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 A1.1a: ADMS – Direct pool source: Key fixed parameters and assumptions

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

Table A1.1b: ADMS – Direct pool source: Parameters varied

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

Table A1.2a DEGADIS – Direct pool source: Key fixed parameters and assumptions

Parameter	Values used	Notes
Source type	Ground-level, low initial momentum (non-jet) release	
Substances modelled	LNG, chlorine	

Table A1.2b: DEGADIS – Direct pool source: Parameters varied

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass flow rate	kg/s	2, 10, 50	
Dimensions of pool	Pool radius	m	1, 5, 10	

Table A1.3a DRIFT – Direct pool source: Key fixed parameters and assumptions

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

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

General parameter	Model input parameter(s)	Units	Values	Notes
Dimensions of pool	Source Diameter	m	2, 5, 10, 20	
Release amount	Release Rate	kg/s	2, 5, 10, 20, 50	

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

Parameter	Values used	Notes
Release type	'Continuous'	
Averaging time	10 minutes	
Duration	Continuous	
Substances modelled	Methane (buoyant) Ethylene (neutrally buoyant) Chlorine (dense)	

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

General parameter	Model input parameter(s)	Units	Values	Notes
Dimensions of pool	Initial plume width	m	2, 5, 10, 20	
Release amount	Mass flux	kg/s	2, 5, 10, 20, 50	
Emission temperature		K	Methane: 111.7, 116.7, 121.7 Ethylene: 169.4, 174.4, 179.4 Chlorine: 238.7, 243.7, 248.7	Equivalent to: Boiling point (bp), bp + 5 , bp + 10

Table A1.5a: SLAB – Direct pool source: Key fixed parameters and assumptions

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

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

General parameter	Model input parameter(s)	Units	Values	Notes
Dimensions of pool	Area source	m^2	3.1, 19.6, 78.5, 314	Modelled as a square area source. Equivalent diameters: 2, 5 , 10, 20m
Release amount	Mass flux from pool	kg/s	2, 5, 10, 20, 50	

A.1.2 Bunded pool source

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

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

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

General parameter	Model input parameter(s)	Units	Values	Notes
Dimensions of pool	Diameter	m	2, 4, 5, 8, 10 (methane) 4,8,10,16,20 (pentane)	
Release amount	Mass flux	tonnes	1, 10, 100	
Initial liquid temperature		°C	-161.6, -162, -165, -170, -180	Varied for methane only For pentane, set to be the same as the base case air and ground temperature (15 °C)
Air temperature		°C	5, 15, 30	
Wind speed		m/s	1, 2, 5, 10 , 20	

Table A1.7a: GASP/DRIFT – Bunded pool source: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties (SPI files source)
Surface type	Land	
Substrate type	Concrete	Using inbuilt substrate properties
Release type (GASP)	Instantaneous	
Pool geometry	Circular	Inbuilt assumption in GASP
Initial pool radius	Set equal to the bund radius	
Initial ground temperature	Equal to the air temperature	Inbuilt assumption in GASP
Pool spreading constraints	Bunded	
Pool surface roughness length	0.23 mm	GASP default
Heat transfer mode	Perfect thermal contact, temperature varying substrate	GASP default
Thermodynamic options	Calculated pool temperature, 3-dimension conduction from ground (true), convection from atmosphere (true)	GASP defaults
Additional heat flux into pool	0 kW/m^2	GASP default
Release type (DRIFT)	Time Varying Release	DRIFT default
Include Dilution Over Pool (DRIFT)	True	DRIFT default

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

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

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

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) Pentane (non-cryogenic)	
Substrate type	‘concrete’ option	
Bund information	‘Dike present’ option	Composition same as substrate (concrete)

Table A1.8b: HGSYSTEM (LPOOL) – Bunded pool source: Parameters varied

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Volume flow rate	m^3/s	2, 20 , 200	Released over one second
Initial liquid temperature - methane		°C	-161, -170, -180	
Initial liquid temperature - pentane		°C	0, 15, 30	
Dimensions of pool	Radius	m	2, 5, 10	
Air temperature		°C	5, 15, 30	
Wind speed		m/s	1, 2, 5, 10 , 20	5m/s for D5 conditions, 2m/s for F2 conditions

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

Parameter	Values used	Notes
Source configuration	'Dam break' (instantaneous)	
Bund information	'Bund present' option	Bund height set to be equivalent to a bund capacity that is 25% larger than the liquid volume level
Substances modelled	Methane (cryogenic) Butane (non-cryogenic)	
Substrate type	'Homogeneous/impermeable'	
Base case 'A' (methane only)	Thermal properties set to represent 'Standard concrete' substrate and bund as the base case	Normal situation, to test most parameters
Base case 'B' (methane only)	Set thermal properties of substrate and bund to represent an insulating bund	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

Table A1.9b: LSMS – Bunded pool source: Parameters varied

General parameter	Model input parameter(s)	Units	Values	Notes
Initial mass in pool – methane (Base Case 'A')	Vertical size	m	0.03, 0.30, 3.0	Varied by varying the vertical size of the liquid and the bund dimensions (and keeping the pool and bund radius constant at 5m)
	Bund depth		0.04, 0.4, 3.8	
Initial mass in pool- butane (Base Case 'A')	Vertical size	m	0.022, 0.22, 2.2	Equivalent to 1, 10,100 tonnes
	Bund depth		0.027, 0.27, 2.7	
Initial liquid temperature – methane (Base Case 'A')		K	111.67, 111.15, 108.15, 103.15, 93.15	111.67 K is the value obtained when the 'set to boiling' option is checked
Initial liquid temperature – butane (Base Case 'A')		K	273.12, 283.12, 288.12, 293.12, 303.12	The substrate temperature was also set to these values, as this represents an ambient storage temperature
Pool and bund radius – methane (Base Case 'A')	Pool radius	m	2, 4, 5, 8, 10	Keeping released mass constant – therefore varying the liquid and bund depth accordingly
	Liquid depth		1.9, 0.47, 0.3, 0.12, 0.08	
	Bund depth		2.4, 0.6, 0.4, 0.15, 0.09	
Pool and bund radius – butane	Pool radius	m	2, 4, 5, 8, 10	
	Liquid depth		1.4, 0.3, 0.2, 0.09, 0.05	
	Bund depth		1.7, 0.4, 0.3, 0.11, 0.07	
Substrate and bund properties (Base Case 'A')			'Standard concrete', 'BG1' concrete, 'GdF' concrete	Different parameters to represent the wide variation of values used for concrete. 'Standard concrete' is the default substrate setting in LSMS. 'BG1' and 'GdF' refer to test cases (taken from LSMS documentation)
Substrate temperature (Base Case 'A', methane)		K	273.12, 283.12, 288.12, 293.12, 303.12	
Solar flux (Base case 'B' only)		kW/m^2	0, 5, 10	
Wind speed (Base cases 'A' and 'B')		m/s	1, 2, 5, 10 , 20	

Table A1.10a: PHAST – Bunded pool source: Key fixed parameters and assumptions

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

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

General parameter	Model input parameter(s)	Units	Values	Notes
Dimensions of bund	Diameter	m	4, 5, 8, 10, 20	
Release amount	Mass	tonnes	1, 10, 100	
Storage temperature		°C	-162.4 to -180 for methane 5, 15, 30 for n-pentane	
Ground temperature		°C	5, 15, 30	
Air temperature		°C	5, 15, 30	
Wind speed		m/s	1, 2, 5, 7, 10 , 20	

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

Parameter	Values used	Notes
Release type	Release from reservoir	
Substances modelled	Methane (cryogenic) Pentane (non-cryogenic)	Using inbuilt substance properties
Release duration	1 second	To approximate an instantaneous release

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

General parameter	Model input parameter(s) varied	Units	Values	Notes
Mass flow into pool	Volume spill rate	m^3/s	2.0, 20.0, 200.0	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
	Orifice diameter	m	0.309, 0.976, 3.124	
Initial liquid temperature - methane		°C	-162, -170, -180	
Initial liquid temperature - pentane		°C	0, 15, 30	Reflects the storage temperature, so the ambient temperature also set to the same values
Ground type		n/a	'insulated concrete', 'wet sand','dry sand'	
Ground temperature		°C	0, 15, 30	
Spreading constraints	Minimum thickness of pool	mm	0.5, 1.0, 2.0	
Wind speed		m/s	1, 2, 5, 10 , 20	

LSMS

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

Parameter	Values used	Notes
Source configuration	'Dam break'	Instantaneous release
Substances modelled	Methane (cryogenic) Butane (non-cryogenic)	
Substrate type	'Homogeneous/impermeable'	
Outputs	Vaporisation rate Pool duration (methane only) Maximum pool radius	

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

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

A.1.4. Continuously released pool source on land

Table A1.13a: ALOHA – Continuously released pool source on land: Key fixed parameters and assumptions

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

Table A1.13b: ALOHA – Continuously released pool source on land: Parameters varied

