</td>
<td>Area</td>
<td>m²</td>
<td>10, 100, 2000, 50, 100</td>
<td></td>
</tr>
<tr>
<td>Pool depth</td>
<td>cm</td>
<td></td>
<td>0.5, 1, 5, 10, 100</td>
<td></td>
</tr>
<tr>
<td>Initial pool temperature</td>
<td>°C</td>
<td></td>
<td>-161.6, -170, -180</td>
<td>This cannot exceed the ambient boiling point (methane = -161.6°C) and has to be above the freezing point (methane = -182°C)</td>
</tr>
</tbody>
</table>
### Table A6.3a: HOTSPOT – Fire plume (outside burning pool): Key fixed parameters and assumptions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Values used</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source type</td>
<td>‘Plutonium fire’</td>
<td></td>
</tr>
<tr>
<td>Radionuclide</td>
<td>‘Weapons grade plutonium’</td>
<td></td>
</tr>
<tr>
<td>‘Material at risk’</td>
<td>3 kg</td>
<td>Total activity of the nuclide involved in the fire</td>
</tr>
<tr>
<td>Damage ratio</td>
<td>1</td>
<td>Default value – This is the fraction of the ‘material at risk’ actually impacted in the release scenario</td>
</tr>
<tr>
<td>Airborne fraction</td>
<td>0.01</td>
<td>Fraction of the ‘material at risk’ that is released to the atmosphere</td>
</tr>
<tr>
<td>Respirable fraction</td>
<td>0.05</td>
<td></td>
</tr>
<tr>
<td>Deposition velocity</td>
<td>0.3 cm/sec</td>
<td></td>
</tr>
<tr>
<td>Height</td>
<td>0m</td>
<td></td>
</tr>
<tr>
<td>Air temperature</td>
<td>15°C</td>
<td></td>
</tr>
</tbody>
</table>

### Table A6.3b: HOTSPOT – Fire plume (outside burning pool): Parameters varied

<table>
<thead>
<tr>
<th>Model input parameter(s)</th>
<th>Units</th>
<th>Values</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius</td>
<td>m</td>
<td>10, 20, 50, 100</td>
<td>This is the effective radius of the fire</td>
</tr>
<tr>
<td>Fuel volume</td>
<td>gallons</td>
<td>3000, 10000, 30000, 50000</td>
<td>This is the total amount of fuel burned in the fire</td>
</tr>
<tr>
<td>Burn duration</td>
<td>minutes</td>
<td>5, 20, 60, 90</td>
<td>Calculated based on HOTSPOT advice that “pool depth burn rates are 1 - 5mm/min”</td>
</tr>
<tr>
<td>Heat of combustion</td>
<td>cal/g</td>
<td>6000, 12000, 30000</td>
<td>Values roughly representative of methanol, ethanol and ammonia</td>
</tr>
</tbody>
</table>
### APPENDIX B: SENSITIVITY TESTS RESULTS TABLES

#### B.1. Evaporating pools

##### B.1.1 Direct pool source

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area of source</td>
<td>Equivalent diameters: 2, 5, 10, 20m</td>
<td>Concentrations at 100m are not sensitive for D5 conditions, but very sensitive for F2 conditions. Concentrations at 1000m are not sensitive for either D5 or F2 conditions. Non linear relationship</td>
</tr>
<tr>
<td>Released amount</td>
<td>Emission rate and mass flux</td>
<td>Concentrations are very sensitive at both 100 and 1000m, and for both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Emission height</td>
<td></td>
<td>Concentrations at 100m and 1000m are not sensitive for D5 conditions, and moderately sensitive for F2 conditions. Linear/almost linear negative relationship</td>
</tr>
<tr>
<td>Emission temperature</td>
<td></td>
<td>Concentrations at 100m are very sensitive, for both D5 and F2 conditions. Concentrations at 1000m are moderately sensitive for D5, and very sensitive for F2 conditions. This sensitivity is only really apparent at very low temperatures.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Input varied: rate of mass release to air</td>
<td>For both D5 and F2 conditions, and for both LNG and chlorine, concentrations at 100m and 1000m are very sensitive to the mass release rate.</td>
</tr>
<tr>
<td>Pool dimensions</td>
<td>Input varied: pool radius</td>
<td>For both D5 and F2 conditions, concentrations at 100m and 1000m are only slightly sensitive to the pool radius</td>
</tr>
<tr>
<td>Stability class/wind speed</td>
<td>D5 and F2 conditions</td>
<td>LNG concentrations at 100m show little sensitivity to the stability class/wind speed, whereas chlorine concentrations at 100m are very sensitive to the stability class/wind speed. Concentrations of both LNG and chlorine at 1000m show moderate sensitivity</td>
</tr>
</tbody>
</table>
Table B1.3: DRIFT – Direct pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>DRIFT Input / Source Parameter</th>
<th>Run cases</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release rate</td>
<td>2kg/s, 5kg/s, 10kg/s, 20kg/s and 50kg/s</td>
<td>Higher release rate from the same area generally lead to higher concentrations with the following exceptions. For dense area sources increasing the release rate increases the gravity spreading at the source. For buoyant sources increasing the release rate enhances buoyant rise – this effect, particularly in low wind speeds can lead to lower ground-level concentrations than at lower rates.</td>
</tr>
<tr>
<td>Source diameter</td>
<td>2m, 5m, 10m, 20m</td>
<td>Larger source area for the same flow rate leads to greater dilution close to the source. For dense releases in low wind the effect of source size is less marked due to dense gas spreading over the source. Smaller source diameter for buoyant releases enhances the effect of buoyant rise in leading to smaller ground-level concentrations at distances between the source and the downstream ground-level maximum.</td>
</tr>
<tr>
<td>Source density</td>
<td>Mw=16, 28, 71</td>
<td>Weak dependence of centreline in D5 conditions, more marked in F2 conditions due to effect of buoyant plume rise and dense gas suppression of mixing. Marked effect on ground-level concentration for buoyant release due to buoyant rise. Note ppm or mol/mol concentrations include a dependence upon molecular weight of the released substance.</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D5, F2</td>
<td>For ambient density release F2 gives higher concentrations at all downstream distances. Dense releases show enhanced spreading over the source and higher downwind concentrations. Buoyant releases show initially higher dilution in F2 and reduction in ground-level concentration due to plume rise, subsequently diluting more slowly in the far field (passive limit).</td>
</tr>
</tbody>
</table>
### Table B1.4: GASTAR – Direct pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dimensions of pool</td>
<td>Input varied: Initial plume width</td>
<td>For both D5 and F2 conditions, in both the near and far field, concentrations of methane, ethylene and chlorine are not very sensitive; the little sensitivity seen is restricted to the near field.</td>
</tr>
<tr>
<td>Release amount</td>
<td>Input varied: Mass flux</td>
<td>For both D5 and F2 conditions, in both the near and far field, concentrations of all three substances are very sensitive - strong positive, non-linear dependence</td>
</tr>
<tr>
<td>Emission temperature</td>
<td></td>
<td>For both D5 and F2 conditions, in both the near and far field: There is almost no sensitivity, except for methane, where concentrations are very sensitive close to the boiling point (where increasing temperatures increase the concentrations)</td>
</tr>
</tbody>
</table>

### Table B1.5: SLAB – Direct pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>Input varied: Mass flux from area source</td>
<td>For both D5 and F2 conditions concentrations of methane, HCN and chlorine at both 100m and 1000m are very sensitive to the release amount. The relationship between the concentration and the release rate is very linear for all substances.</td>
</tr>
<tr>
<td>Dimensions of pool</td>
<td>Input varied: area of source</td>
<td>For both D5 and F2 conditions concentrations of methane, HCN and chlorine at 100m are moderately sensitive. Concentrations at 1000m are not sensitive for any of the cases. Increasing the area decreases the concentrations.</td>
</tr>
<tr>
<td>Stability class/wind speed</td>
<td>D5 and F2</td>
<td>The concentrations of methane, HCN and chlorine at both 100m and 1000m are very sensitive to the stability class/wind speed.</td>
</tr>
</tbody>
</table>
B.1.2 Bunded pool source

