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

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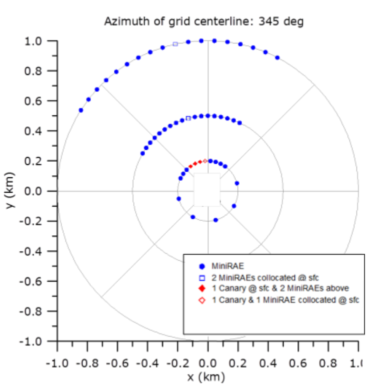
Contents

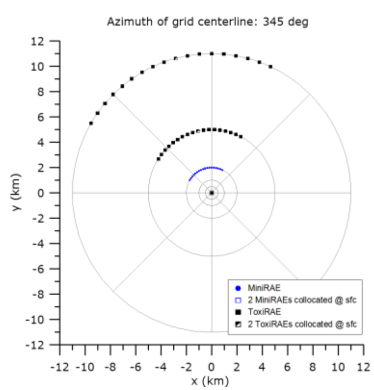
- Objectives
- Jack Rabbit II experiments
- PHAST and DRIFT models
- Discharge
- Dispersion
- Conclusions

Objectives

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

<u>Sensor locations:</u>





<u>Sensor saturation concentrations:</u>

- Jaz = 100,000 ppmv
- Canary = 10,000 ppmv
- MiniRAE = 2,000 ppmv
- ToxiRAE = 50 ppmv

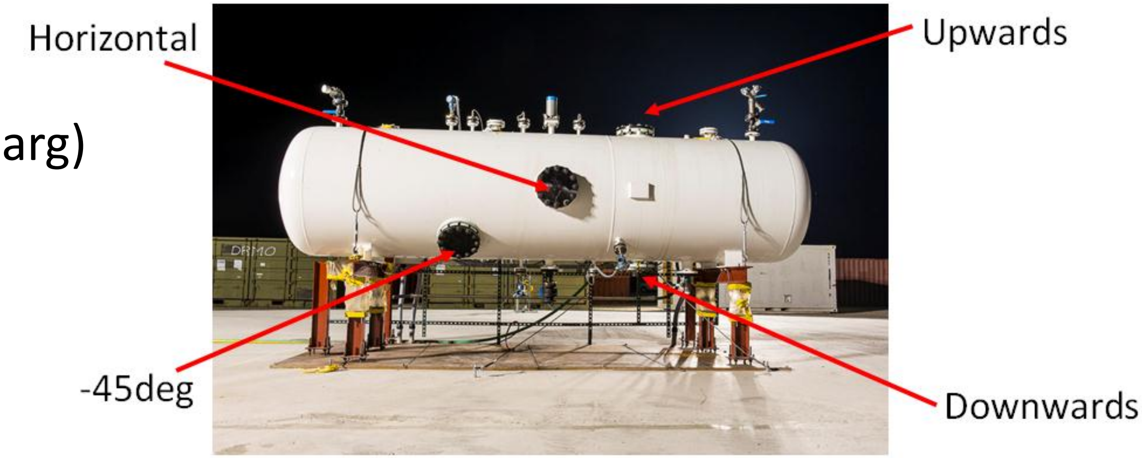
For context: IDLH = 10 ppmv

- Modelling methodology: predict reasonably conservative estimates and run sensitivity tests

Jack Rabbit II Experiments

Chlorine Release

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



Terrain

Surface roughness z_0 = 1mm

Weather

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

2015 Experiments

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

Tests modelled (2016)

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

* Metastable liquid (agreed by the MWG)

** Models are conservative if assuming no rainout

PHAST Model

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

DRIFT model

- Constant release rate
  - HSE Stream release rate calculation
- DRIFT finite-duration dispersion model accounts for:
  - Additional gravity spreading and dilution over the source
  - Along-wind diffusion
  - Along-wind gravity spreading
  - Limitations: may over-predict concentrations for short duration releases in far-field due to use of smaller Froude number for gravity spreading derived for continuous releases