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

Table A1.14a: GASP/DRIFT – Continuously released pool source on land: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties (SPI files source)
Release type (GASP)	Continuous	
Aperture diameter (GASP)	0.05 m	
Release duration	1800 s	The duration of the release into the pool
Maximum pool age	3600 s	GASP runs until 99% if the spilled substance is vaporised or the maximum pool age is reached.
Pool geometry	Circular	Inbuilt assumption in GASP
Surface type	Land	
Pool spreading constraints	Puddle depth	Only the part of the pool above the puddle depth contributes to the pool spread
Initial ground temperature	Equal to the air temperature	Inbuilt assumption in GASP
Pool surface roughness length	0.23 mm	GASP default
Heat transfer mode	Perfect thermal contact, temperature varying substrate	GASP default
Thermodynamic options	Calculated pool temperature, 3-dimension conduction from ground (true), convection from atmosphere (true)	GASP defaults
Additional heat flux into pool	0 kW/m^2	GASP default
Release type (DRIFT)	Time Varying Release	DRIFT default
Include Dilution Over Pool (DRIFT)	True	DRIFT default

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

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

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

Parameter	Values used	Notes
Source type	Release from reservoir	
Substances modelled	Methane , pentane	Using inbuilt substance properties

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

General parameter	Model input parameter(s) varied	Units	Values	Notes
Mass flow into pool	Volume spill rate	m3/s	0.002, 0.02, 0.2, 2.0	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
	Orifice diameter	cm	0.97, 3.1, 9.81, 31.0	
Duration of release	Spill duration	s	900, 1800, 3600	
Initial liquid temperature - methane		°C	-162, -170, -180	
Initial liquid temperature - pentane			0,15,30	Reflects the storage temperature, so the ambient temperature also set to the same values
Ground type		n/a	'insulated concrete', 'wet sand','dry sand',	
Ground temperature		°C	0, 15, 30	
Spreading constraints	Minimum thickness of pool	mm	0.5, 1.0, 2.0	
Wind speed		m/s	1, 2, 5, 10 , 20	

Table A1.16a: LSMS – Continuously released pool source on land: Key fixed parameters and assumptions

Parameter	Values used	Notes
Source configuration	'Constant inflow' option, with axisymmetric geometry	Continuous release
Substances modelled	Methane (cryogenic) Butane (non-cryogenic)	
Release duration	3600s	The duration of the liquid release into the pool

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

General parameter	Model input parameter(s)	Units	Values	Notes
Flow into pool – methane	Volume flow into pool	m^3/s	0.0024, 0.024, 0.24, 2.4	Equivalent to 1, 10, 100, 1000 kg/s Keeping velocity of liquid flow constant
	Source radius	m	0.09, 0.28, 0.86, 2.7	
Flow into pool – butane	Volume flow into pool	m^3/s	0.0017, 0.017, 0.17, 1.7	
	Source radius	m	0.074, 0.23, 0.74, 2.3	
Initial liquid temperature – methane		K	111.67, 108.15, 93.15	111.67 K is the value obtained when the 'set to boiling' option is checked
Initial liquid temperature – butane		K	283.12, 288.12, 293.12	The substrate temperature was also set to these values, as this represents an ambient storage temperature
Substrate properties		n/a	'Standard concrete', 'non-porous sand', 'soil'	Set thermal parameters to represent these (taken from LSMS documentation)
Substrate temperature		K	283.12, 288.12, 293.12	
Spreading constraints	Turbulent drag	n/a	0.005, 0.01, 0.02	An advanced option controlling the dynamic spreading of the pool
Wind speed		m/s	1, 2, 5, 10 , 20	

Table A1.17a: PHAST – Continuously released pool source on land: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties
Inventory type	Atmospheric storage tank	
Inventory mass	1000 te	
Release type	Continuous spill	User defined spill rate
Release phase	Liquid	
Surface type	User defined (land)	
Surface roughness length	10 cm	
Solar radiation flux	0 kW/m^2	

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

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

A.1.5. Instantaneously released pool source on water

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

Parameter	Values used	Notes
Source type	'Puddle' option used	Using the 'Puddle' option means that no spreading is modelled
Release duration	1 minute	1 minute is the minimum allowed release duration
Orifice	Circular	
Ground type	'Water'	
Surface roughness length	0.1 cm	

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

General parameter	Model input parameter(s) varied	Units	Values	Notes
Mass of spill	Pool mass	tonnes	1, 10, 100	Varied the initial pool diameter to ensure that the pool depth was constant (1 cm)
	Diameter	m	17, 55, 174	
Initial diameter		m	50, 54.9, 60, 70	Keeping mass constant, so effectively varying the pool depth
Convective heat from water	Water temperature	°C	10, 15, 20	Can only vary the temperature (ALOHA calculates the heat flux from this).
Initial liquid temperature		°C	-162, -165, -170, -180	
Substances modelled			Methane, hydrogen(cryogenic)	Using inbuilt substance properties

Table A1.19a: GASP/DRIFT – Instantaneously released pool source on water: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties (SPI files source)
Release type (GASP)	Instantaneous	
Pool geometry	Circular	Inbuilt assumption in GASP
Surface type	Deep water	
Heat transfer coefficient	500 $W/m^2/K$	GASP default for deep water
Pool spreading constraints	Capillary depth = 0.2 mm	Surface tension provides restoring force for pool spreading on water
Water temperature	Equal to the air temperature	Inbuilt assumption in GASP
Pool surface roughness length	0.23 mm	GASP default
Thermodynamic options	Calculated pool temperature, convection from atmosphere (true)	GASP defaults
Additional heat flux into pool	0 kW/m^2	GASP default
Release type (DRIFT)	Time Varying Release	DRIFT default
Include Dilution Over Pool (DRIFT)	True	DRIFT default

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	tonnes	1, 10, 100	Input as mass with initial pool depth of 1 cm.
Dimensions of pool	Diameter	m	50, 55, 60, 70	
Initial liquid temperature		°C	-162.4, -163, -165, -170, -180 for methane 5, 15, 30 for n-pentane	
Ambient temperature		°C	10, 15, 20, 30 for methane 5, 15, 20 for n-pentane	Water and air temperature
Wind speed		m/s	1, 2, 5, 7, 10 , 20	

Table A1.20a: HGSYSTEM (LPOOL) – Instantaneously released pool source on water: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane	Using inbuilt substance properties from DATAPROP
Release duration	1 second	Approximating an instantaneous release
Orifice	Circular	
Ground type	'Water'	
Surface roughness length	0.1 cm	

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

General parameter	Model input parameter(s) varied	Units	Values	Notes
Release amount	Volume spill rate	m^3/s	2.0, 20.0, 200.0	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
	Orifice diameter	cm	0.309, 0.976, 3.124	
Initial liquid temperature - methane		°C	-162, -170, -180	
Substrate temperature		°C	0, 15, 30	

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

Parameter	Values used	Notes
Source configuration	'Dam break'	Instantaneous release
Substances modelled	Methane (cryogenic) Butane (non-cryogenic)	
Substrate	'Water'	
Initial liquid temperature	'Set to boiling'	111.67
Surface roughness length	0.001 m	

Table A1.21b: LSMS – Instantaneously released pool source on water: Parameters varied

General parameter	Model input parameter(s)	Units	Values	Notes
Mass of spill – methane	Vertical size	m	0.91, 1.96, 4.2	Keeping aspect ratio constant (height:width of 0.5) Equivalent to 1, 10, 100 tonnes
	Initial radius		0.91, 1.96, 4.2	
Initial mass in pool – hydrogen	Vertical size	m	1.6, 3.6, 7.7	
	Initial radius		1.6, 3.6, 7.7	
Initial pool radius - methane		m	0.5, 1.96, 4.0	Keeping the initial height constant. ∴ Also effectively varying the mass
Initial pool radius - hydrogen		m	0.9, 3.6, 7.0	
Convective heat flux from water	Initial heat flux	kW/m^2	5, 50, 500	
Roughness length		m	0.0001, 0.001, 0.1	

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

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties
Inventory type	Atmospheric storage tank	
Release type	Catastrophic rupture	Release height set to zero
Release phase	Liquid	
Release temperature	-162.4 °C for methane 15 °C for n-pentane	
Surface type	Deep water or channel	
Surface roughness length	1 mm	
Solar radiation flux	0 kW/m^2	
Air temperature	15 °C	

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	tonnes	1, 10, 100	Input as inventory mass
Water temperature		°C	5, 15, 30	
Wind speed		m/s	1, 2, 5, 7, 10 , 20	

A.1.6. Continuously released pool source on water

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

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

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

General parameter	Model input parameter(s) varied	Units	Values	Notes
Mass flow into pool	Chemical mass in tank	tonnes	1, 10, 100, 1000	Varied the orifice diameter to ensure that the release duration was constant (30 minutes)
	Tank volume		2.625, 26.25, 262.5, 2625	
	Orifice diameter	cm	3.55, 9.7, 24.92, 62	
Duration of release	Orifice diameter	cm	14, 9.7, 6.88	Hole diameter adjusted to give the required duration: 15, 30, 60 minutes
Convective heat from water	Water temperature	°C	10, 15, 20	Can only vary the temperature (ALOHA calculates the heat flux from this).
Initial liquid temperature		°C	-162, -165, -170, -180	