Table B1.6: ALOHA – Bunded pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter</td>
<td></td>
<td>The vaporisation rates and both concentration-based outputs are very sensitive for both methane and pentane.</td>
</tr>
<tr>
<td>Mass released</td>
<td></td>
<td>The vaporisation rates are not very sensitive for methane (cryogenic) or pentane (non-cryogenic). Concentration-based outputs in the near field (distance to LEL) and far field (distance to 10% LEL) are only slightly sensitive for both methane and pentane.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>Varied for methane only</td>
<td>The vaporisation rates and both concentration-based outputs are very sensitive. They are particularly sensitive where the temperatures are close to the boiling temperatures.</td>
</tr>
<tr>
<td>Air temperature</td>
<td></td>
<td>The vaporisation rates and both concentration-based outputs are not very sensitive, for both methane and pentane.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, the vaporisation rate is not sensitive up to around 5m/s, and moderately sensitive between 5 and 20m/s. Interesting patterns (see results summary text) For pentane, the vaporisation rate is highly sensitive, with an almost linear, positive relationship. For both methane and pentane, the concentration-based outputs are moderately sensitive.</td>
</tr>
</tbody>
</table>
## Table B1.7: GASP – Bunded pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>GASP Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source properties</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spill mass</td>
<td>1te, 10te, 100te</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vaporisation reduces with increased spill mass. Distance to LFL and 10% LFL decrease significantly with increasing spill mass.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td>Weak</td>
<td>Peak vaporisation rate from GASP insensitive to spill mass. Segment peak rate in DRIFT increases slowly with spill mass. Distance to LFL equal to bund radius, distance to 10% LFL increases slowly with spill mass.</td>
</tr>
<tr>
<td>Spill temperature</td>
<td>-162.4°C to -180°C</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vaporisation rate, distances to LFL and 10% LFL all decrease with decreasing spill temperature. Effect is most strong for initial temperatures close to the boiling temperature.</td>
</tr>
<tr>
<td></td>
<td>5°C, 15°C, 30°C</td>
<td>n-Pentane</td>
<td>Strong</td>
<td>Peak vaporisation rate very sensitive to the spill temperature. Distance to 10% LFL is very sensitive, but change in distance to LFL is limited to be close to the edge of the bund.</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>4m, 5m, 8m, 10m, 20m</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vaporisation rate increases markedly with increased bund diameter – at a greater rate than in proportion to the increase in pool area. Distance to LFL and 10% LFL increases with increasing bund diameter.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td>Strong</td>
<td>Peak vaporisation rate increases in direct proportion to bund area. Distance to LFL and 10% LFL increases with increasing bund diameter.</td>
</tr>
<tr>
<td>Substrate properties</td>
<td>5°C, 15°C, 30°C</td>
<td>In GASP the ground temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Atmospheric properties</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vapourisation weakly dependent upon wind speed decreasing at large wind speeds with a maximum between 5m/s and 2m/s. Distance to LFL and 10% LFL decrease strongly with increasing wind speed.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td>Moderate</td>
<td>Peak vapourisation rate is a strong function of wind speed - increasing with (wind speed)^0.87. Distance to LFL remains at or near bund radius. Distance to 10% LFL decreases with increasing wind speed with only a small change between 7m/s and 20 m/s wind speeds.</td>
</tr>
<tr>
<td>Temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
<td>Peak vapourisation rate increases with ground/air temperature. Distance to LFL and 10% LFL may increase or decrease with air/ground temperature. A weaker effect than for spill temperature.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td>Weak</td>
<td>Peak vapourisation insensitive to air/ground temperature. Distances to LFL and 10% LFL increase with air/ground temperature. Less of an effect than for spill temperature.</td>
</tr>
</tbody>
</table>
### Table B1.8: HGSYSTEM (LPOOL) – Bunded pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume flow rate</td>
<td>Released over one second</td>
<td>For methane, the vaporisation rate/time plots show very different behaviours for different release volumes, with varying delays in the occurrence of the peak vaporisation rate. For the base case, the vaporisation rate is very low until around 100s after the start of the release. The maximum vaporisation rate is very sensitive, with increasing release volumes resulting in decreasing vaporisation rates. The sensitivity of the vaporisation rate decreases with increasing averaging time. For pentane, when averaged over 10 minutes or less, the vaporisation rate is not sensitive to the amount released into the bund. When averaged over longer averaging times, the vaporisation rate is moderately sensitive. The sensitivity increases over time. These observations apply to both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td></td>
<td>The vaporisation rates are very sensitive for both D5 and F2 conditions. The vaporisation rate for the base case (-162°C) shows a distinct peak in the first few minutes, while the vaporisation rates for the other two temperatures (-170 and -180°C) are almost constant throughout the modelling period.</td>
</tr>
<tr>
<td>Initial liquid temperature - pentane</td>
<td></td>
<td>The vaporisation rates are very sensitive for both D5 and F2 conditions. The vaporisation rates are almost constant over time for all cases.</td>
</tr>
<tr>
<td>Pool radius</td>
<td></td>
<td>The vaporisation rates are very sensitive for both D5 and F2 conditions and both methane and pentane. The sensitivity is greater for methane than for pentane.</td>
</tr>
<tr>
<td>Air temperature</td>
<td></td>
<td>The vaporisation rate of both methane and pentane, and both D5 and F2 conditions is not sensitive to this parameter.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, the vaporisation rate is very sensitive for D5 conditions and moderately sensitive for F2 conditions. For pentane, the vaporisation rate is highly sensitive, with an almost linear, positive relationship, for both D5 and F2 conditions.</td>
</tr>
</tbody>
</table>
### Table B1.9: LSMS – Bunded pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill</td>
<td>Base Case ‘A’ only Varied the vertical size of pool and bund</td>
<td>Very different behaviour for cryogenic and non-cryogenic substances: Methane (cryogenic): Negative relationship (increasing mass gives decreasing concentrations) Vaporisation rate is moderately sensitive – more so at lower mass values Butane (non-cryogenic): Positive relationship (increasing mass gives increasing concentrations) Vaporisation rate is very sensitive – more so at higher mass values</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>Base Case ‘A’ only</td>
<td>Methane: Very sensitive; positive, almost linear relationship. Butane: Only slightly sensitive</td>
</tr>
<tr>
<td>Pool and bund radius</td>
<td>Base Case ‘A’ only</td>
<td>Both methane and butane: Very sensitive, generally positive relationship.</td>
</tr>
<tr>
<td>Substrate and bund properties</td>
<td>Base Case ‘A’ only</td>
<td>Methane: The vaporisation rate is moderately sensitive over the range tested (all variations of ‘concrete’). Sensitivity decreases over time Butane: The vaporisation rate shows no sensitivity – values are identical for each type.</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td>Base Case ‘A’ and methane only</td>
<td>The vaporisation rate is only slightly sensitive to this parameter</td>
</tr>
<tr>
<td>Solar flux</td>
<td>Base case ‘B’ only (methane only)</td>
<td>The vaporisation rate only slightly sensitive. Sensitivity increases over time.</td>
</tr>
<tr>
<td>Wind speed</td>
<td>Base cases ‘A’ and ‘B’</td>
<td>Base case ‘A’, methane: the vaporisation rate is not very sensitive Base case ‘A’, butane: the vaporisation rate is moderately sensitive – sensitivity decreases over time. Base case ‘B’ (methane): the vaporisation rate is moderately sensitive</td>
</tr>
</tbody>
</table>
Table B1.10: PHAST – Bunded pool source: Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spill mass</td>
<td>1te, 10te, 100te</td>
<td>Methane</td>
<td>Moderate</td>
<td>Negative relationship (increasing mass gives decreasing concentrations) Vaporisation rate is moderately sensitive – more so at lower mass values</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td>Positive relationship (increasing mass gives increasing concentrations). Vaporisation rate is very sensitive – more so at higher mass values</td>
</tr>
<tr>
<td>Spill temperature</td>
<td>-162.4°C to -180°C</td>
<td>Methane</td>
<td>Weak</td>
<td>Peak vaporisation rate and concentration insensitive to initial spill temperature except very close to boiling point.</td>
</tr>
<tr>
<td></td>
<td>5°C, 15°C, 30°C</td>
<td>n-Pentane</td>
<td></td>
<td>Peak vaporisation rate and concentration slightly sensitive to initial spill temperature – increasing with increasing temperature</td>
</tr>
<tr>
<td><strong>Spreading constraints</strong></td>
<td>4m, 5m, 8m, 10m, 20m</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vaporisation rate increases markedly with increased bund diameter. Distance to LFL and 10% LFL increases with increasing bund diameter.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Substrate properties</strong></td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
<td>Only very small effect on LFL and 10% LFL distances</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Moderate</td>
<td>Peak vaporisation rate increases with wind speed. Distance to LFL and 10% LFL decreases with wind speed with a strong dependence at low wind speeds.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
**B.1.3. Instantaneously released pool source on land**

Table B1.11: HGSYSTEM (LPOOL) – Instantaneously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume flow rate</td>
<td>Released over one second</td>
<td>Both the vaporisation rate and the maximum pool diameter, for both methane and pentane, and for D5 and F2 conditions, are very sensitive to this parameter. There is a very linear dependency of vaporisation rate and release amount for all cases.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for both methane and pentane, and for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td></td>
<td>For methane, the vaporisation rate and the maximum pool diameter are only slightly sensitive to this parameter, for both D5 and F2 conditions. For pentane, the vaporisation rate is moderately sensitive, and the maximum pool diameter is not sensitive to this parameter, for both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Substrate type</td>
<td>‘insulated concrete’, ‘wet sand’, ‘dry sand’</td>
<td>For methane, the vaporisation rate is very sensitive, and the maximum pool diameter is moderately sensitive, for this range of substrate types. The vaporisation rate/time plots show very different behaviours for different substrate types, with varying delays in the occurrence of the peak vaporisation rate. For pentane, the vaporisation rate is moderately sensitive, and the maximum pool diameter is not sensitive, for this range of substrate types, for both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Varied the minimum thickness of the pool</td>
<td>For methane, the vaporisation rate is very sensitive, and the maximum pool diameter is only slightly sensitive, for this range of substrate types, for both D5 and F2 conditions. For pentane, the vaporisation rate and the maximum pool diameter are moderately sensitive, for this range of substrate types, for both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, the vaporisation rate is very sensitive, and the maximum pool diameter is only slightly sensitive, for both D5 and F2 conditions. For pentane, the vaporisation rate is very sensitive, and the maximum pool diameter is moderately sensitive, for both D5 and F2 conditions.</td>
</tr>
</tbody>
</table>


Table B1.12: LSMS – Instantaneously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill</td>
<td>Varied the initial source radius and height (kept aspect ratio constant)</td>
<td>For both methane and butane, all outputs are all very sensitive to this parameter.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>For methane, all outputs are only slightly sensitive, while for butane, all outputs are moderately sensitive.</td>
</tr>
<tr>
<td>Initial pool radius</td>
<td>Keeping the initial height constant (therefore, effectively varying the mass)</td>
<td>For both methane and butane, all outputs are all very sensitive to this parameter, with a linear/almost linear relationship.</td>
</tr>
<tr>
<td>Substrate properties</td>
<td></td>
<td>The vaporisation rates are moderately sensitive to this parameter for methane, and only slightly sensitive for butane. The pool duration for methane is only moderately sensitive. The maximum pool radius is not very sensitive for either methane or butane.</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td>Varied for methane only</td>
<td>All outputs are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Varied the turbulent drag parameter</td>
<td>For methane, the vapourisation rate and pool duration are moderately sensitive, and the maximum pool radius is only slightly sensitive to this parameter. For butane, the vapourisation rate is moderately sensitive, and the maximum pool radius is only slightly sensitive.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, the vapourisation rate and the maximum pool radius are only slightly sensitive; the duration of the pool is sensitive up to 5m/s, and not at all sensitive above 5m/s. For butane, the vapourisation rate is not sensitive until the wind speed is greater than around 5m/s; above 5m/s, it becomes very sensitive, and linear. The maximum pool radius is only slightly sensitive.</td>
</tr>
</tbody>
</table>
B.1.4. Continuously released pool source on land