Discharge Predictions

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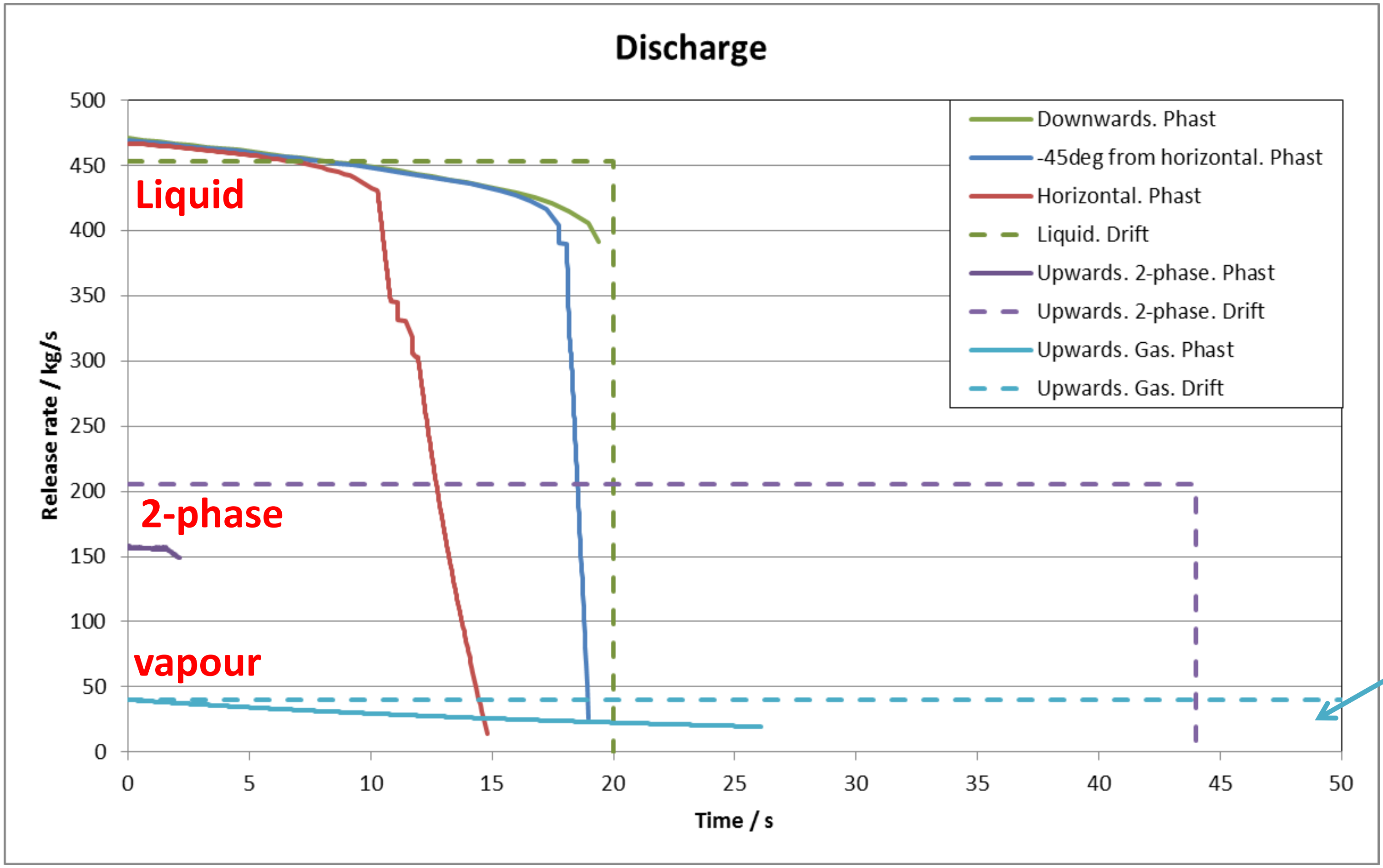