Table A1.24a: GASP/DRIFT – Continuously released pool source on water: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties (SPI files source)
Release type (GASP)	Continuous	
Aperture diameter (GASP)	0.05 m	
Release duration	1800 s	The duration of the release into the pool
Maximum pool age	3600 s	GASP runs until 99% if the spilled substance is vaporised or the maximum pool age is reached.
Pool geometry	Circular	Inbuilt assumption in GASP
Surface type	Deep water	
Heat transfer coefficient	500 $W/m^2/K$	GASP default for deep water
Pool spreading constraints	Capillary depth = 0.2 mm	Surface tension provides restoring force for pool spreading on water
Water temperature	Equal to the air temperature	Inbuilt assumption in GASP
Pool surface roughness length	0.23 mm	GASP default
Thermodynamic options	Calculated pool temperature, convection from atmosphere (true)	GASP defaults
Additional heat flux into pool	0 kW/m^2	GASP default
Release type (DRIFT)	Time Varying Release	DRIFT default
Include Dilution Over Pool (DRIFT)	True	DRIFT default

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	tonnes	1, 10, 100, 1000	Input as mass release rate in kg/s
Release duration	Time limited spill	min	15, 30, 60	Input as time limited spill in s
Initial liquid temperature		°C	-162.4, -163, -165, -170, -180 for methane 5, 15, 30 for n-pentane	
Ambient temperature		°C	5, 15, 30	Water and air temperature
Wind speed		m/s	1, 2, 5, 7, 10 , 20	

Table A1.25a: HGSYSTEM (LPOOL) – Continuously released pool source on water: Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic)	Using inbuilt substance properties from DATAPROP
Ground type	'Water'	
Surface roughness length	0.1 cm	

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

General parameter	Model input parameter(s) varied	Units	Values	Notes
Mass flow into pool	Volume spill rate	m^3/s	0.0024, 0.024, 0.24, 2.4	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
	Orifice diameter	cm	0.309, 0.976, 3.124	
Duration of release	Spill duration	s	900, 1800, 3600	
Initial liquid temperature - methane		°C	-162, -170, -180	
Water temperature		°C	0, 15, 30	

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

Parameter	Values used	Notes
Source configuration	'Constant inflow' option, with axisymmetric geometry	Continuous release
Substances modelled	Methane (cryogenic)	Using inbuilt substance properties
Release type	'Constant inflow'	
Release duration	3600 s	The duration of the liquid release into the pool
Substrate	'Water'	
Initial liquid temperature	'Set to boiling'	111.67
Surface roughness length	0.001 m	

Table A1.26b: LSMS – Continuously released pool source on water: Parameters varied

General parameter	Model input parameter(s)	Units	Values	Notes
Flow into pool	Volume flow into pool	m^3/s	0.0024, 0.024, 0.24, 2.4	Equivalent to 1, 10, 100, 1000 kg/s Keeping velocity of liquid flow constant
	(initial) source radius	m	0.09, 0.28, 0.86, 2.7	
Convective heat flux from water	Initial heat flux	kW/m^2	5, 50, 500	

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

Parameter	Values used	Notes
Substances modelled	Methane (cryogenic) n-Pentane (non-cryogenic)	Using inbuilt substance properties
Inventory type	Atmospheric storage tank	
Release type	Liquid spill	Specified rate for a given duration
Release phase	Liquid	
Surface type	Deep water or channel	
Surface roughness length	1 mm	
Solar radiation flux	0 kW/m^2	
Air temperature	15 °C	

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	tonnes	1, 10, 100	Input as inventory mass
Release duration	Time limited spill	min	15, 30, 60	Input as duration of spill in s
Release temperature		°C	-162.4 to -180 for methane 5, 15, 30 for n-pentane	
Water temperature		°C	5, 15, 30	
Wind speed		m/s	1, 2, 5, 7, 10 , 20	

A.2. Pressurised catastrophic failure (flashing)

A.2.1 Direct source

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

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

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	kg	100, 1000, 10000, 100000, 1000000	

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

Parameter	Values used	Notes
Substance modelled	Chlorine	
Release type	'Instantaneous'	
Release phase	Superheated Liquid/Two-Phase	
Release temperature	238.7 K	Taken from GASTAR's flash calculation utility, based on storage temperature of 15 °C and atmospheric pressure of 1013mb
Hazardous fraction	1000000 ppm	Fraction of initial release that is hazardous (determines the initial quantity of air in the instantaneous cloud)
Initial cloud radius	Based on jet output parameter values extracted from ACE model runs	
Momentum initially well mixed option	Selected	This should only be deselected if the release has zero ambient velocity

Table A2.2b: GASTAR – Pressurised catastrophic failure (flashing): Parameters varied

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	kg	1000, 10000, 100000	
Initial liquid fraction		kg/kg	0.5, 0.8, 0.847, 0.9	Base case value was taken from GASTAR's flash calculation utility, based on storage temperature of 15°C and atmospheric pressure of 1013mb
Aspect ratio	Diameter	m	23.8, 34.5, 52	Equivalent aspect ratios: 1, 0.33, 0.1
Mass of entrained air		kg	3000, 15000, 75000	Also varying the diameter to keep the aspect ratio constant

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

Parameter	Values used	Notes
Substance modelled	Chlorine	
Release type	Release in HEGABOX	
Initial air entrainment	0.33 mole pollutant/mole total mixture.	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."

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release amount	Mass	kg	1000, 10000, 100000, 1000000	Wet pollutant
Aspect ratio	Initial cloud radius	m	24.0, 35.0, 52.0	Equivalent aspect ratios: 1, 0.33, 0.1
Initial air entrainment	0.064, 0.32	mole pollutant/mole total mixture		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."

A.2.2 Catastrophic failure source term models

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

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

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

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

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

Parameter	Values used	Notes
Substance modelled	Chlorine	Using inbuilt substance properties
Inventory type	Pressure vessel	
Release type	Catastrophic rupture	
Surface type	User defined (land)	
Surface roughness length	10 cm	
Solar radiation flux	0 kW/m^2	

Table A2.5b: PHAST– Pressurised catastrophic failure (flashing): Parameters varied

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

A.3. Jet releases

A.3.1. Direct source

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

Parameter	Values used	Notes
Substance modelled	Methane, air	
Release type	'jet' source type	
Release phase	Gaseous	
Release temperature	15 °C	
Release heat capacity	Methane: 2220 J/°C/kg Air: 1012 J/°C/kg	
Release molecular mass	Methane: 16 Air: 28.97	

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

General parameter	Model input parameter(s)	Units	Values	Notes
Pseudo diameter - methane		m	0.01, 0.05, 0.1199, 0.2, 0.5	Keeping velocity value constant (at 652 m/s for methane and 479m/s for air). Effectively varying volume (and mass) flow rates
Pseudo diameter - air			0.01, 0.05, 0.1199, 0.2, 0.5	
Mass flow-methane	velocity	m/s	130, 261, 652, 977	Keeping pseudo diameter constant
Mass flow-air	velocity		95.7, 192, 479, 719, 957	
Release height		m	1, 10	
Release direction			Horizontal, vertical	Downwind for horizontal, Upwards for vertical
Duration		s	Continuous, 1800, 180, 18	Plume run for continuous, puff run otherwise
Averaging time		s	600, 1	

Table A3.2a: DRIFT – Direct jet source (no expansion): Key fixed parameters and assumptions

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

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

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

Table A3.3a: GASTAR – Direct jet source (no expansion): Key fixed parameters and assumptions

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

Table A3.3b: GASTAR – Direct jet source (no expansion): Parameters varied

<table>
<tr><th>General parameter</th><th>Model input parameter(s)</th><th>Units</th><th>Values</th><th>Notes</th></tr>
<tr><td colspan="2">Pseudo diameter: gaseous chlorine</td><td>m</td><td>0.01, 0.05, 0.084, 0.1, 0.5</td><td rowspan="3">Keeping mass flow rate constant. Base case values based on output from DRIFT</td></tr>
<tr><td colspan="2">Pseudo diameter: gaseous methane</td><td>m</td><td>0.01, 0.05, 0.120, 0.2, 0.5</td></tr>
<tr><td colspan="2">Pseudo diameter: two-phase chlorine</td><td>m</td><td>0.01, 0.05, 0.113, 0.1, 0.5</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 rowspan="2">Diameter and release rate</td><td>Diameter</td><td>m</td><td>0.084, 0.115, 0.160, 0.250</td><td rowspan="2">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>Mass flow rate</td><td>kg/s</td><td>5, 10, 20, 50</td></tr>
<tr><td colspan="2">Release height</td><td>m</td><td>1, 10</td><td></td></tr>
<tr><td colspan="2">Release direction</td><td></td><td>Horizontal, vertical</td><td>Downwind for horizontal</td></tr>
<tr><td colspan="2">Aerosol liquid fraction (two-phase chlorine only)</td><td></td><td>0.7, 0.8, 0.9</td><td></td></tr>
<tr><td colspan="2">Averaging time</td><td>s</td><td>600, 1</td><td></td></tr>
<tr><td colspan="2">Wind speed and stability</td><td></td><td>D5, F2</td><td></td></tr>
</table>