Table B1.13: ALOHA – Continuously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill</td>
<td>Varied mass in tank, tank volume and orifice diameter</td>
<td>All model outputs (the vaporisation rate, maximum pool diameter and the distances to the LEL and 10% LEL) are very sensitive to this parameter, for both methane and pentane, and for both D5 and F2 conditions. There is a linear dependency between the vaporisation rate and release amount for all cases. The maximum pool diameter and the distance to the LEL and 10% LEL are more sensitive at the lower end of the range.</td>
</tr>
<tr>
<td>Duration</td>
<td>Varied orifice diameter</td>
<td>All model outputs (the vaporisation rate, maximum pool diameter and the distance to the LEL and 10% LEL) are very sensitive to this parameter, for both methane and pentane, and for both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Initial liquid temperature - methane</td>
<td></td>
<td>The vaporisation rate and the distances to both the LEL and to the 10% LEL are all very sensitive when the temperature is very close to the boiling point. Below around -163°C, these outputs show only slight sensitivity. The maximum pool diameter is only slightly sensitive for the whole range of temperature values.</td>
</tr>
<tr>
<td>Initial liquid temperature - pentane</td>
<td></td>
<td>The vaporisation rate, the maximum pool diameter and the distance to the 10% LEL are only slightly sensitive, while the distance to the LEL is moderately sensitive.</td>
</tr>
<tr>
<td>Ground type</td>
<td></td>
<td>For both methane and pentane, there is an overall moderate sensitivity to varying the substrate type. Most substrate types give similar results (particularly ‘concrete’ and ‘soil’ substrate types). An exception to this is the ‘sandy dry soil’ substrate, which is a noticeable outlier.</td>
</tr>
<tr>
<td>Ground temperature</td>
<td></td>
<td>For both methane and pentane, all model outputs are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Varied maximum pool diameter</td>
<td>For methane, the vaporisation rate and the distances to both the LEL and to the 10% LEL are all moderately sensitive to the user-specified maximum diameter. For pentane, these outputs are all very sensitive.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, the vaporisation rate is moderately sensitive to the wind speed, and the maximum pool diameter and the distances to the LEL and 10% LEL are very sensitive. For pentane, all outputs are very sensitive, particularly at lower wind speeds.</td>
</tr>
</tbody>
</table>
Table B1.14: GASP/DRIFT Continuously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>GASP Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spill rate</td>
<td>0.556kg/s, 5.5 kg/s, 55.6 kg/s, 556 kg/s</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vapourisation rate is directly proportional and almost equal to the spill rate (constant of proportionality 0.9-0.93). The maximum pool radius varies approximately as the square root of the spill rate. Distance to LFL and 10% LFL varies approximately as (spill rate)^q with q=0.56.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spill temperature</td>
<td>-162.4°C to -180°C</td>
<td>Methane</td>
<td>Weak</td>
<td>The peak vapourisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the released liquid – decreasing slightly as the storage temperature decreases.</td>
</tr>
<tr>
<td>5°C, 15°C, 30°C</td>
<td>n-Pentane</td>
<td></td>
<td></td>
<td>The peak vapourisation rate, maximum pool size and distances to LFL and 10% LFL are very weakly dependent on the temperature of the released liquid, increasing slightly as the storage temperature increases.</td>
</tr>
<tr>
<td>Spill duration</td>
<td>15min, 30min, 60min</td>
<td>Methane</td>
<td>Strong</td>
<td>Spilling the same release quantity (10te) over different durations introduces a strong dependence upon spill duration (spill rate)</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Spreading constraints</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Puddle depth</td>
<td>2mm, 1cm, 2cm, 5cm, 10cm</td>
<td>Methane</td>
<td>Strong</td>
<td>The peak vapourisation rate, maximum pool radius, distance to LFL and distance to 10% LFL all decrease with increasing puddle depth. The peak vapourisation rate divided by the maximum pool area is approximately constant.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td>The peak vapourisation rate divided by the maximum pool area increases with increasing puddle depth.</td>
</tr>
<tr>
<td><strong>Substrate properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ground temperature</td>
<td>In GASP the ground temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>asphalt, concrete, dry soil, wet soil</td>
<td>Methane</td>
<td>Strong</td>
<td>The maximum vapourisation rate is insensitive to the substrate type, whereas the maximum pool radius is moderately sensitive to substrate type. The distances to LFL and 10% LFL vary significantly between substrates, with wet soil giving maximum ranges.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td>Moderate</td>
<td>The maximum vapourisation rate is sensitive to the substrate type, whereas the maximum pool radius is fairly insensitive to substrate type. The overall effect is for the distance to LFL and 10% LFL to be moderately sensitive to the substrate type.</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Strong</td>
<td>The maximum vapourisation is insensitive to wind speed. The maximum pool radius depends weakly on wind speed – decreasing with increased wind speed. The distance to LFL and 10% LFL depend strongly on wind speed with higher wind speeds giving a reduction in distance.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td>The peak vapourisation rate increases with increasing wind speed. The maximum pool radius decreases slowly with increasing wind speed. Distances to LFL and 10% LFL reduce with increasing wind speed.</td>
</tr>
<tr>
<td>Temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
<td>The peak vapourisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the ambient temperature – increasing slightly as the ground temperature increases.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td>The results for n-Pentane show a greater sensitivity to ambient temperature than methane. The sensitivity to variation in ambient temperature is greater than to the spill temperature.</td>
</tr>
</tbody>
</table>

54
Table B1.15: HGSYSTEM (LPOOL) – Continuously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume flow rate</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for both methane and pentane, and for D5 and F2 conditions, are very sensitive to this parameter. There is a linear dependency of vaporisation rate and release amount for all cases.</td>
</tr>
<tr>
<td>Release duration</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for both methane and pentane, and for D5 and F2 conditions, are only slightly sensitive to this parameter</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for both methane and pentane, and for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for both methane and pentane, and for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Substrate type</td>
<td>‘insulated concrete’, ‘wet sand’, ‘dry sand’</td>
<td>The vaporisation rate is not sensitive, and the maximum pool diameter is moderately sensitive, for both methane and pentane, and both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Varied the minimum thickness of the pool</td>
<td>For methane, the average vaporisation rate is not sensitive to this spreading constraint, but the maximum vaporisation rate is moderately sensitive, for both D5 and F2 conditions. For pentane, the opposite is observed; the average vaporisation rate is moderately sensitive, but the average vaporisation rate is moderately sensitive, for both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter. For pentane, the vaporisation rate is moderately sensitive, and the maximum pool diameter is only slightly sensitive, for both D5 and F2 conditions. The vaporisation/time plots for methane and pentane are very different. Methane displays a pattern of a high initial peak in vaporisation rate, followed by much lower vaporisation. Pentane shows a gradual increase in vaporisation rate, reaching a plateau later in the release period.</td>
</tr>
</tbody>
</table>
Table B1.16: LSMS – Continuously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume flow into pool</td>
<td>Also varied the initial source radius (kept velocity of liquid flow constant)</td>
<td>For both methane and butane, the vaporisation rate and the maximum pool radius are very sensitive to this parameter.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td>Varied for methane only</td>
<td>Both the vaporisation rate and the maximum pool radius are only slightly sensitive.</td>
</tr>
<tr>
<td>Substrate properties</td>
<td></td>
<td>For both methane and butane, the vaporisation rate and the maximum pool radius are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Substrate temperature</td>
<td></td>
<td>For both methane and butane, both outputs are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Spreading constraints</td>
<td>Varied the turbulent drag parameter</td>
<td>For both methane and butane, neither of the outputs is sensitive to this parameter.</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>For methane, both the vaporisation rate and the maximum pool radius are only slightly sensitive. For butane, both outputs are moderately sensitive.</td>
</tr>
</tbody>
</table>
Table B1.17: PHAST – Continuously released pool source on land: Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spill rate</td>
<td>0.556kg/s, 5.5 kg/s, 55.6 kg/s, 556 kg/s</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vaporisation rate is directly proportional and almost equal to the spill rate (constant of proportionality 0.95-1). The maximum pool radius varies approximately as (spill rate)$^{n}$ with $q=0.40$ and 0.49 respectively.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td>Peak vaporisation rate is approximately proportional to the spill rate with a constant of proportionality of approximately 0.7-0.8. The maximum pool radius increases with approximately the square root of the release rate. The distance to LFL and 10% LFL is a strong function of the spill rate.</td>
</tr>
<tr>
<td>Spill temperature</td>
<td>162.4°C to 180°C, 5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
<td>The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the released liquid – decreasing slightly as the storage temperature decreases.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td>The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are very weakly dependent on the temperature of the released liquid, increasing slightly as the storage temperature increases.</td>
</tr>
<tr>
<td>Spill duration</td>
<td>15min, 30min, 60min</td>
<td>Methane</td>
<td>Strong</td>
<td>Spilling the same release quantity (10te) over different durations introduces a strong dependence upon spill duration (spill rate)</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Minimum pool depth</td>
<td>2mm, 1cm, 2cm, 5cm, 10cm</td>
<td>Methane</td>
<td>Moderate – different behaviour close to the pool</td>
<td>The peak vaporisation rate is insensitive to the minimum pool depth. The maximum pool radius depends approximately as (minimum pool depth)$^{1/2}$. Distance to LFL and 10% LFL increase as the pool minimum depth is increased.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ground temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
<td>The results for n-Pentane show a greater sensitivity to ground temperature than methane. The sensitivity to variation in ground temperature is greater than to the spill temperature.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substrate type</td>
<td>asphalt, concrete, dry soil, wet soil</td>
<td>Methane</td>
<td>Strong</td>
<td>The maximum vapourisation rate is insensitive to the substrate type, whereas the maximum pool radius is very sensitive to substrate type. The overall effect is for the distance to LFL and 10% LFL to be strongly sensitive to the substrate type.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
<td>The maximum vapourisation rate is insensitive to the substrate type, whereas the maximum pool radius is moderately sensitive to substrate type. The overall effect is for the distance to LFL and 10% LFL to be moderately sensitive to the substrate type.</td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Strong</td>
<td>The maximum vapourisation is insensitive to wind speed. The maximum pool radius depends weakly on wind speed – decreasing with increased wind speed. The distance to LFL and 10% LFL depend strongly on wind speed with higher wind speeds giving a reduction in distance.</td>
</tr>
</tbody>
</table>
### B.1.5. Instantaneously released pool source on water

#### Table B1.18: – ALOHA - Instantaneously released pool source on water. Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill</td>
<td>Varied mass and diameter</td>
<td>All model outputs (the vaporisation rate and the distances to both the LEL and 10% LEL) are very sensitive to this parameter</td>
</tr>
<tr>
<td>Initial diameter</td>
<td></td>
<td>None of the model outputs are sensitive to this parameter</td>
</tr>
<tr>
<td>Water temperature</td>
<td></td>
<td>None of the model outputs are sensitive to this parameter</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>None of the model outputs are sensitive to this parameter; there is no effect at all on the results.</td>
</tr>
<tr>
<td>Substance</td>
<td>Modelled a hydrogen spill</td>
<td>When an equivalent mass of hydrogen is released, the vaporisation rate is the same as that for methane</td>
</tr>
</tbody>
</table>
Table B1.19: GASP - Instantaneously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spill mass (and diameter)</td>
<td>1te, 10te, 100te</td>
<td>Methane</td>
<td>Strong</td>
<td>The distance to LFL and 10% LFL varies approximately as (spill mass)$^{1/3}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td>The distance to LFL and 10% LFL varies with spill mass as (spill mass)$^q$ where q=0.5 and 0.44 respectively.</td>
</tr>
<tr>
<td>Initial spill diameter</td>
<td>50m, 55m, 60m, 70m</td>
<td>Methane</td>
<td>Moderate – different behaviour for methane and n-pentane</td>
<td>Increased spill diameter leads to decreased distance to LFL and 10% LFL</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td>Increased spill diameter leads to increased distance to LFL and 10% LFL. This is the opposite behaviour to methane.</td>
</tr>
<tr>
<td>Spill temperature</td>
<td>-162.4°C to -180°C</td>
<td>Methane</td>
<td>Negligible</td>
<td>Variation of the initial spill temperature has negligible effect on the distance to LFL and 10% LFL</td>
</tr>
<tr>
<td></td>
<td>5°C, 15°C, 30°C</td>
<td>n-Pentane</td>
<td>Weak</td>
<td>The distance to LFL and 10% LFL show small increases with increased spill temperature.</td>
</tr>
<tr>
<td><strong>Substrate properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water temperature</td>
<td></td>
<td></td>
<td></td>
<td>In GASP the water temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Strong – different behaviour for methane and n-pentane</td>
<td>The vaporisation rate from the pool is independent of wind speed. The distance to LFL and 10% LFL are predicted to increase with increasing wind speed and then decrease – the worst case for these runs being a 7m/s wind.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
<td>The vaporisation rate increases with increasing wind speed. The distances to LFL and 10% LFL are predicted to decrease with increasing wind speed.</td>
</tr>
<tr>
<td>Temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Moderate</td>
<td>The distance to LFL is predicted to decrease with slightly increasing ambient temperature whereas the distance to 10% LFL increases and then decreases.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>n-Pentane</td>
<td>Strong</td>
<td>The distances to LFL and 10% LFL are predicted to increase significantly with ambient temperature.</td>
</tr>
</tbody>
</table>
### Table B1.20: HGSYSTEM (LPOOL) – Instantaneously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume flow rate</td>
<td>Released over one second</td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are very sensitive to this parameter. There is a linear dependency of vaporisation rate and release amount for both cases.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Water temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
</tbody>
</table>