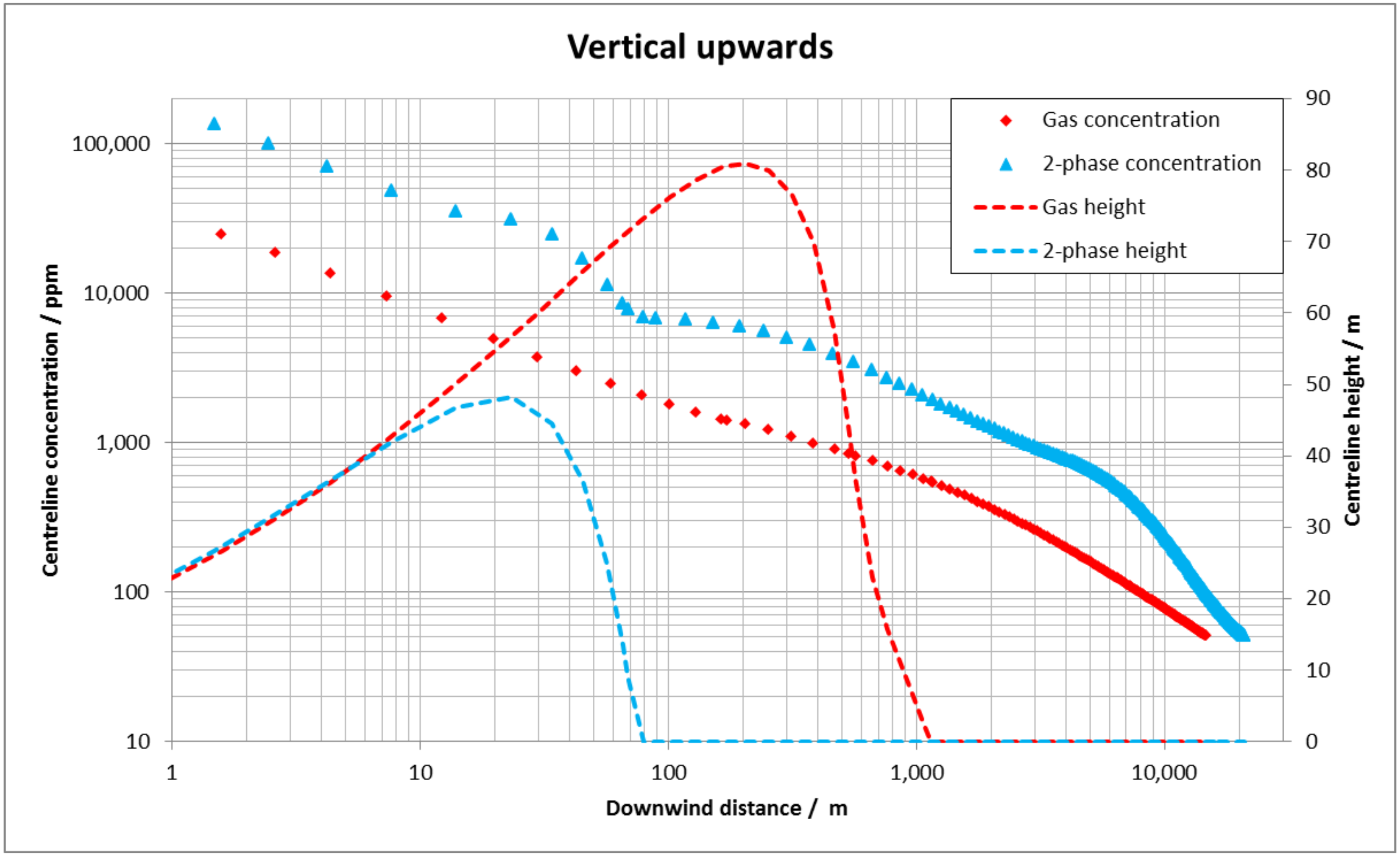
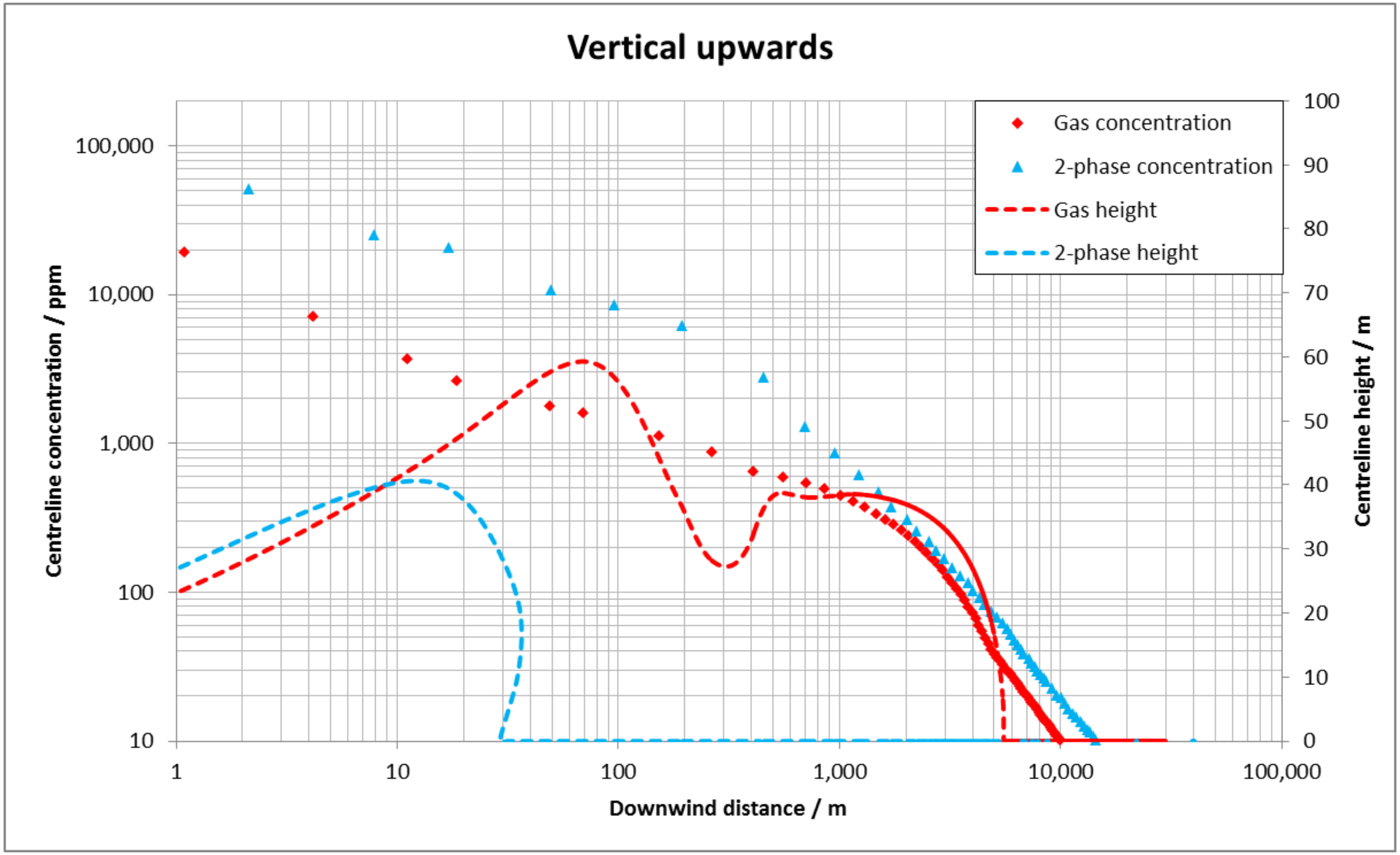