Table A3.4a: SLAB – Direct jet source (no expansion): Key fixed parameters and assumptions

Parameter	Values used	Notes
Spill type	Type '2' (for base case)	horizontal jet release: area with plane perpendicular to ambient wind direction, velocity pointing downwind
Substances modelled (Source density)	Methane (buoyant gas) Chlorine (dense gas)	
Release phase	Gaseous	

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

General parameter	Model input parameter(s)	Units	Values	Notes
Release rate		kg/s	2, 5, 10, 20, 50	
Jet radius - methane		m	0.005, 0.025, 0.060, 0.1, 0.25	
Jet radius - chlorine		m	0.005, 0.025, 0.042, 0.05, 0.25	
Jet radius and release rate - methane	Radius	m	0.060, 0.084, 0.117, 0.185	
	Mass flow rate	kg/s	5, 10, 20, 50	
Jet radius and release rate - chlorine	Radius	m	0.084, 0.115, 0.160, 0.25	
	Mass flow rate	kg/s	5, 10, 20, 50	
Release direction			Horizontal, vertical	Downwind for horizontal
Release height		m	1, 10	

A.3.2. Source term jet models

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

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

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

General parameter	Model input parameter(s)	Units	Values	Notes
Orifice diameter: gaseous chlorine		m	0.001, 0.01, 0.05, 0.1, 0.5	Keeping storage pressure constant (at 2.78 atm)
Orifice diameter: gaseous methane		m	0.001, 0.01, 0.05, 0.1, 0.5	Keeping storage pressure constant (at 23.3 atm)
Orifice diameter: two-phase chlorine		m	0.001, 0.01, 0.05, 0.1, 0.5	
Release rate – gaseous chlorine	Storage pressure	atm	1.29, 2.78, 5.48	Equivalent to 2, 5 and 10 kg/s release rate
Release rate – gaseous methane			9.45, 23.3, 45.7, 88.0, 220.5	Equivalent to 2, 5, 10, 20 and 50 kg/s release rate
Storage temperature – two-phase chlorine		°C	0, 15, 30	
Orifice type			Circular hole / Pipe or valve	

Table A3.6a: DRIFT – Jet source (with expansion): Key fixed parameters and assumptions

Parameter	Values used	Notes
Substances modelled (Source density)	Methane (buoyant gas) Air (neutrally buoyant gas) Chlorine (dense gas) Chlorine (two-phase flashing)	
Release type	Finite duration Steady continuous (for infinite duration)	
Release phase	Gaseous Superheated Liquid/Two-phase	Using inbuilt jet expansion model
Source type	Momentum jet	
Release rate	User specified or Calculated	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)
Release temperature	15 °C	
Release pressure	101325 Pa for metastable liquid Choke pressure for choked two-phase flow	Calculated by DRIFT for gaseous discharge. 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.
Liquid fraction	0.0 for gaseous 1.0 for metastable liquid Calculated liquid fraction at exit for choked two-phase flow	Liquid fraction for choked two-phase flow calculated using 'Omega' discharge model.
Rainout fraction	0.0	No rainout included

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

Model input parameter(s)	Units	Values	Notes
Orifice diameter	m	0.001, 0.01, 0.05, 0.1, 0.5	
Release rate	kg/s	2, 5, 10, 20, 50, Calculated	Varied for fixed orifice diameter or varied with orifice diameter based upon flow rate model (gaseous, liquid, two-phase)
Release duration	s	18, 180, 1800, infinite	
Wind speed and stability		D5, F2	
Ambient temperature	°C	15, 30	
Discharge coefficient		0.6 (liquid), 0.8 (gaseous), 1.0	

Table A3.7a: HGSYSTEM (AEROPLUME) – Jet source (with expansion): Key fixed parameters and assumptions

Parameter	Values used	Notes
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

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

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

Parameter	Values used	Notes
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/m^2	

Table A3.8b: PHAST – Jet source (with expansion): Parameters varied

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

A.4. Spray releases

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

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

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

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

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

Parameter	Values used	Notes
Substances modelled	m-xylene water	Using inbuilt substance properties
Inventory type	Pressure Vessel	
Inventory mass	1000 te	
Storage and release phase	Liquid	
Discharge coefficient	0.6	
Surface type	User defined (land)	
Surface roughness length	0.1 m	
Solar radiation flux	0 kW/m^2	
Air temperature	15°C	
Relative humidity	70%	

Table A4.2b: PHAST – Jet source (with expansion): Parameters varied

Model input parameter(s)	Units	Values	Notes
Storage temperature	°C	15, 30, 100	
Storage pressure	barg	5, 10, 20, 50, 100	
Orifice diameter	m	0.001, 0.01, 0.1	
Release elevation	m	1, 10	
Release direction		Horizontal, up	
Wind speed and stability		D2, D5, D10, F2	

A.5. Fire plume (warehouse)

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

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

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

Model input parameter(s)	**Units**	**Values**	**Notes**
Temperature (high temperature case)	°C	50, 100, 300, 400, 600	
Temperature (low temperature case)		15, 30, 50, 100	
Velocity (high temperature case)	m/s	5, 10, 20, 30	
Velocity (low temperature case)		0.2, 2, 5, 10	
Source diameter	m	0.5, 2, 4, 10	
No of openings (sources)		1, 2, 5, 10	The single source was located in the centre of the warehouse roof. Multiple sources located at regular intervals along building centreline
Building downwash		Modelled, not modelled	Building of 10m height, 30m width and 100m length
Building alignment		Aligned with wind, perpendicular to wind	
Wind speed	m/s	1, 2, 5, 10, 15	
Particle diameter	m	1×10^{6}, 1×10^{5}	Affects dry deposition of particulates only
Wind speed and stability		D5, F2, D15	

Table A5.2a: HOTSPOT – Warehouse fire: Key fixed parameters and assumptions for cases (a) and (b)

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

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

Case	Model input parameter(s)	Units	Values	Notes
a	Height	m	0, 5, 10	This is the 'elevation of burning debris'
	Radius	m	10, 20, 50, 100	This is the effective radius of the fire
	Cloud top	m	10, 20, 50	This is the cloud top of the plume
b	Heat emission rate	cal/g	4.78×10^6, 9.56×10^6, 1.91×10^7	Equivalent to 20, 40 and 80 MW

A.6. Fire plume (outside burning pool)

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

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

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

Model input parameter(s)	Units	Values	Notes
Temperature	°C	100, 200, 300, 400, 500	
Velocity	m/s	5, 10, 20, 30	
Source diameter	m	2, 10, 30, 50	Equivalent areas: 3, 79, 707, 1963 m^2
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

Parameter	Values used	Notes
Source type	'Burning puddle (pool fire)' source	
Fuels modelled	Methane	
Outputs	Flame length, burn duration, burn rate, total amount burned	

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

General parameter	Model input parameter(s)	Units	Values	Notes
Pool size	Area	m^2	10, 100, 2000, 50, 100	
Pool depth		cm	0.5, 1, 5, 10, 100	
Initial pool temperature		°C	-161.6, -170, -180	This cannot exceed the ambient boiling point (methane = -161.6°C) and has to be above the freezing point (methane = -182°C)

Table A6.3a: HOTSPOT – Fire plume (outside burning pool): Key fixed parameters and assumptions

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

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

Model input parameter(s)	Units	Values	Notes
Radius	m	10, 20, 50, 100	This is the effective radius of the fire
Fuel volume	gallons	3000, 10000, 30000, 50000	This is the total amount of fuel burned in the fire
Burn duration	minutes	5, 20, 60, 90	Calculated based on HOTSPOT advice that "pool depth burn rates are 1 - 5mm/min"
Heat of combustion	cal/g	6000, 12000, 30000	Values roughly representative of methanol, ethanol and ammonia

APPENDIX B: SENSITIVITY TESTS RESULTS TABLES

B.1. Evaporating pools

B.1.1 Direct pool source

Table B1.1: ADMS – Direct pool source: Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Area of source	Equivalent diameters: 2, 5, 10, 20m	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
Released amount	Emission rate and mass flux	Concentrations are very sensitive at both 100 and 1000m, and for both D5 and F2 conditions.
Emission height		Concentrations at 100m and 1000m are not sensitive for D5 conditions, and moderately sensitive for F2 conditions. Linear/almost linear negative relationship
Emission temperature		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.