### Table B1.21: LSMS – Instantaneously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass of spill</td>
<td>Varied the initial source radius and height (kept aspect ratio constant)</td>
<td>The average and maximum vaporisation rates, the pool duration and the maximum pool radius are all very sensitive to this parameter, for both methane and hydrogen. The evaporation rate is most sensitive.</td>
</tr>
<tr>
<td>Initial pool radius</td>
<td></td>
<td>The average and maximum vaporisation rates, the pool duration and the maximum pool radius are all very sensitive to this parameter, for both methane and hydrogen. The duration of the pool is particularly sensitive for hydrogen.</td>
</tr>
<tr>
<td>Convective heat flux from water</td>
<td>By specifying the initial heat flux from the water</td>
<td>The average and maximum vaporisation rates and the pool duration are very sensitive to this parameter, with a large effect on the pool duration. The maximum pool radius is only moderately sensitive.</td>
</tr>
<tr>
<td>Roughness length</td>
<td></td>
<td>The vaporisation rate and maximum pool radius are not sensitive to this parameter. The pool duration is moderately sensitive for methane and very sensitive for hydrogen.</td>
</tr>
</tbody>
</table>
Table B1.22: PHAST – Instantaneously released pool source on water. Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td>Spill mass</td>
<td>1te, 10te, 100te</td>
<td>Methane</td>
<td>Strong</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
</tr>
<tr>
<td><strong>Substrate properties</strong></td>
<td>Water temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>n-Pentane</td>
<td>Moderate</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td>Wind speed and stability</td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Strong – different behaviour for methane and n-pentane</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>n-Pentane</td>
<td></td>
</tr>
</tbody>
</table>
### B.1.6. Continuously released pool source on water

#### Table B1.23: ALOHA – Continuously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow into pool</td>
<td>Varying mass in tank, tank volume and orifice diameter</td>
<td>All model outputs (the vaporisation rate, maximum pool diameter and the distances to the LEL and 10% LEL) are very sensitive to this parameter. There is a linear dependency between the vaporisation rate and release amount. The maximum pool diameter and the distance to the LEL and 10% LEL are more sensitive at the lower end of the range.</td>
</tr>
<tr>
<td>Duration of release</td>
<td>Varying orifice diameter</td>
<td>The vaporisation rate is very sensitive to this parameter, while the maximum pool diameter and the distances to the LEL and 10% LEL are moderately sensitive.</td>
</tr>
<tr>
<td>Convective heat from water</td>
<td>Varying water temperature</td>
<td>All of the model outputs are only slightly sensitive to the water temperature. The distance to the LFL does show some sensitivity above 15/20 °C, but there is no corresponding sensitivity in the evaporation rate, however, suggesting that this might be a dispersion effect.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>When the temperature is very close to the boiling point, the vaporisation rate and the maximum pool diameter are very sensitive, and the distances to the LEL and to the 10% LEL are moderately sensitive. Below around -163°C, none of these outputs are sensitive.</td>
</tr>
</tbody>
</table>
Table B1.24: GASP – Continuously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>GASP Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source properties</td>
<td>Spill rate</td>
<td>Methane</td>
<td>Strong</td>
<td>Peak vaporisation rate is directly proportional and almost equal to the spill rate. The maximum pool radius, distance to LFL and distance to 10% LFL vary strongly with the spill rate.</td>
</tr>
<tr>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Spill temperature</td>
<td>Methane</td>
<td>Negligible</td>
<td>The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the released liquid – decreasing slightly as the storage temperature decreases.</td>
</tr>
<tr>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Spill duration</td>
<td>Methane</td>
<td>Strong</td>
<td>Spilling the same release quantity (10t) over different durations introduces a strong dependence upon spill duration (spill rate)</td>
</tr>
<tr>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substrate properties</td>
<td>Water temperature</td>
<td>In GASP the water temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Atmospheric properties</td>
<td>Wind speed and stability</td>
<td>Methane</td>
<td>Strong</td>
<td>The maximum vaporisation is insensitive to wind speed. The maximum pool radius depends weakly on wind speed – decreasing with increased wind speed. The distance to LFL and 10% LFL depend strongly on wind speed with higher wind speeds giving a reduction in distance.</td>
</tr>
<tr>
<td></td>
<td>n-Pentane</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Temperature</td>
<td>Methane</td>
<td>Weak</td>
<td>The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the water – increasing slightly as the water temperature increases.</td>
</tr>
</tbody>
</table>

| Spill rate | 0.556kg/s, 5.56 kg/s, 55.6 kg/s, 556 kg/s | Methane | Strong | Peak vaporisation rate is directly proportional and almost equal to the spill rate. The maximum pool radius, distance to LFL and distance to 10% LFL vary strongly with the spill rate. |
| n-Pentane  |                                         |         |        |                                 |
| Spill temperature | -162.4°C to -180°C | Methane | Negligible | The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the released liquid – decreasing slightly as the storage temperature decreases. |
| n-Pentane  |                                         |         |        |                                 |
| Spill duration | 15min, 30min, 60min | Methane | Strong | Spilling the same release quantity (10t) over different durations introduces a strong dependence upon spill duration (spill rate) |
| n-Pentane  |                                         |         |        |                                 |
| Water temperature | In GASP the water temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below. | | | |
| Wind speed and stability | D1, D2, D5, D7, D10, D20, F2 | Methane | Strong | The maximum vaporisation is insensitive to wind speed. The maximum pool radius depends weakly on wind speed – decreasing with increased wind speed. The distance to LFL and 10% LFL depend strongly on wind speed with higher wind speeds giving a reduction in distance. |
| n-Pentane  |                                         |         |        |                                 |
| Temperature | 5°C, 15°C, 30°C | Methane | Weak   | The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the water – increasing slightly as the water temperature increases. |
### Table B1.25: HGSYSTEM (LPOOL) – Continuously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate</td>
<td>Varied the volume spill rate and the orifice diameter</td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are very sensitive to this parameter. There is a linear dependency of vaporisation rate.</td>
</tr>
<tr>
<td>Spill duration</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Initial liquid temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
<tr>
<td>Water temperature</td>
<td></td>
<td>Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.</td>
</tr>
</tbody>
</table>

### Table B1.26: LSMS – Continuously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Volume flow into pool</td>
<td>Also varied the initial source radius (kept velocity of liquid flow constant)</td>
<td>The average vaporisation rate is very sensitive to this parameter, even over long averaging times, with a linear/almost linear dependency. The maximum radius of the pool is very sensitive to the volume flow</td>
</tr>
<tr>
<td>Convective heat flux from water</td>
<td>By specifying the initial heat flux from the water</td>
<td>The average vaporisation rate is very sensitive to this parameter, but only over shorter averaging time; the sensitivity is negligible after around 15 minutes, after which there is no dependence on the initial heat flux. Particularly sensitive at lower end of value range. The maximum radius of the pool is very sensitive to the initial heat flux.</td>
</tr>
</tbody>
</table>
Table B1.27: PHAST – Continuously released pool source on water: Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Spill rate</td>
<td>0.556 kg/s, 5.56 kg/s, 55.6 kg/s, 556 kg/s</td>
<td>Methane, n-Pentane</td>
<td>Strong</td>
<td>Peak vaporisation rate is directly proportional and almost equal to the spill rate. The maximum pool radius, distance to LFL and distance to 10% LFL vary strongly with the spill rate.</td>
</tr>
<tr>
<td>Spill temperature</td>
<td>-162.4°C to -180°C, 5°C, 15°C, 30°C</td>
<td>Methane, n-Pentane</td>
<td>Negligible</td>
<td>The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the released liquid – decreasing slightly as the storage temperature decreases.</td>
</tr>
<tr>
<td>Spill duration</td>
<td>15min, 30min, 60min</td>
<td>Methane, n-Pentane</td>
<td>Strong</td>
<td>Spilling the same release quantity (10te) over different durations introduces a strong dependence upon spill duration (spill rate)</td>
</tr>
<tr>
<td><strong>Substrate properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Water temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Methane</td>
<td>Weak</td>
<td>The peak vaporisation rate, maximum pool size and distances to LFL and 10% LFL are insensitive to the temperature of the water – increasing slightly as the water temperature increases.</td>
</tr>
<tr>
<td>n-Pentane</td>
<td></td>
<td>Moderate</td>
<td></td>
<td>The maximum vaporisation rate is insensitive to wind speed. The maximum pool radius decreases as the water temperature increases. The distance to LFL and 10% LFL increases significantly with increased water temperature.</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D1, D2, D5, D7, D10, D20, F2</td>
<td>Methane</td>
<td>Strong</td>
<td>The maximum vaporisation is insensitive to wind speed. The maximum pool radius depends weakly on wind speed – decreasing with increased wind speed. The distance to LFL and 10% LFL depend strongly on wind speed with higher wind speeds giving a reduction in distance.</td>
</tr>
</tbody>
</table>
B.2. Pressurised catastrophic failure (flashing)

B.2.1. Direct source

Table B2.1: ALOHA – Pressurised catastrophic failure (flashing): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>By specifying the mass released</td>
<td>The concentrations at 100m are extremely sensitive at the lower end of the range of release mass values, but they show little sensitivity for the larger release mass values. At this higher end of the range, there is also a difference in behaviour between D5 and F2 conditions; increasing the release mass from 100 to 1000 tonnes gives slightly lower concentrations for D5 conditions, but slightly higher concentrations for F2 conditions. The concentrations at 1000m are very sensitive for all release mass values. For D5 conditions, the relationship is almost linear, but for F2 conditions, the sensitivity is greater at the lower end of the range of release mass values.</td>
</tr>
</tbody>
</table>

Table B2.2: GASTAR – Pressurised catastrophic failure (flashing): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>By specifying the mass released</td>
<td>For both D5 and F2 conditions, the concentrations at 100m are very sensitive. For both D5 and F2 conditions, the concentrations at 1000m are very sensitive for all release mass values; the relationship is almost linear. The sensitivity increases with increasing distance downwind; the concentration/distance plots diverge significantly.</td>
</tr>
<tr>
<td>Initial liquid fraction</td>
<td></td>
<td>The concentrations at both 100 and 1000m are not very sensitive to this parameter, for either D5 or F2 conditions.</td>
</tr>
<tr>
<td>Aspect ratio</td>
<td>By specifying the diameter</td>
<td>For both D5 and F2 conditions, the concentrations at 100m are moderately sensitive to this parameter, while concentrations at 1000m are only slightly sensitive. Although the initial sensitivity drops off around 1000m, the plots diverge again further downwind.</td>
</tr>
<tr>
<td>Mass of entrained air</td>
<td>Also varying the diameter to keep the aspect ratio constant</td>
<td>For both D5 and F2 conditions, the concentrations at 100m are very sensitive to this parameter, while concentrations at 1000m are only slightly sensitive. The initial sensitivity drops off before 1000m downwind.</td>
</tr>
</tbody>
</table>
Table B2.3: HGSYSTEM (HEGABOX) – Pressurised catastrophic failure (flashing): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release amount</td>
<td>By specifying the mass released</td>
<td>Initial concentrations are moderately sensitive to the release mass</td>
</tr>
<tr>
<td>Initial cloud radius</td>
<td></td>
<td>Initial concentrations are very sensitive to the initial cloud radius</td>
</tr>
<tr>
<td>Mass of entrained air</td>
<td></td>
<td>Initial concentrations are very sensitive to the values tested mass of entrained air</td>
</tr>
</tbody>
</table>
### B.2.2. Source term