Table B1.2: DEGADIS – Direct pool source: Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Release amount	Input varied: rate of mass release to air	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.
Pool dimensions	Input varied: pool radius	For both D5 and F2 conditions, concentrations at 100m and 1000m are only slightly sensitive to the pool radius
Stability class/wind speed	D5 and F2 conditions	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

Table B1.3: DRIFT – Direct pool source: Sensitivity summary

DRIFT Input / Source Parameter		Run cases	Summary of Observed Sensitivity
Source properties	Release rate	2kg/s, 5kg/s, 10kg/s, 20kg/s and 50kg/s	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.
	Source diameter	2m, 5m, 10m, 20m	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.
	Source density	Mw=16, 28, 71	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.
Atmospheric properties	Wind speed and stability	D5, F2	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).

Table B1.4: GASTAR – Direct pool source: Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Dimensions of pool	Input varied: Initial plume width	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.
Release amount	Input varied: Mass flux	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
Emission temperature		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)

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

Model parameter varied	Notes	Summary of observed sensitivity
Release amount	Input varied: Mass flux from area source	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.
Dimensions of pool	Input varied: area of source	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.
Stability class/wind speed	D5 and F2	The concentrations of methane, HCN and chlorine at both 100m and 1000m are very sensitive to the stability class/wind speed.

B.1.2 Bunded pool source

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

Model parameter varied	Notes	Summary of observed sensitivity
Diameter		The vaporisation rates and both concentration-based outputs are very sensitive for both methane and pentane.
Mass released		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.
Initial liquid temperature	Varied for methane only	The vaporisation rates and both concentration-based outputs are very sensitive. They are particularly sensitive where the temperatures are close to the boiling temperatures.
Air temperature		The vaporisation rates and both concentration-based outputs are not very sensitive, for both methane and pentane.
Wind speed		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.

Table B1.7: GASP – Bunded pool source: Sensitivity summary

GASP Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill mass	1te, 10te, 100te	Methane	Strong	Peak vaporisation reduces with increased spill mass. Distance to LFL and 10% LFL decrease significantly with increasing spill mass.
			n-Pentane	Weak	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
	Spill temperature	-162.4C to -180°C	Methane	Strong	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.
		5°C, 15°C, 30°C	n-Pentane		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.
Spreading constraints	Bund diameter	4m, 5m, 8m, 10m, 20m	Methane	Strong	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.
			n-Pentane		Peak vaporisation rate increases in direct proportion to bund area. Distance to LFL and 10% LFL increases with increasing bund diameter.
Substrate properties	Ground temperature	5°C, 15°C, 30°C	In GASP the ground temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.		
Atmospheric properties	Wind speed and stability	D1, D2, D5, D7, D10, D20, F2	Methane	Strong	Peak vaporisation 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.
			n-Pentane	Moderate	Peak vaporisation rate is a strong function of wind speed - increasing with $(\text{wind speed})^{0.87}$. 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.
	Temperature	5°C, 15°C, 30°C	Methane	Weak	Peak vaporisation 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.
			n-Pentane	Weak	Peak vaporisation insensitive to air/ground temperature. Distances to LFL and 10% LFL increase with air/ground temperature. Less of an effect than for spill temperature.

Table B1.8: HGSYSTEM (LPOOL) – Bunded pool source: Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Volume flow rate	Released over one second	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.
Initial liquid temperature - methane		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.
Initial liquid temperature - pentane		The vaporisation rates are very sensitive for both D5 and F2 conditions. The vaporisation rates are almost constant over time for all cases.
Pool radius		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.
Air temperature		The vaporisation rate of both methane and pentane, and both D5 and F2 conditions is not sensitive to this parameter.
Wind speed		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.

Table B1.9: LSMS – Bunded pool source: Sensitivity summary

Model parameter varied	**Notes**	**Summary of observed sensitivity**
Mass of spill	Base Case 'A' only Varied the vertical size of pool and bund	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
Initial liquid temperature	Base Case 'A' only	Methane: Very sensitive; positive, almost linear relationship. Butane: Only slightly sensitive
Pool and bund radius	Base Case 'A' only	Both methane and butane: Very sensitive, generally positive relationship.
Substrate and bund properties	Base Case 'A' only	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.
Substrate temperature	Base Case 'A' and methane only	The vaporisation rate is only slightly sensitive to this parameter
Solar flux	Base case 'B' only (methane only)	The vaporisation rate only slightly sensitive. Sensitivity increases over time.
Wind speed	Base cases 'A' and 'B'	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

Table B1.10: PHAST – Bunded pool source: Sensitivity summary

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill mass	1te, 10te, 100te	Methane	Moderate	Negative relationship (increasing mass gives decreasing concentrations) Vaporisation rate is moderately sensitive – more so at lower mass values
			n-Pentane		Positive relationship (increasing mass gives increasing concentrations). Vaporisation rate is very sensitive – more so at higher mass values
	Spill temperature	-162.4°C to -180°C	Methane	Weak	Peak vaporisation rate and concentration insensitive to initial spill temperature except very close to boiling point.
		5°C , 15°C, 30°C	n-Pentane		Peak vaporisation rate and concentration slightly sensitive to initial spill temperature – increasing with increasing temperature
Spreading constraints	Bund diameter	4m, 5m, 8m, 10m, 20m	Methane	Strong	Peak vaporisation rate increases markedly with increased bund diameter. Distance to LFL and 10% LFL increases with increasing bund diameter.
			n-Pentane		
Substrate properties	Ground temperature	5°C, 15°C , 30°C	Methane	Weak	Only very small effect on LFL and 10% LFL distances
			n-Pentane		
Atmospheric properties	Wind speed and stability	D1, D2, D5, D7, D10, D20, F2	Methane	Moderate	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.
			n-Pentane		

B.1.3. Instantaneously released pool source on land

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

Model parameter varied	Notes	Summary of observed sensitivity
Volume flow rate	Released over one second	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.
Initial liquid temperature		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.
Substrate temperature		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.
Substrate type	'insulated concrete', 'wet sand', 'dry sand'	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.
Spreading constraints	Varied the minimum thickness of the pool	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.
Wind speed		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.

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

Model parameter varied	Notes	Summary of observed sensitivity
Mass of spill	Varied the initial source radius and height (kept aspect ratio constant)	For both methane and butane, all outputs are all very sensitive to this parameter.
Initial liquid temperature		For methane, all outputs are only slightly sensitive, while for butane, all outputs are moderately sensitive.
Initial pool radius	Keeping the initial height constant (therefore, effectively varying the mass)	For both methane and butane, all outputs are all very sensitive to this parameter, with a linear/almost linear relationship.
Substrate properties		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.
Substrate temperature	Varied for methane only	All outputs are only slightly sensitive to this parameter.
Spreading constraints	Varied the turbulent drag parameter	For methane, the vaporisation rate and pool duration are moderately sensitive, and the maximum pool radius is only slightly sensitive to this parameter. For butane, the vaporisation rate is moderately sensitive, and the maximum pool radius is only slightly sensitive
Wind speed		For methane, the vaporisation 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 vaporisation 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.

B.1.4. Continuously released pool source on land

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

Model parameter varied	Notes	Summary of observed sensitivity
Mass of spill	Varied mass in tank, tank volume and orifice diameter	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.
Duration	Varied orifice diameter	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.
Initial liquid temperature - methane		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.
Initial liquid temperature - pentane		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.
Ground type		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.
Ground temperature		For both methane and pentane, all model outputs are only slightly sensitive to this parameter.
Spreading constraints	Varied maximum pool diameter	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.
Wind speed		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.

Table B1.14: GASP/DRIFT Continuously released pool source on land: Sensitivity summary

GASP Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill rate	0.556kg/s, 5.5 kg/s, 55.6 kg/s, 556 kg/s	Methane	Strong	Peak vaporisation 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.
			n-Pentane		Peak vaporisation rate is approximately proportional to the spill rate with a constant of proportionality of approximately 0.6. 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.
	Spill temperature	-162.4°C to -180°C	Methane	Weak	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.
		5°C, 15°C, 30°C	n-Pentane		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.
	Spill duration	15min, 30min, 60min	Methane	Strong	Spilling the same release quantity (10te) over different durations introduces a strong dependence upon spill duration (spill rate)
			n-Pentane		
Spreading constraints	Puddle depth	2mm, 1cm, 2cm, 5cm, 10cm	Methane	Strong	The peak vaporisation rate, maximum pool radius, distance to LFL and distance to 10% LFL all decrease with increasing puddle depth. The peak vaporisation rate divided by the maximum pool area is approximately constant.
			n-Pentane		The peak vaporisation rate, maximum pool radius, distance to LFL and distance to 10% LFL all decrease with increasing puddle depth. The peak vaporisation rate divided by the maximum pool area increases with increasing puddle depth.
Substrate properties	Ground temperature	In GASP the ground temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.			
	Substrate type	asphalt, concrete, dry soil, wet soil	Methane	Strong	The maximum vaporisation 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.
			n-Pentane	Moderate	The maximum vaporisation 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.
Atmospheric properties	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		The peak vaporisation 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.
	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 ambient temperature – increasing slightly as the ground temperature increases.
			n-Pentane		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.

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

Model parameter varied	Notes	Summary of observed sensitivity
Volume flow rate		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.
Release duration		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
Initial liquid temperature		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.
Substrate temperature		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.
Substrate type	'insulated concrete', 'wet sand','dry sand'	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.
Spreading constraints	Varied the minimum thickness of the pool	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.
Wind speed		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.

Table B1.16: LSMS – Continuously released pool source on land: Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Volume flow into pool	Also varied the initial source radius (kept velocity of liquid flow constant)	For both methane and butane, the vaporisation rate and the maximum pool radius are very sensitive to this parameter.
Initial liquid temperature	Varied for methane only	Both the vaporisation rate and the maximum pool radius are only slightly sensitive.
Substrate properties		For both methane and butane, the vaporisation rate and the maximum pool radius are only slightly sensitive to this parameter.
Substrate temperature		For both methane and butane, both outputs are only slightly sensitive to this parameter.
Spreading constraints	Varied the turbulent drag parameter	For both methane and butane, neither of the outputs is sensitive to this parameter.
Wind speed		For methane, both the vaporisation rate and the maximum pool radius are only slightly sensitive. For butane, both outputs are moderately sensitive.

Table B1.17: PHAST – Continuously released pool source on land: Sensitivity summary

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill rate	0.556kg/s, 5.5 kg/s, 55.6 kg/s, 556 kg/s	Methane	Strong	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)$^{0.6}$. Distance to LFL and 10% LFL varies approximately as (spill rate)^{q} with q=0.40 and 0.49 respectively.
			n-Pentane		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.
	Spill temperature	-162.4°C to -180°C	Methane	Weak	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.
		5°C , 15°C , 30°C	n-Pentane		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.
	Spill duration	15min, 30min, 60min	Methane	Strong	Spilling the same release quantity (10te) over different durations introduces a strong dependence upon spill duration (spill rate)
			n-Pentane		
Spreading constraints	Minimum pool depth	2mm, 1cm, 2cm, 5cm, 10cm	Methane	Moderate – different behaviour close to the pool	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.
			n-Pentane		The peak vaporisation is sensitive to the minimum pool depth – decreasing with increasing pool depth. The maximum pool radius also decreases with increasing minimum pool depth. The distance to LFL increases as the minimum pool depth is increased. Whereas the distance to 10% LFL decreases as minimum pool depth is increased. This different behaviour might be due to sensitivity to maximum pool size close to the pool and sensitivity to vaporisation rate at greater distances.
Substrate properties	Ground 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 ground – increasing slightly as the ground temperature increases.
			n-Pentane	Moderate	The results fort 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.
	Substrate type	asphalt, concrete, dry soil, wet soil	Methane	Strong	The maximum vaporisation 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.
			n-Pentane		The maximum vaporisation 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.
Atmospheric properties	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.

B.1.5. Instantaneously released pool source on water

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

Model parameter varied	Notes	Summary of observed sensitivity
Mass of spill	Varied mass and diameter	All model outputs (the vaporisation rate and the distances to both the LEL and 10% LEL) are very sensitive to this parameter
Initial diameter		None of the model outputs are sensitive to this parameter
Water temperature		None of the model outputs are sensitive to this parameter
Initial liquid temperature		None of the model outputs are sensitive to this parameter; there is no effect at all on the results.
Substance	Modelled a hydrogen spill	When an equivalent mass of hydrogen is released, the vaporisation rate is the same as that for methane

Table B1.19: GASP - Instantaneously released pool source on water: Sensitivity summary

Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill mass (and diameter)	1te, 10te, 100te	Methane	Strong	The distance to LFL and 10% LFL varies approximately as (spill mass)$^{1/3}$
			n-Pentane		The distance to LFL and 10% LFL varies with spill mass as (spill mass)^{q} where q=0.5 and 0.44 respectively.
	Initial spill diameter	50m, 55m, 60m, 70m	Methane	Moderate – different behaviour for methane and n-pentane	Increased spill diameter leads to decreased distance to LFL and 10% LFL
		40m, 45m, 50m, 60m	n-Pentane		Increased spill diameter leads to increased distance to LFL and 10% LFL. This is the opposite behaviour to methane.
	Spill temperature	-162.4°C to -180°C	Methane	Negligible	Variation of the initial spill temperature has negligible effect on the distance to LFL and 10% LFL
		5°C, 15°C, 30°C	n-Pentane	Weak	The distance to LFL and 10% LFL show small increases with increased spill temperature.
Substrate properties	Water temperature	In GASP the water temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.			
Atmospheric properties	Wind speed and stability	D1, D2, D5, D7, D10, D20, F2	Methane	Strong – different behaviour for methane and n-pentane	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.
			n-Pentane		The vaporisation rate increases with increasing wind speed. The distances to LFL and 10% LFL are predicted to *decrease* with increasing wind speed.
	Temperature	5°C, 15°C, 30°C	Methane	Moderate	The distance to LFL is predicted to decrease with slightly increasing ambient temperature whereas the distance to 10% LFL increases and then decreases.
			n-Pentane	Strong	The distances to LFL and 10% LFL are predicted to increase significantly with ambient temperature.

Table B1.20: HGSYSTEM (LPOOL) – Instantaneously released pool source on water: Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Volume flow rate	Released over one second	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.
Initial liquid temperature		Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.
Water temperature		Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.

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

Model parameter varied	Notes	Summary of observed sensitivity
Mass of spill	Varied the initial source radius and height (kept aspect ratio constant)	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.
Initial pool radius		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.
Convective heat flux from water	By specifying the initial heat flux from the water	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.
Roughness length		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.

Table B1.22: PHAST – Instantaneously released pool source on water. Sensitivity summary

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill mass	1te, 10te, 100te	Methane	Strong	The distance to LFL and 10% LFL varies strongly with spill mass
			n-Pentane		
Substrate properties	Water temperature	5°C , 15°C , 30°C	Methane	Weak	Slight decrease in distance to LFL with increasing water temperature whereas the distance to 10% LFL increases slightly.
			n-Pentane	Moderate	The distances to LFL and 10% LFL are predicted to increase with water temperature.
Atmospheric properties	Wind speed and stability	D1, D2, D5, D7, D10, D20, F2	Methane	Strong – different behaviour for methane and n-pentane	The distance to LFL and 10% LFL are predicted to *increase* with increasing wind speed.
			n-Pentane		The distance to LFL and 10% LFL are predicted to *decrease* with increasing wind speed.

B.1.6. Continuously released pool source on water

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

Model parameter varied	**Notes**	**Summary of observed sensitivity**
Mass flow into pool	Varying mass in tank, tank volume and orifice diameter	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.
Duration of release	Varying orifice diameter	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.
Convective heat from water	Varying water temperature	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.
Initial liquid temperature		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.

Table B1.24: GASP – Continuously released pool source on water: Sensitivity summary

GASP Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	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 (10te) over different durations introduces a strong dependence upon spill duration (spill rate)
			n-Pentane		
Substrate properties	Water temperature	In GASP the water temperature is the same as the air temperature. See sensitivities to Temperature in Atmospheric properties below.			
Atmospheric properties	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

Model parameter varied	Notes	Summary of observed sensitivity
Mass flow rate	Varied the volume spill rate and the orifice diameter	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.
Spill duration		Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter
Initial liquid temperature		Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter.
Water temperature		Both the vaporisation rate and the maximum pool diameter, for D5 and F2 conditions, are only slightly sensitive to this parameter

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

Model parameter varied	Notes	Summary of observed sensitivity
Volume flow into pool	Also varied the initial source radius (kept velocity of liquid flow constant)	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
Convective heat flux from water	By specifying the initial heat flux from the water	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.

Table B1.27: PHAST – Continuously released pool source on water: Sensitivity summary

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Spill rate	0.556 kg/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 -180C	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.
		5°C, 15°C, 30°C	n-Pentane		
	Spill duration	15min, 30min, 60min	Methane	Strong	Spilling the same release quantity (10te) over different durations introduces a strong dependence upon spill duration (spill rate)
			n-Pentane		
Substrate properties	Water 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.
			n-Pentane	Moderate	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.
Atmospheric properties	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.

B.2. Pressurised catastrophic failure (flashing)

B.2.1. Direct source

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

Model parameter varied	Notes	Summary of observed sensitivity
Release amount	By specifying the mass released	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.

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

Model parameter varied	Notes	Summary of observed sensitivity
Release amount	By specifying the mass released	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.
Initial liquid fraction		The concentrations at both 100 and 1000m are not very sensitive to this parameter, for either D5 or F2 conditions.
Aspect ratio	By specifying the diameter	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.
Mass of entrained air	Also varying the diameter to keep the aspect ratio constant	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.