#### Table B2.4: ACE/DRIFT – Pressurised catastrophic failure (flashing) source term: Sensitivity summary

<table>
<thead>
<tr>
<th>ACE Input / Source Parameter</th>
<th>Run cases</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance properties</td>
<td>Substance</td>
<td>Chlorine</td>
</tr>
<tr>
<td></td>
<td>Phase</td>
<td>Two-phase</td>
</tr>
<tr>
<td>Storage properties</td>
<td>Mass</td>
<td>1 te, 10 te, 100 te</td>
</tr>
<tr>
<td></td>
<td>Temperature</td>
<td>0°C, 15°C, 30°C</td>
</tr>
<tr>
<td></td>
<td>Pressure</td>
<td>Run cases covered by temperature variation (above) and padding (below)</td>
</tr>
<tr>
<td></td>
<td>Enhanced pressure from added gas</td>
<td>+1 bar pad pressure</td>
</tr>
<tr>
<td>Release properties</td>
<td>Initial turbulent velocity</td>
<td>No run cases</td>
</tr>
<tr>
<td></td>
<td>Directional release</td>
<td>Down (default), omni</td>
</tr>
<tr>
<td></td>
<td>Release height</td>
<td>No run cases</td>
</tr>
<tr>
<td>Atmospheric properties</td>
<td>Wind speed and stability</td>
<td>D5, F2</td>
</tr>
<tr>
<td></td>
<td>Roughness length</td>
<td>0.1 m</td>
</tr>
<tr>
<td></td>
<td>Temperature</td>
<td>0°C, 15°C, 30°C</td>
</tr>
<tr>
<td></td>
<td>Relative humidity</td>
<td>No runs</td>
</tr>
<tr>
<td>Other</td>
<td>Rainout</td>
<td>Including rainout, no pool</td>
</tr>
<tr>
<td></td>
<td>Dilution at source</td>
<td>Dilution (by ACE), no dilution</td>
</tr>
</tbody>
</table>
Table B2.5: PHAST – Pressurised catastrophic failure (flashing) source term: Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Substance properties</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Substance</td>
<td>Chlorine</td>
<td></td>
</tr>
<tr>
<td>Phase</td>
<td>Two-Phase</td>
<td></td>
</tr>
<tr>
<td>Mass</td>
<td>10te, 100te, 1000te</td>
<td>Strong dependence on spill mass, distance to 1000 ppm varies as $\sim(mass)^{1/3}$, distance to 100 ppm varies slightly more strongly with $\sim(mass)^{0.4}$</td>
</tr>
<tr>
<td>Temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Distance to 1000 ppm increases slowly in D5 conditions with increasing storage temperature (3% increase over temperature range for 1000 te base case) with a more marked increase (7% increase over temperature range) in F2 conditions. Distance to 100 ppm insensitive in D5 conditions, decreased distance (8% decrease over temperature range) to 100 ppm in F2 conditions</td>
</tr>
<tr>
<td>Pressure</td>
<td>Run cases covered by temperature variation (above) and padding (below)</td>
<td>See above for saturated conditions (storage pressure = saturated vapour pressure) and below for the effect of padding pressure.</td>
</tr>
<tr>
<td>Enhanced pressure from added gas</td>
<td>+1, +2, +3 bar pad pressure</td>
<td>Negligible effect (&lt;0.1% change) on distance to 1000 ppm and 100 ppm for 1000 te base case</td>
</tr>
<tr>
<td><strong>Storage properties</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D2, D5, D10, F2</td>
<td>Strong effect of increased wind speed giving increased distance to 1000 ppm and 100 ppm. F2 gives shorter distance to 1000 ppm than D2, whereas this is reversed for distance to 100 ppm.</td>
</tr>
<tr>
<td>Roughness length</td>
<td>0.001m, 0.01m, 0.1m, 1m</td>
<td>Strong effect on decreased distance to 1000 ppm with increasing roughness length. Opposite behaviour for 100 ppm where distance increases with increasing roughness length.</td>
</tr>
<tr>
<td>Temperature</td>
<td>5°C, 15°C, 30°C</td>
<td>Distance to 1000 ppm and 100 ppm increases slowly in D5 conditions with increasing ambient temperature. The effect of varying ambient temperature is slightly stronger than the effect of varying storage temperature.</td>
</tr>
<tr>
<td>Relative humidity</td>
<td>0%, 50%, 70%, 95%</td>
<td>0%, 50% and 70% relative humidity have weak effect on distances to 1000 ppm and 100 ppm, with a tendency for higher humidity to slightly increase the distances. For 95% relative humidity there is larger effect with an increase of approximately 3% in distance to 1000 ppm over the 70% base case.</td>
</tr>
</tbody>
</table>
B.3. Jet releases

B.3.1. Direct source jet models

Table B3.1: ADMS – Direct jet source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pseudo diameter</td>
<td>Keeping velocity value constant - effectively varying volume (and mass) flow rates</td>
<td>Concentrations are very sensitive over this range of pseudo diameters, for both methane and air, and D5 and F2 conditions. Linear/almost linear dependence.</td>
</tr>
<tr>
<td>Mass flow rate (velocity)</td>
<td>In ADMS, for jet sources, the efflux rate is specified by entering the velocity. Keeping pseudo diameter constant</td>
<td>Concentrations are very sensitive to this parameter, for both methane and air, and D5 and F2 conditions. The sensitivity of the concentrations is not evident until after the initial jet region (concentrations independent of velocity until after the first few metres).</td>
</tr>
<tr>
<td>Release height</td>
<td></td>
<td>Concentrations in the jet regime region and the far field region are not very sensitive to the release height for any of the cases. Concentrations in the near field dispersion (non-jet) region are very sensitive for the air D5 case, moderately sensitive for the methane D5 case, and not very sensitive for the methane F2 case. Note that the plume impacts the ground for the release of air under F2 conditions, so calculations stop</td>
</tr>
<tr>
<td>Release direction</td>
<td>Horizontal /vertical</td>
<td>For the air releases, concentrations are very sensitive in both the near and far field. For the methane releases, concentrations are very sensitive in the near field, but less sensitive in the far field. The sensitivity is apparent from the point of release i.e. concentrations are sensitive to release direction even in the jet regime.</td>
</tr>
<tr>
<td>Averaging time</td>
<td>Generally, concentrations are not very sensitive to the averaging times; there is slightly more sensitivity in F2 conditions in the far field.</td>
<td></td>
</tr>
<tr>
<td>Duration</td>
<td>Tested plume release and puff releases of various durations</td>
<td>There is a large variation in the dose values (but this only scales proportionally to the exposure time)</td>
</tr>
</tbody>
</table>
### Table B3.2: DRIFT – Direct Jet Source: Sensitivity summary