Table B2.3: HGSYSTEM (HEGABOX) – Pressurised catastrophic failure (flashing): Sensitivity summary

Model parameter varied	**Notes**	**Summary of observed sensitivity**
Release amount	By specifying the mass released	Initial concentrations are moderately sensitive to the release mass
Initial cloud radius		Initial concentrations are very sensitive to the initial cloud radius
Mass of entrained air		Initial concentrations are very sensitive to the values tested mass of entrained air

B.2.2. Source term

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

ACE Input / Source Parameter		Run cases	Summary of Observed Sensitivity
Substance properties	Substance	Chlorine	
	Phase	Two-phase	
Storage properties	Mass	1te, 10te, 100te	Strong dependence of concentration on release mass, concentration ~ $(mass)^{2/3}$
	Temperature	0°C , 15°C, 30°C	The effect on downstream concentrations of temperature is small for the cases considered
	Pressure	Run cases covered by temperature variation (above) and padding (below)	See above for saturated conditions (storage pressure = saturated vapour pressure) and below for the effect of padding pressure
	Enhanced pressure from added gas	+1 bar pad pressure	Negligible effect on downstream concentrations is small for the cases considered
Release properties	Initial turbulent velocity	No run cases	Not changeable for standard users
	Directional release	Down (default), omni	Factor of two decrease in concentration at source due to additional air entrained for the omni-directional release (spherical) compared with the default down direction (hemisphere). The effect of this decays with distance as more air is entrained
	Release height	No run cases	There is no release height dependence in ACE, other than the possibility of specifying release direction. DRIFT only allows ground based instantaneous releases.
Atmospheric properties	Wind speed and stability	D5, F2	The ACE source term is independent of wind speed and stability. However pool vaporisation and dispersion gives sensitivity to wind speed and stability. Toxic dose is more sensitive to wind speed due to entrainment of air at source. In some circumstances instantaneous dense releases in D5 can give shorter hazard ranges than F2 conditions.
	Roughness length	0.1m	The ACE source term is independent of roughness length. Dispersion however depends strongly upon roughness particularly in the far field.
	Temperature	0°C , 15°C, 30°C	Atmospheric temperature assumed to equal storage temperature. See temperature variation for storage temperature.
	Relative humidity	No runs	The ACE source term is independent of humidity. Typically dispersion has little dependence upon humidity, except possible for condensation in cold clouds which are marginally buoyant.
Other	Rainout	Including rainout, no pool	Small difference between concentration results including pool or not within the dispersion calculations. The effect on toxic dose is more marked due to the extended release duration from the pool.
	Dilution at source	Dilution (by ACE), no dilution	The results with no dilution are significantly higher close to the source but are similar at downwind distances corresponding to 1000 ppm or less.

Table B2.5: PHAST – Pressurised catastrophic failure (flashing) source term: Sensitivity summary

PHAST Input / Source Parameter		Run cases	Summary of Observed Sensitivity
Substance properties	Substance	**Chlorine**	
	Phase	**Two-Phase**	
Storage properties	Mass	10te, 100te, 1000te	Strong dependence on spill mass, distance to 1000 ppm varies as ~$(mass)^{1/3}$, distance to 100 ppm varies slightly more strongly with ~$(mass)^{0.4}$
	Temperature	5°C , 15°C, 30°C	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
	Pressure	Run cases covered by temperature variation (above) and padding (below)	See above for saturated conditions (storage pressure = saturated vapour pressure) and below for the effect of padding pressure.
	Enhanced pressure from added gas	+1, +2, +3 bar pad pressure	Negligible effect (<0.1% change) on distance to 1000 ppm and 100 ppm for 1000 te base case
Atmospheric properties	Wind speed and stability	D2, D5, D10, F2	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.
	Roughness length	0.001m, 0.01m, 0.1m, 1m	Strong effect on decreased distance to 1000 ppm with increasing roughness length. Opposite behaviour for 100 ppm where distance increases with increasing roughness length.
	Temperature	5°C , 15°C , 30°C	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.
	Relative humidity	0%, 50%, 70%, 95%	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.

B.3. Jet releases

B.3.1. Direct source jet models

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

Model parameter varied	Notes	Summary of observed sensitivity
Pseudo diameter	Keeping velocity value constant - effectively varying volume (and mass) flow rates	Concentrations are very sensitive over this range of pseudo diameters, for both methane and air, and D5 and F2 conditions. Linear/almost linear dependence.
Mass flow rate (velocity)	In ADMS, for jet sources, the efflux rate is specified by entering the velocity. Keeping pseudo diameter constant	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).
Release height		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
Release direction	Horizontal /vertical	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.
Averaging time		Generally, concentrations are not very sensitive to the averaging times; there is slightly more sensitivity in F2 conditions in the far field.
Duration	Tested plume release and puff releases of various durations	There is a large variation in the dose values (but this only scales proportionally to the exposure time)

Table B3.2: DRIFT – Direct Jet Source: Sensitivity summary

DRIFT Input / Source Parameter		Run cases	Summary of Observed Sensitivity
Source properties	Release rate	2kg/s, 5kg/s, 10kg/s, 20kg/s and 50kg/s	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 ~ (release rate). For downwind directed jets the jet regime covers a greater distance in low wind conditions.
	Release duration	18s, 180s, 1800s and infinite	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.
	Source density	Mw=16,28,71 for gaseous releases 2-phase chlorine (80% liquid, 239K)	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.
	Release diameter	1mm, 1cm, 5cm, 10cm, 50cm	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 ~ (release diameter). Beyond the jet regime the concentration becomes independent of release diameter for the same release rate.
	Release height	1m, 10m	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.
	Release direction	Horizontal, vertical	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.
Atmospheric properties	Wind speed and stability	D5, F2	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.
	Roughness length	0.001m, 0.01m, 0.1m, 1m	Negligible effect on concentration predictions in the jet regime. The effect increases at greater distances with lower roughness giving higher concentrations.
	Temperature	0°C , 15°C, 30°C	Negligible effect on concentration predictions
	Relative humidity	0%, 50%, 70%, 95%	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.
	Inversion height	F2 50m, 100m, 200m	Negligible effect exception at very low concentrations

Table B3.3: GASTAR – Direct jet source: Sensitivity summary

Model input parameter(s)	Notes	Summary of observed sensitivity
Pseudo diameter	Keeping mass flow constant	**Gaseous releases**: 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.
		Two-phase release: 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
Mass flow rate	Keeping pseudo diameter constant	**Gaseous releases:** 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.
		Two-phase releases: Concentrations and jet outputs are very sensitive to this parameter. The sensitivity of the concentrations is not evident until after jet transition point.
Diameter and mass flow rate	Effectively varying the storage pressure	**Gaseous releases:** Very sensitive for both methane and chlorine, and both D5 and F2 conditions. Greater sensitivity in the chlorine case.
		Two-phase releases: The concentrations are moderately sensitive to this combination of parameters, but jet parameters not very sensitive.
Release height		**Gaseous releases** Jet outputs are very sensitive to the release height for both methane and chlorine and both D5 and F2 conditions. Concentrations only moderately sensitive
		Two-phase releases: 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
Release direction	Horizontal /vertical	**Gaseous releases:** Jet outputs and concentrations are all very sensitive to the release direction. Concentrations sensitive in both the near and far fields. The jet does not touch down for methane in F2 conditions.
		Two-phase releases: 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
Aerosol liquid fraction	Two-phase release only	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.
Averaging time		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.
Wind speed and stability		Jet outputs show no sensitivity to the stability /wind speed categories tested. Concentrations are very sensitive to this

Table B3.4: SLAB – Direct jet source. Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Release rate		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.
Diameter	Input as the jet area	Concentrations are not sensitive to this parameter, for any of the cases.
Diameter and release rate		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.
Release direction	Horizontal /vertical	Concentrations are not sensitive to this parameter, for any of the cases, in neither the near- nor the far-field
Release height		Concentrations are not very sensitive to this parameter, for any of the cases. There is slightly more sensitivity in the near-field results

B.3.2. Source term jet models

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

Model parameter varied	Notes	Summary of observed sensitivity
Orifice diameter	Keeping the storage pressure constant	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.
		Two-phase jet: Concentrations are extremely sensitive to this parameter for both D5 and F2 conditions. Less sensitivity towards the smaller diameter values.
Mass flow rate (gaseous jets only)	Set by varying the storage pressure. Keeping diameter constant	Concentrations are very sensitive, with a linear/almost linear relationship, for both methane and chlorine and for D5 and F2 conditions.
Storage temperature (two-phase jets only)		Concentrations are very sensitive, with a linear/almost linear relationship, for D5 and F2 conditions.
Orifice type	Circular hole / Pipe or valve	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"

Table B3.6: DRIFT – Jet Source (with expansion): Sensitivity summary

DRIFT Input / Source Parameter		Run cases	Summary of Observed Sensitivity
Source properties	Release rate	2kg/s, 5kg/s, 10kg/s, 20kg/s and 50kg/s	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.
	Release duration	18s, 180s, 1800s and infinite	As for unexpanded jet source
	Source density	Mw=16,28,71 for gaseous releases 2-phase chlorine (flashing liquid)	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.
	Release diameter	1mm, 1cm, 5cm, 10cm, 50cm	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.
	Release height	No runs	See unexpanded jet source
	Release direction	No runs	See unexpanded jet source
	Discharge coefficient	0.6 (default for liquid), 0.8 (default for gas), 1	Weak dependence on discharge coefficient for gaseous releases. Stronger dependence for flashing liquid releases with concentration ~ (discharge coefficient)
Atmospheric properties	Wind speed and stability	D5, F2	As for unexpanded jet source
	Roughness length	No runs	See unexpanded jet source
	Temperature	15°C , 30°C	As for unexpanded jet source
	Relative humidity	No runs	See unexpanded jet source
	Inversion height	No runs	See unexpanded jet source