<table>
<thead>
<tr>
<th>DRIFT Input / Source Parameter</th>
<th>Run cases</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source properties</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release rate</td>
<td>2kg/s, 5kg/s, 10kg/s, 20kg/s and 50kg/s</td>
<td>Concentration independent of release rate in the jet dispersion regime (when velocity is much greater than wind speed). At greater distances where the jet has slowed to close to the wind speed then concentration develops a strong dependence on release rate, concentration ( \sim ) (release rate). For downwind directed jets the jet regime covers a greater distance in low wind conditions.</td>
</tr>
<tr>
<td>Release duration</td>
<td>18s, 180s, 1800s and infinite</td>
<td>Concentration independent of release duration at distances where the travel time is much shorter than the release duration. Concentration decreases with decreasing duration at greater distances due to the effects of longitudinal dispersion. Toxic dose depends directly upon release duration.</td>
</tr>
<tr>
<td>Source density</td>
<td>Mw=16,28,71 for gaseous releases 2-phase chlorine (80% liquid, 239K)</td>
<td>Weak dependence for gaseous releases in the jet dispersion regime (when velocity is much greater than wind speed), 2 phase jet shows higher concentration for the same flow rate. Note ppm or mol/mol concentrations include a dependence upon molecular weight of the released substance.</td>
</tr>
<tr>
<td>Release diameter</td>
<td>1mm, 1cm, 5cm, 10cm, 50cm</td>
<td>Strong dependence of concentration on release diameter for the same release rate in the jet dispersion regime (when velocity is much greater than wind speed) with concentration ( \sim ) (release diameter). Beyond the jet regime the concentration becomes independent of release diameter for the same release rate.</td>
</tr>
<tr>
<td>Release height</td>
<td>1m, 10m</td>
<td>Weak dependence of centreline concentration at plume height. Strong dependence of ground level concentration at distances less than the distance of the ground level maximum, subsequently little or no effect.</td>
</tr>
<tr>
<td>Release direction</td>
<td>Horizontal, vertical</td>
<td>Significant reduction in centreline concentration as a function of downwind distance due to the initial vertical motion of the jet. Strong dependence on ground level concentration on direction at distances less than the distance of the ground level maximum, subsequently little or no effect.</td>
</tr>
<tr>
<td>Atmospheric properties</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D5, F2</td>
<td>Concentration independent of wind speed and atmospheric stability in the jet dispersion region (when velocity is much greater than wind speed). At greater distances where the jet has slowed to close to the wind speed then concentration develops a strong dependence on wind speed and stability with F2 giving slower decay with distance.</td>
</tr>
<tr>
<td>Roughness length</td>
<td>0.001m, 0.01m, 0.1m, 1m</td>
<td>Negligible effect on concentration predictions in the jet regime. The effect increases at greater distances with lower roughness giving higher concentrations.</td>
</tr>
<tr>
<td>Temperature</td>
<td>0°C, 15°C, 30°C</td>
<td>Negligible effect on concentration predictions</td>
</tr>
<tr>
<td>Relative humidity</td>
<td>0%, 50%, 70%, 95%</td>
<td>Modelled cases show negligible dependence upon humidity. There is a possible significant effect when condensation in cold clouds leads to an otherwise dense/neutral cloud having a transient buoyant phase.</td>
</tr>
<tr>
<td>Inversion height</td>
<td>F2 50m, 100m, 200m</td>
<td>Negligible effect exception at very low concentrations</td>
</tr>
<tr>
<td>Model input parameter(s)</td>
<td>Notes</td>
<td>Summary of observed sensitivity</td>
</tr>
<tr>
<td>--------------------------</td>
<td>-------</td>
<td>---------------------------------</td>
</tr>
<tr>
<td>Pseudo diameter</td>
<td>Keeping mass flow constant</td>
<td><strong>Gaseous releases</strong>: Concentrations very sensitive to this parameter, with a non-linear relationship. Concentrations more sensitive in the near field. The sensitivities of the jet output parameters (touchdown and jet transition distances) vary between the chlorine and methane cases, and between D5 and F2 conditions — the sensitivity for methane is only seen for larger diameter values, particularly under F2 conditions. <strong>Two-phase release</strong>: Concentrations and jet outputs are very sensitive to this parameter, with non-linear relationships. Concentrations more sensitive in the lower end of the diameter value range, and in the near field. The jet output parameters (touchdown and jet transition distances) are also very sensitive to this parameter.</td>
</tr>
<tr>
<td>Mass flow rate</td>
<td>Keeping pseudo diameter constant</td>
<td><strong>Gaseous releases</strong>: Concentration outputs: sensitivity increases with distance downwind for both methane and chlorine and both D5 and F2 conditions. Greater sensitivity in the methane case. Jet outputs: Touchdown distances only moderately sensitive, but transition distance very sensitive, for both substances and both D5 and F2 conditions. <strong>Two-phase release</strong>: Concentrations and jet outputs are very sensitive to this parameter. The sensitivity of the concentrations is not evident until after jet transition point.</td>
</tr>
<tr>
<td>Diameter and mass flow rate</td>
<td>Effectively varying the storage pressure</td>
<td><strong>Gaseous releases</strong>: Very sensitive for both methane and chlorine, and both D5 and F2 conditions. Greater sensitivity in the chlorine case. <strong>Two-phase release</strong>: The concentrations are moderately sensitive to this combination of parameters, but jet parameters not very sensitive.</td>
</tr>
<tr>
<td>Release height</td>
<td>Horizontal /vertical</td>
<td><strong>Gaseous releases</strong> Jet outputs are very sensitive to the release height for both methane and chlorine and both D5 and F2 conditions. Concentrations only moderately sensitive <strong>Two-phase release</strong>: Sensitivity of concentrations is greater in the near field, and jet outputs very sensitive. Also, the concentration /distance plots converge downwind. Sensitivity dominated by source term effects</td>
</tr>
<tr>
<td>Aerosol liquid fraction</td>
<td>Two-phase release only</td>
<td>Concentrations show significant sensitivity in the near field dispersion (non-jet) regime, but there is little dependence on liquid aerosol fraction further downwind. The jet touchdown and the transition distance show significant sensitivity; the latter being more sensitive for D5 conditions.</td>
</tr>
<tr>
<td>Averaging time</td>
<td></td>
<td>Averaging time – the results are all identical for some cases (two-phase and gaseous chlorine releases under F2 conditions). For other cases, the results diverge after the jet transition point.</td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td></td>
<td>Jet outputs show no sensitivity to the stability /wind speed categories tested. Concentrations are very sensitive to this</td>
</tr>
</tbody>
</table>
Table B3.4: SLAB – Direct jet source. Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release rate</td>
<td></td>
<td>Concentrations are very sensitive to this parameter, for all cases. There is a similar degree of sensitivity for all cases, and in both the near- and far-field.</td>
</tr>
<tr>
<td>Diameter</td>
<td>Input as the jet area</td>
<td>Concentrations are not sensitive to this parameter, for any of the cases.</td>
</tr>
<tr>
<td>Diameter and release rate</td>
<td></td>
<td>The concentrations are moderately sensitive to this combination of parameters for chlorine under D5 conditions, and very sensitive for chlorine under F2, and methane under both D5 and F2 conditions.</td>
</tr>
<tr>
<td>Release direction</td>
<td>Horizontal /vertical</td>
<td>Concentrations are not sensitive to this parameter, for any of the cases, in neither the near- nor the far-field</td>
</tr>
<tr>
<td>Release height</td>
<td></td>
<td>Concentrations are not very sensitive to this parameter, for any of the cases. There is slightly more sensitivity in the near-field results</td>
</tr>
</tbody>
</table>
### B.3.2. Source term jet models

#### Table B3.5: ALOHA – Source term jet source: Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Orifice diameter</td>
<td>Keeping the storage pressure constant</td>
<td>Gaseous jet: Concentrations are extremely sensitive to this parameter, with a linear/almost linear relationship, for both methane and chlorine, and for D5 and F2 conditions.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Two-phase jet: Concentrations are extremely sensitive to this parameter for both D5 and F2 conditions. Less sensitivity towards the smaller diameter values.</td>
</tr>
<tr>
<td>Mass flow rate (gaseous jets only)</td>
<td>Set by varying the storage pressure. Keeping diameter constant</td>
<td>Concentrations are very sensitive, with a linear/almost linear relationship, for both methane and chlorine and for D5 and F2 conditions.</td>
</tr>
<tr>
<td>Storage temperature (two-phase jets only)</td>
<td></td>
<td>Concentrations are very sensitive, with a linear/almost linear relationship, for D5 and F2 conditions.</td>
</tr>
<tr>
<td>Orifice type</td>
<td>Circular hole / Pipe or valve</td>
<td>Concentrations are not at all sensitive to this parameter for gaseous jets, but very sensitive for two-phase jets. This is an known feature of ALOHA: The online User Guide explains that “In [two phase flow] release cases, your choice of opening type can have an important effect on ALOHA's release rate computations...The type of opening does not make a difference in pure gas or unpressurized liquid releases”</td>
</tr>
</tbody>
</table>
Table B3.6: DRIFT – Jet Source (with expansion): Sensitivity summary

<table>
<thead>
<tr>
<th>DRIFT Input / Source Parameter</th>
<th>Run cases</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release rate</td>
<td>2kg/s, 5kg/s, 10kg/s, 20kg/s and 50kg/s</td>
<td>Differs from unexpanded source. Expansion, even when from the same hole size, introduces a strong dependence of concentration upon release rate even in the jet regime.</td>
</tr>
<tr>
<td>Release duration</td>
<td>18s, 180s, 1800s and infinite</td>
<td>As for unexpanded jet source</td>
</tr>
<tr>
<td>Source density</td>
<td>Mw=16,28,71 for gaseous releases 2-phase chlorine (flashing liquid)</td>
<td>Similar effect of density to unexpanded jet source, except that the concentration from the 2-phase flashing release decays significantly more slowly with distance in the jet regime - due flashing leading to a large expanded jet diameter in this case. At greater distances, in the passive limit, the 2-phase chlorine concentrations asymptote towards the gaseous (Mw=71) results.</td>
</tr>
<tr>
<td>Release diameter</td>
<td>1mm, 1cm, 5cm, 10cm, 50cm</td>
<td>Differs from unexpanded source. In the case that the same release rate occurs through different release diameters then expansion can lead to a similar expanded diameter and a weak dependence upon release diameter. In the case that the release rate per unit area is the same (corresponding to the same upstream conditions) then there is a strong dependence upon release diameter with concentration ~ (release diameter) but decaying more slowly than the unexpanded case.</td>
</tr>
<tr>
<td>Release height</td>
<td>No runs</td>
<td>See unexpanded jet source</td>
</tr>
<tr>
<td>Release direction</td>
<td>No runs</td>
<td>See unexpanded jet source</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.6 (default for liquid), 0.8 (default for gas), 1</td>
<td>Weak dependence on discharge coefficient for gaseous releases. Stronger dependence for flashing liquid releases with concentration ~ (discharge coefficient)</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D5, F2</td>
<td>As for unexpanded jet source</td>
</tr>
<tr>
<td>Roughness length</td>
<td>No runs</td>
<td>See unexpanded jet source</td>
</tr>
<tr>
<td>Temperature</td>
<td>15°C , 30°C</td>
<td>As for unexpanded jet source</td>
</tr>
<tr>
<td>Relative humidity</td>
<td>No runs</td>
<td>See unexpanded jet source</td>
</tr>
<tr>
<td>Inversion height</td>
<td>No runs</td>
<td>See unexpanded jet source</td>
</tr>
</tbody>
</table>
### Table B3.7: HGSYSTEM (AEROPLUME) – Jet Source (with expansion): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
</table>
| Release rate           | Varying the orifice diameter and the mass flow rate | Gaseous jet: For both methane and chlorine, the jet touchdown distance is moderately sensitive. The transition point and the concentrations are very sensitive to this parameter, for both D5 and F2 conditions.  
Two phase jets: Two-phase jets: The jet touchdown distance, transition point and concentrations are all very sensitive to this parameter. |
| Release duration       | None of the outputs are sensitive to this parameter; results are identical |
| Discharge coefficient  | Two-phase release only | The jet touchdown distance is not at all sensitive to this parameter. The transition point is not at all sensitive in D5 conditions, but moderately sensitive in F2 conditions. The concentrations are moderately sensitive to this parameter. |
| Release direction      | Gaseous jets: No clear jet touchdown occurs for the vertical jet, for either methane or chlorine, for D5 or F2 conditions. Concentrations are very sensitive to this parameter, for both D5 and F2 conditions.  
Two-phase jets: The jet touchdown distance and concentrations are very sensitive to this parameter; the transition point is moderately sensitive. |
| Release height         | Gaseous jets: For chlorine, there is no clear jet touchdown for the 10m high release, for D5 or F2 conditions. For methane, the touchdown distance is very sensitive to the release height, but the jet transition point is only slightly sensitive. Concentrations of both methane and chlorine are very sensitive to the release height.  
Two-phase jets: The jet touchdown distance and the concentrations are very sensitive to this parameter for both D5 and F2 conditions. Concentrations are much more sensitive in the near field than in the far field. The transition point is very sensitive for D5 conditions, but not sensitive for F2 conditions. |
| Reservoir pressure     | Gaseous jet: The jet touchdown distances are only slightly sensitive for methane, and moderately sensitive for chlorine. The transition point and concentrations are very sensitive.  
Two phase jets: The jet touchdown distance and transition point are only slightly sensitive. Concentrations are moderately sensitive. |
| Reservoir temperature  | Two-phase release only | The jet touchdown distance is only slightly sensitive to this parameter, while the transition point and concentrations are moderately sensitive. |
### Table B3.8: PHAST – Source term (Expanded) Jet Source: Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Release diameter</td>
<td>1mm, 1cm, 5cm, 10cm</td>
<td>Methane Gas, Chlorine Gas, 2-Phase Chlorine</td>
<td>Strong</td>
<td>Release rate increases with square of release diameter. Strong dependence of concentration on release diameter. Generally for the same release conditions distances to fixed concentrations scale approximately in direct proportion with release diameter, i.e. according to the square root of the release rate.</td>
</tr>
<tr>
<td>Storage temperature</td>
<td>5°C, 15°C and 30°C</td>
<td>Methane Gas, 2-Phase Chlorine</td>
<td>Weak</td>
<td>Release rate decreases with increased storage temperature. Distance to LFL scales in proportion with the square root of the release rate. Distances to 10% LFL at a height of 1m deviate from this proportionality – results here may be affected by the upward trajectory of the buoyant jet.</td>
</tr>
<tr>
<td>Pad pressure</td>
<td>Sat, +1bar, +2bar, +3bar</td>
<td>2-Phase Chlorine</td>
<td>Moderate</td>
<td>For saturated storage conditions storage pressure increases with storage temperature according to the vapour pressure. Liquid release rate scales with the square root of storage pressure (gauge). Distances to fixed concentration increased – scaling with approximately with the square root of release rate, i.e. as the ( (\text{storage pressure})^{1/4} ).</td>
</tr>
<tr>
<td>Release phase</td>
<td>Liquid, 2-phase</td>
<td>2-Phase Chlorine</td>
<td>Strong</td>
<td>Release rate significantly reduced (by approx. factor of 3) by flashing prior to release. Distance to fixed concentration scales in proportion to the square root of the release rate giving a significant reduction (2-phase release distances approx. 0.6 x liquid release distances)</td>
</tr>
<tr>
<td>Discharge coefficient</td>
<td>0.6, 0.8, 1</td>
<td>Methane Gas, 2-Phase Chlorine</td>
<td>Moderate</td>
<td>Release rate and expanded jet diameter increases in direct proportion to discharge coefficient. Distances to fixed concentrations vary ( \sim (\text{discharge coefficient})^{1/2} ).</td>
</tr>
<tr>
<td>Release elevation</td>
<td>1m, 10m</td>
<td>Methane Gas, Air, Chlorine Gas</td>
<td>Weak</td>
<td>Negligible effect before touchdown. Large differences (up to a factor of 4) in centreline concentration at intermediate distances. Little difference in far-field where the plume has reached the ground.</td>
</tr>
<tr>
<td>Release direction</td>
<td>Horizontal, up, down</td>
<td>Methane Gas</td>
<td>Strong, particularly in</td>
<td>Large difference in centreline concentration as a function of horizontal distance. Downwards and impinged releases give significantly higher centreline concentrations than horizontal</td>
</tr>
<tr>
<td>PHAST Input / Source Parameter</td>
<td>Run cases</td>
<td>Substance</td>
<td>Effect</td>
<td>Summary of Observed Sensitivity</td>
</tr>
<tr>
<td>---------------------------------</td>
<td>-----------</td>
<td>-----------------</td>
<td>------------------------------------------</td>
<td>--------------------------------------------------------------------------------------------------</td>
</tr>
<tr>
<td></td>
<td>impinged</td>
<td></td>
<td></td>
<td>As for methane, except that results for horizontal, down and impinged releases converge at approximately 2000ppm. Vertical releases give significantly lower centreline concentrations at all modelled distances.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Air</td>
<td>near-field</td>
<td>As for methane, except that results for horizontal, down and impinged releases converge at approximately 1000ppm. Vertical releases give significantly lower centreline concentrations at all modelled distances.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Chlorine Gas</td>
<td></td>
<td>As for chlorine gas, except that results for horizontal, down and impinged releases converge sooner, at approximately 10000ppm.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2-Phase Chlorine</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D2, D5, D10, F2</td>
<td>Methane Gas</td>
<td>Weak in near-field (jet), Strong in far-field (passive)</td>
<td>Increased wind speed leads to small reduction in distance to LFL. Distance to 10% LFL increases with wind speed – this might be related to distances being at a receiver height of 1m. D5 and F2 give almost centreline concentrations down to 10,000 ppm, between 10,000 ppm and 600 ppm F2 gives lower concentrations, subsequently dilution is greater in D5 than F2.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Air</td>
<td></td>
<td>D5 and F2 give almost identical centreline concentrations down to 5000 ppm, subsequently dilution is greater in D5 than F2.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Chlorine Gas</td>
<td></td>
<td>D5 and F2 give almost identical centreline concentrations down to 3000 ppm, subsequently dilution is greater in D5 than F2.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2-Phase Chlorine</td>
<td></td>
<td>D5 and F2 give almost identical centreline concentrations down to 10000 ppm, subsequently dilution is greater in D5 than F2.</td>
</tr>
<tr>
<td>Atmospheric properties</td>
<td>Roughness length</td>
<td>Methane Gas</td>
<td>Weak in near-field (jet), Strong in far-field (dense and passive)</td>
<td>Increased roughness gives slightly decreased distance to LFL and more marked decrease to 10% LFL.</td>
</tr>
<tr>
<td></td>
<td>0.001m, 0.01m, 0.1m, 1m</td>
<td>2-Phase Chlorine</td>
<td></td>
<td>Increased roughness gives rise to a marked reduction in distances to 1000ppm and lower concentrations.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Methane Gas</td>
<td>Weak</td>
<td>Distance to LFL and 10% LFL increase weakly with increased ambient temperature – this might be related to distances being at a receiver height of 1m. Higher ambient temperature gives a small reduction in distances to a given concentration.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2-Phase Chlorine</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Methane Gas</td>
<td>Weak</td>
<td>Negligible dependence of distance to LFL and 10% LFL upon relative humidity. Exception is 95% relative humidity which leads to a 13% reduction in distance to 10% LFL in D5 conditions.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2-Phase Chlorine</td>
<td></td>
<td>Reduced humidity reduces distance to concentration levels by a maximum of approx. 10% at 1000ppm. Smaller differences at lower concentrations.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
# B.4. Spray releases