Table B3.7: HGSYSTEM (AEROPLUME) – Jet Source (with expansion): Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
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

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Release diameter	1mm, 1cm, 5cm, 10cm	Methane Gas Chlorine Gas 2-Phase Chlorine	Strong	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.
	Storage temperature	5°C , 15°C and 30°C	Methane Gas	Weak	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.
			2-Phase Chlorine	Moderate	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 (storage pressure)$^{1/4}$
	Pad pressure	Sat, +1bar, +2bar, +3bar	2-Phase Chlorine	Moderate	Liquid release rate scales with the square root of storage pressure (gauge). Distances to fixed concentration increase with pad pressure, scaling with approximately with the square root of release rate i.e. as the (storage pressure)$^{1/4}$
	Release phase	Liquid, 2-phase	2-Phase Chlorine	Strong	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)
	Discharge coefficient	0.6, 0.8, 1	Methane Gas 2-Phase Chlorine	Moderate	Release rate and expanded jet diameter increases in direct proportion to discharge coefficient. Distances to fixed concentrations vary ~(discharge coefficient)$^{1/2}$
	Release elevation	1m, 10m	Methane Gas Air Chlorine Gas	Weak in near-field (jet), Strong at intermediate distances, Weak in far-field (passive)	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.
	Release direction	Horizontal, up, down,	Methane Gas	Strong, particularly in	Large difference in centreline concentration as a function of horizontal distance. Downwards and impinged releases give significantly higher centreline concentrations than horizontal

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
		impinged		near-field	release. Vertical releases give significantly lower centreline concentrations.
			Air		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.
			Chlorine Gas		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.
			2-Phase Chlorine		As for chlorine gas, except that results for horizontal, down and impinged releases converge sooner, at approximately 10000ppm.
Atmospheric properties	Wind speed and stability	D2, D5, D10, F2	Methane Gas	Weak in near-field (jet), Strong in far-field (passive)	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.
			Air		D5 and F2 give almost identical centreline concentrations down to 5000 ppm, subsequently dilution is greater in D5 than F2.
			Chlorine Gas		D5 and F2 give almost identical centreline concentrations down to 3000 ppm, subsequently dilution is greater in D5 than F2.
			2-Phase Chlorine		D5 and F2 give almost identical centreline concentrations down to 10000 ppm, subsequently dilution is greater in D5 than F2.
	Roughness length	0.001m, 0.01m, 0.1m, 1m	Methane Gas	Weak in near-field (jet), Strong in far-field (dense and passive)	Increased roughness gives slightly decreased distance to LFL and more marked decrease to 10% LFL.
			2-Phase Chlorine		Increased roughness gives rise to a marked reduction in distances to 1000ppm and lower concentrations.
	Temperature	5°C , 15°C and 30°C	Methane Gas	Weak	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.
			2-Phase Chlorine		Higher ambient temperature gives a small reduction in distances to a given concentration.
	Relative humidity	0%, 50%, 70%, 95%	Methane Gas	Weak	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.
			2-Phase Chlorine		Reduced humidity reduces distance to concentration levels by a maximum of approx. 10% at 1000ppm. Smaller differences at lower concentrations.

B.4. Spray releases

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

DRIFT Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Release diameter	1mm, 1cm, 10cm	m-Xylene	Strong	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)
			Water		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.
	Storage temperature	15°C ,30°C and 100°C	m-Xylene	Negligible	Changing the release temperature has negligible effect on distance to LFL and 10% LFL (and equivalents for water).
			Water		
	Storage pressure	5barg, 10barg, 20barg, 50barg, 100barg	m-Xylene	Strong	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.
			Water		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.
	Release elevation	1m, 10m	m-Xylene	Weak	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.
			Water		
	Release direction	Horizontal, vertical	m-Xylene	Strong	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.
			Water		
Atmospheric properties	Wind speed and stability	D1, D2, D5, D7, D10, D20 F2	m-Xylene	Strong	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.
			Water		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.
	Temperature	5°C , 15°C and 30°C	m-Xylene	Weak	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.
			Water		

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

PHAST Input / Source Parameter		Run cases	Substance	Effect	Summary of Observed Sensitivity
Source properties	Release diameter	1mm, 1cm, 10cm	Xylene	Strong	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.
			Water		Droplet diameter independent of release diameter. Rainout fraction increases with increasing release diameter. Water droplets larger than xylene droplets for the same flow rate.
	Storage temperature	15°C, 30°C and 100°C	Xylene	Moderate	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 15C and zero rainout for 100C. Distance to LFL insensitive to storage temperature. Distance to 10% LFL significantly increased at 100C.
			Water		Rainout fraction and initial droplet size decreases with increased temperature. Rainout fraction varies between 0.8 and 0.71.
	Storage pressure	5barg, 10barg, 20barg, 50barg, 100barg	Xylene	Strong	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
			Water		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.
	Release elevation	1m, 10m	Xylene	Strong	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.
			Water		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.
	Release direction	Horizontal, vertical	Xylene	Strong	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.
			Water		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
Atmospheric properties	Wind speed and stability	D2, D5, D10, F2	Xylene	Strong	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,
			Water		Rainout decreases from 0.84 in D1 conditions to zero D20.

B.5. Fire plume (warehouse)

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

Model parameter varied	Notes	Summary of observed sensitivity
Temperature		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.
Velocity		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.
Source diameter		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.
No of openings (sources)		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).
Building downwash	Building downwash included in base case	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
Building alignment		Concentrations at 10om are moderately sensitive, and those at 1000m not sensitive, for both D5 and F2 conditions
Wind speed		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.
Particle diameter	To assess the effect on dry deposition rates	Dry deposition rates at both 100m and 1000m, and for D5 and F2 conditions, are very sensitive to the particle diameter
Stability and wind speed	D5, F2, D15	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.

Table B5.2: ADMS - Fire plume (warehouse). Sensitivity summary for enclosed, low temperature case

Model parameter varied	Notes	Summary of observed sensitivity
Temperature		Concentrations at both 100 m and 1000m downwind are moderately sensitive for D5 conditions. For F2 conditions, concentrations at 100 m are very sensitive, and those at 1000m only moderately sensitive. For D5, almost linear negative relationship; for F2, non-linear, with sharper decrease at lower end of parameter range.
Velocity		Concentrations at both 100 m and 1000m downwind are very sensitive for F2 conditions. For D5 conditions, concentrations at 10om are moderately sensitive, and those at 1000m not sensitive. For D5, almost linear negative relationship; for F2, non-linear, with sharper decrease at lower end of parameter range.
Source diameter		For D5 conditions, concentrations at both 100 m and 1000m downwind are moderately sensitive. For F2 conditions, concentrations at both 100 m and 1000m downwind are very sensitive. For D5, almost linear negative relationship; for F2, non-linear, with sharper decrease at lower end of parameter range.
No of openings (sources)		For D5 conditions, concentrations at 100 m are moderately sensitive, while for F2 conditions they are very sensitive. Concentrations at 1000m 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.
Building downwash	Building downwash included in base case	Concentrations are not sensitive both 100 m and 1000m downwind for D5 conditions, and 1000m downwind for F2 conditions. Concentrations at 100m are, however, very sensitive for F2 conditions.
Building alignment		For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000m are moderately sensitive. For F2 conditions, the inverse is true, with concentrations at 100 m moderately sensitive, and those at 1000m very sensitive.
Wind speed		For D5 conditions, concentrations at 100 m are very sensitive, and those at 1000m are moderately sensitive. For F2 conditions, concentrations at both 100m and 1000m are very sensitive to the wind speed. Very non-linear relationship; dramatic increase in concentrations between 1 and 2m/s (5m/s for F2 conditions), and then a steady decrease after this.
Particle diameter	To assess the effect on dry deposition rates	Dry deposition rates at both 100m and 1000m, and for D5 and F2 conditions are very sensitive to the particle diameter, and

Table B5.3: HOTSPOT – Fire plume (warehouse) Cases (a) and (b): Sensitivity summary

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

B.6. Fire plume (outside burning pool)

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

Model parameter varied	**Notes**	**Summary of observed sensitivity**
Temperature		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.
Velocity		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.
Source diameter	Equivalent areas: 3, 79, 707, 1963 m^2	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.
Source height		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.
Stability and wind speed	D5, F2, D15	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.

Table B6.2: ALOHA – Fire plume (outside burning pool): Sensitivity summary

Model parameter varied	Notes	Summary of observed sensitivity
Pool area	Note: the observed sensitivities apply to all stability conditions tested (D5, F2 and D15). All outputs show very little sensitivity to the stability.	The flame length, burn rate and total amount burned are very sensitive. The burn duration is not at all sensitive (no variation at all)
Pool depth		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).
Initial pool temperature		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.

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

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