## Table B4.1: DRIFT – Spray release: Sensitivity summary

<table>
<thead>
<tr>
<th>DRIFT Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Release diameter</strong></td>
<td>1mm, 1cm, 10cm</td>
<td>m-Xylene</td>
<td>Strong</td>
<td>The initial droplet size is independent of release diameter. Increasing release diameter increases flow rate and distance to LFL and 10% LFL. The effect of deposition is greater for greater travel distances (i.e. greater for distance to 10% LFL and for larger release diameter)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Storage temperature</strong></td>
<td>15°C, 30°C and 100°C</td>
<td>m-Xylene</td>
<td>Negligible</td>
<td>The initial droplet size for water is larger than for m-xylene – presumably due to the higher surface tension of water. The same dispersion trends as m-xylene are observed for water, except there is a greater effect due to deposition which is probably associated with the larger droplet sizes.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Storage pressure</strong></td>
<td>5 barg, 10 barg, 20 barg, 50 barg, 100 barg</td>
<td>m-Xylene</td>
<td>Strong</td>
<td>The effect of deposition is most marked at lower pressure where the initial droplet sizes are larger. For example distances to 10% LFL is decreased by approx. a factor of 3 at 5 barg, whereas for 100 barg there is only a 20% change.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>The same trend is observed for water, except the effect of deposition is more marked at low pressure, e.g. a factor of 8 difference in distance to 10% LFL equivalent at low pressure.</td>
</tr>
<tr>
<td><strong>Release elevation</strong></td>
<td>1 m, 10 m</td>
<td>m-Xylene</td>
<td>Weak</td>
<td>Increased elevation is predicted to produce little change to the distances to LFL and 10% LFL (and equivalents for water). The effect of changing elevation is less than the effect of switching off deposition.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Release direction</strong></td>
<td>Horizontal, vertical</td>
<td>m-Xylene</td>
<td>Strong</td>
<td>Vertically orienting the release leads to a shortening of the distances to LFL and 10% LFL (and equivalents for water). The effect of changing elevation is more than the effect of switching off deposition.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Wind speed and stability</strong></td>
<td>D1, D2, D5, D7, D10, D20 F2</td>
<td>m-Xylene</td>
<td>Strong</td>
<td>Increasing wind speed leads to shortening of the distances to LFL and 10% LFL. The effect being greatest for 10% LFL and high winds. The effect of increased stability (F2) is to lengthen the distance to 10% LFL compared with the neutral equivalent (D5), whereas there is negligible difference for the LFL distance.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>The behaviour for water is similar to m-xylene, except that the higher deposition at lower winds leads to a lesser change between distances in high and low wind speeds.</td>
</tr>
<tr>
<td><strong>Temperature</strong></td>
<td>5°C, 15°C and 30°C</td>
<td>m-Xylene</td>
<td>Weak</td>
<td>Increased ambient temperature slightly increases the distances to LFL and 10% LFL. This is a weak effect, but stronger than the effect of storage temperature.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Note: DRIFT runs based upon flow rates and initial droplet sizes from PHAST. For comparison purposes for water the concentration equivalent m-xylene LFL is used: LFL equivalent = (m-xylene LFL) * (Molecular weight xylene/Molecular weight water)
Table B4.2: PHAST – Spray release: Sensitivity summary

<table>
<thead>
<tr>
<th>PHAST Input / Source Parameter</th>
<th>Run cases</th>
<th>Substance</th>
<th>Effect</th>
<th>Summary of Observed Sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Source properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Release diameter</td>
<td>1mm, 1cm, 10cm</td>
<td>Xylene</td>
<td>Strong</td>
<td>Droplet diameter independent of release diameter. Rainout fraction increases with increasing release diameter. Distance to LFL and 10% LFL depends strongly upon the release diameter.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td>Strong</td>
<td>Droplet diameter independent of release diameter. Rainout fraction increases with increasing release diameter. Water droplets larger than xylene droplets for the same flow rate.</td>
</tr>
<tr>
<td>Storage temperature</td>
<td>15°C, 30°C and 100°C</td>
<td>Xylene</td>
<td>Moderate</td>
<td>Release rate is only a very weak function of storage temperature. Rainout fraction and initial droplet size decreases with increased temperature. 0.45 rainout fraction for 15°C and zero rainout for 100°C. Distance to LFL insensitive to storage temperature. Distance to 10% LFL significantly increased at 100°C.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>Rainout fraction and initial droplet size decreases with increased temperature. Rainout fraction varies between 0.8 and 0.71.</td>
</tr>
<tr>
<td>Storage pressure</td>
<td>5barg, 10barg, 20barg, 50barg, 100barg</td>
<td>Xylene</td>
<td>Strong</td>
<td>Release rate varies with square root of storage pressure (gauge). Droplet diameter and rainout fraction decreases with increasing storage pressure. Rainout fraction varies between 0.94 for 5 barg to zero for 100 barg. Droplet diameters vary from 225 µm for 5 barg to 11 µm for 100 barg. Increased pressure leads to a significant increase in distance to LFL and 10% LFL.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>Release rate varies with square root of storage pressure (gauge). Droplet diameter and rainout fraction decreases with increasing storage pressure. Rainout fraction varies between 0.99 for 5 barg to 0.8 for 100 barg. Droplet diameters vary from 583 µm for 5 barg to 29 µm for 100 barg.</td>
</tr>
<tr>
<td>Release elevation</td>
<td>1m, 10m</td>
<td>Xylene</td>
<td>Strong</td>
<td>Results based upon 100barg release. No rainout predicted. 10% LFL distance decreased in F2 conditions. No results available at 1m receptor height for other cases.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>Results based upon 100barg release. Rainout decreased from 0.85 for 1m elevation to 0.52 for 10m elevation in F2. No rainout in D5 conditions.</td>
</tr>
<tr>
<td>Release direction</td>
<td>Horizontal, vertical</td>
<td>Xylene</td>
<td>Strong</td>
<td>Rainout fraction decreased from 0.45 for horizontal to zero for vertical in D5 conditions and from 0.65 to zero in F2 conditions. No LFL or 10% LFL distances available at 1m height.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>Rainout fraction decreased from 0.8 for horizontal to zero for vertical in D5 conditions and from 0.8 to 0.52 in F2 conditions</td>
</tr>
<tr>
<td><strong>Atmospheric properties</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Wind speed and stability</td>
<td>D2, D5, D10, F2</td>
<td>Xylene</td>
<td>Strong</td>
<td>Rainout decreases from 0.61 in D1 conditions to zero D10. Distance to LFL decreases with increased wind speed. Distance to 10% LFL increases and then decreases with speed,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Water</td>
<td></td>
<td>Rainout decreases from 0.84 in D1 conditions to zero D20.</td>
</tr>
</tbody>
</table>
## B.5. Fire plume (warehouse)

### Table B5.1: ADMS – Fire plume (warehouse): Sensitivity summary for enclosed, high temperature case

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td></td>
<td>The maximum plume height is moderately sensitive to this parameter, for both D5 and F2 conditions. (Ground level) concentrations at both 100 m and 1000m downwind are very sensitive for F2 conditions. For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000m only moderately sensitive. Negative non-linear relationship; results are more sensitive at the lower end of the temperature range.</td>
</tr>
<tr>
<td>Velocity</td>
<td></td>
<td>The maximum plume height is moderately sensitive to this parameter, for both D5 and F2 conditions. Concentrations at both 100 m and 1000m downwind are very sensitive for F2 conditions. For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000m only moderately sensitive. Negative non-linear relationship; results are more sensitive at the lower end of the range.</td>
</tr>
<tr>
<td>Source diameter</td>
<td></td>
<td>Concentrations are extremely sensitive for diameters between 0.5 and 2m, and still very sensitive towards other larger diameter values, for F2 and D5 conditions.</td>
</tr>
<tr>
<td>No of openings (sources)</td>
<td></td>
<td>Concentrations at both 100 m and 1000m downwind are very sensitive for F2 conditions. For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000m only moderately sensitive. Concentrations are more sensitive at lower end of range (fewer openings).</td>
</tr>
<tr>
<td>Building downwash</td>
<td>Building downwash included in base case</td>
<td>Concentrations at 100 m are extremely sensitive for both D5 and F2 conditions. Concentrations at 1000 m are moderately sensitive for F2 conditions, but not sensitive for D5 conditions</td>
</tr>
<tr>
<td>Building alignment</td>
<td></td>
<td>Concentrations at 100m are moderately sensitive, and those at 1000m not sensitive, for both D5 and F2 conditions</td>
</tr>
<tr>
<td>Wind speed</td>
<td></td>
<td>The maximum plume height is very sensitive to this parameter, for both D5 and F2 conditions. Concentrations at both 100m and 1000m, and for D5 and F2 conditions, are very sensitive to the wind speed.</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>To assess the effect on dry deposition rates</td>
<td>Dry deposition rates at both 100m and 1000m, and for D5 and F2 conditions, are very sensitive to the particle diameter</td>
</tr>
<tr>
<td>Stability and wind speed</td>
<td>D5, F2, D15</td>
<td>All model outputs are very sensitive to the stability and wind speed. The maximum plume height is greatest in F2 conditions, and lowest in D15 conditions. The ground level concentrations, correspondingly, are lowest in F2 conditions, and greatest in D15 conditions.</td>
</tr>
</tbody>
</table>
### Table B5.2: ADMS - Fire plume (warehouse). Sensitivity summary for enclosed, low temperature case

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature</td>
<td>Concentrations at both 100 m and 1000 m downwind are moderately sensitive for D5 conditions. For F2 conditions, concentrations at 100 m are very sensitive, and those at 1000 m only moderately sensitive. For D5, almost linear negative relationship; for F2, non-linear, with sharper decrease at lower end of parameter range.</td>
<td></td>
</tr>
<tr>
<td>Velocity</td>
<td>Concentrations at both 100 m and 1000 m downwind are very sensitive for F2 conditions. For D5 conditions, concentrations at 100 m are moderately sensitive, and those at 1000 m not sensitive. For D5, almost linear negative relationship; for F2, non-linear, with sharper decrease at lower end of parameter range.</td>
<td></td>
</tr>
<tr>
<td>Source diameter</td>
<td>For D5 conditions, concentrations at both 100 m and 1000 m downwind are moderately sensitive. For F2 conditions, concentrations at both 100 m and 1000 m downwind are very sensitive. For D5, almost linear negative relationship; for F2, non-linear, with sharper decrease at lower end of parameter range.</td>
<td></td>
</tr>
<tr>
<td>No of openings (sources)</td>
<td>For D5 conditions, concentrations at 100 m are moderately sensitive, while for F2 conditions they are very sensitive. Concentrations at 1000 m are not sensitive for D5 or F2 conditions. Increasing the number of openings increases the concentrations, but not a linear dependency; the concentrations are more sensitive at the lower end of the range, particularly to increasing from one to two openings.</td>
<td></td>
</tr>
<tr>
<td>Building downwash</td>
<td>Building downwash included in base case</td>
<td>Concentrations are not sensitive both 100 m and 1000 m downwind for D5 conditions, and 1000 m downwind for F2 conditions. Concentrations at 100 m are, however, very sensitive for F2 conditions.</td>
</tr>
<tr>
<td>Building alignment</td>
<td>For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000 m are moderately sensitive. For F2 conditions, the inverse is true, with concentrations at 100 m moderately sensitive, and those at 1000 m very sensitive.</td>
<td></td>
</tr>
<tr>
<td>Wind speed</td>
<td>For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000 m are moderately sensitive. For F2 conditions, concentrations at both 100 m and 1000 m are very sensitive to the wind speed. Very non-linear relationship; dramatic increase in concentrations between 1 and 2 m/s (5 m/s for F2 conditions), and then a steady decrease after this.</td>
<td></td>
</tr>
<tr>
<td>Particle diameter</td>
<td>To assess the effect on dry deposition rates</td>
<td>Dry deposition rates at both 100 m and 1000 m, and for D5 and F2 conditions are very sensitive to the particle diameter, and</td>
</tr>
</tbody>
</table>
Table B5.3: HOTSPOT – Fire plume (warehouse) Cases (a) and (b): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Height</td>
<td>Varied in Case (a)</td>
<td>Concentrations at both 100 m and 1000m downwind are not very sensitive to this parameter</td>
</tr>
<tr>
<td></td>
<td>The ‘elevation of burning debris’</td>
<td></td>
</tr>
<tr>
<td>Radius</td>
<td>Varied in Case (a)</td>
<td>Concentrations are very sensitive to this parameter, particularly at 100m, showing an</td>
</tr>
<tr>
<td></td>
<td>The effective radius of the fire</td>
<td>approximately linear, negative relationship.</td>
</tr>
<tr>
<td>Cloud top</td>
<td>Varied in Case (a)</td>
<td>Concentrations are very sensitive at 100m and moderately sensitive at 1000m. As expected, the</td>
</tr>
<tr>
<td></td>
<td>The cloud top of the plume</td>
<td>higher the cloud top, the lower the impact.</td>
</tr>
<tr>
<td>Heat emission rate</td>
<td>Varied in Case (b)</td>
<td>Concentrations are very sensitive at both 100 m and 1000m, and more so at the lower end of the</td>
</tr>
<tr>
<td></td>
<td></td>
<td>range of values.</td>
</tr>
</tbody>
</table>
### B.6. Fire plume (outside burning pool)

**Table B6.1: ADMS – Fire plume (outside burning pool): Sensitivity summary**

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Temperature</strong></td>
<td></td>
<td>The maximum plume height is moderately sensitive to this parameter, for both D5 and F2 conditions. The (ground level) concentrations are very sensitive both 100m and 1000m downwind, for both D5 and F2 conditions. Non-linear relationship, with sharper decrease at lower end of parameter range.</td>
</tr>
<tr>
<td><strong>Velocity</strong></td>
<td></td>
<td>The maximum plume height is moderately sensitive to this parameter, for both D5 and F2 conditions. The concentrations are very sensitive both 100m and 1000m downwind, for both D5 and F2 conditions. Non-linear relationship, with sharper decrease at lower end of parameter range.</td>
</tr>
<tr>
<td><strong>Source diameter</strong></td>
<td>Equivalent areas: 3, 79, 707, 1963 m²</td>
<td>The maximum plume height is very sensitive to this parameter, for both D5 and F2 conditions. The concentrations are very sensitive both 100m and 1000m downwind, for both D5 and F2 conditions. Non-linear relationship, with sharper decrease at lower end of parameter range.</td>
</tr>
<tr>
<td><strong>Source height</strong></td>
<td></td>
<td>The maximum plume height is not sensitive to this parameter, for either or D5 and F2 conditions. The concentrations are very sensitive at 100m downwind and moderately sensitive at 1000m, for both D5 and F2 conditions. Almost linear, negative relationship.</td>
</tr>
<tr>
<td><strong>Stability and wind speed</strong></td>
<td>D5, F2, D15</td>
<td>The maximum plume height and the concentrations 100m downwind are very sensitive to the stability and wind speed, and the concentrations 1000m downwind are moderately sensitive. The maximum plume height is greatest in F2 conditions, and lowest in D15 conditions. The ground level concentrations, correspondingly, are lowest in F2 conditions, and greatest in D15 conditions.</td>
</tr>
</tbody>
</table>
### Table B6.2: ALOHA – Fire plume (outside burning pool): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pool area</td>
<td>Note: the observed sensitivities apply to all stability conditions tested (D5, F2 and D15). All outputs show very little sensitivity to the stability.</td>
<td>The flame length, burn rate and total amount burned are very sensitive. The burn duration is not at all sensitive (no variation at all)</td>
</tr>
<tr>
<td>Pool depth</td>
<td></td>
<td>The burn duration, burn rate and total amount burned are very sensitive. The burn rate is particularly sensitive to depths between 1 and 5cm. The flame length is not sensitive (no variation at all).</td>
</tr>
<tr>
<td>Initial pool temperature</td>
<td></td>
<td>None of the four output parameters are very sensitive to this range of initial pool temperatures. The most sensitive output is the burn rate, although this is minimal.</td>
</tr>
</tbody>
</table>

### Table B6.3: HOTSPOT – Fire plume (outside burning pool): Sensitivity summary

<table>
<thead>
<tr>
<th>Model parameter varied</th>
<th>Notes</th>
<th>Summary of observed sensitivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Radius</td>
<td>The effective radius of the fire</td>
<td>The concentrations are moderately sensitive both 100m and 1000m downwind. The sensitivity becomes much greater further downwind</td>
</tr>
<tr>
<td>Fuel volume</td>
<td>This is the total amount of fuel burned in the fire</td>
<td>The concentrations are extremely sensitive both 100m and 1000m downwind. Increasing the fuel volume decreases the impact.</td>
</tr>
<tr>
<td>Burn duration</td>
<td></td>
<td>The concentrations are very sensitive both 100m and 1000m downwind. The sensitivity becomes much greater further downwind</td>
</tr>
<tr>
<td>Heat of combustion</td>
<td></td>
<td>The concentrations are very sensitive both 100m and 1000m downwind. The sensitivity becomes much greater further downwind</td>
</tr>
</tbody>
</table>