Release duration 229sec

Phast. Vertical upwards, aligned in the wind direction (azimuth of 345 degrees)



Drift. Vertical upwards, aligned in the wind direction (azimuth of 345 degrees)



Phast. Centreline concentration, aligned in the wind direction (azimuth of 345 degrees)

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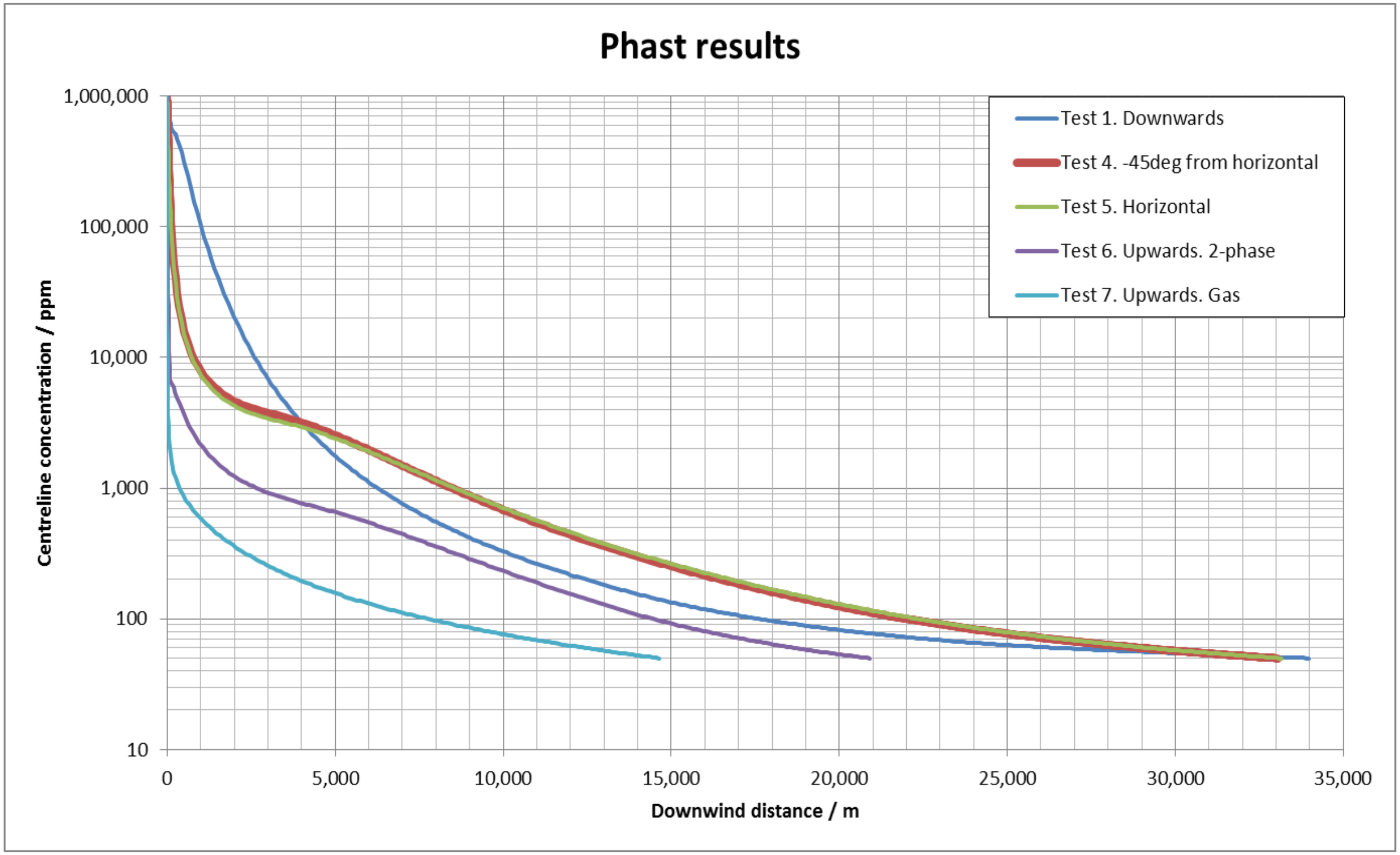
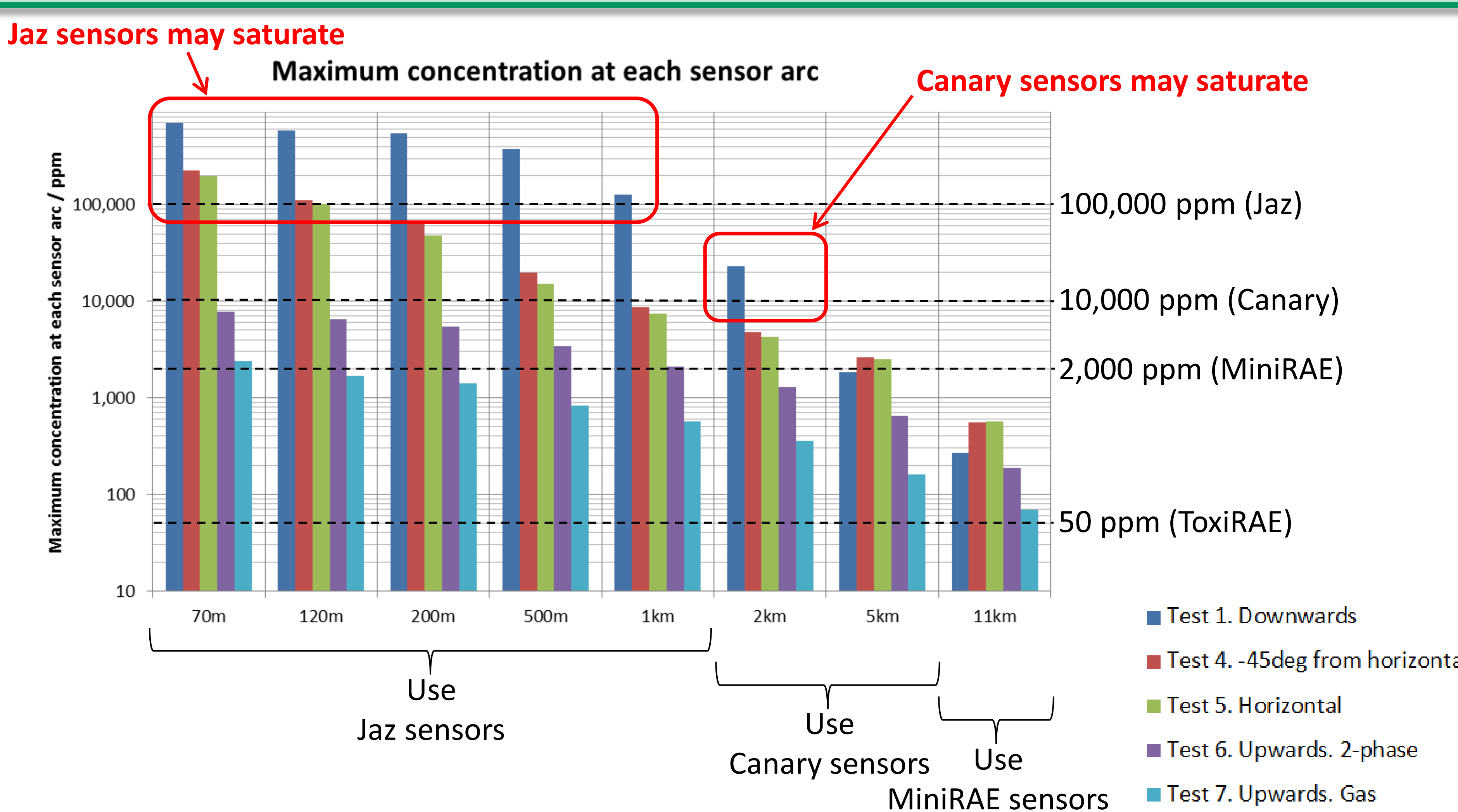
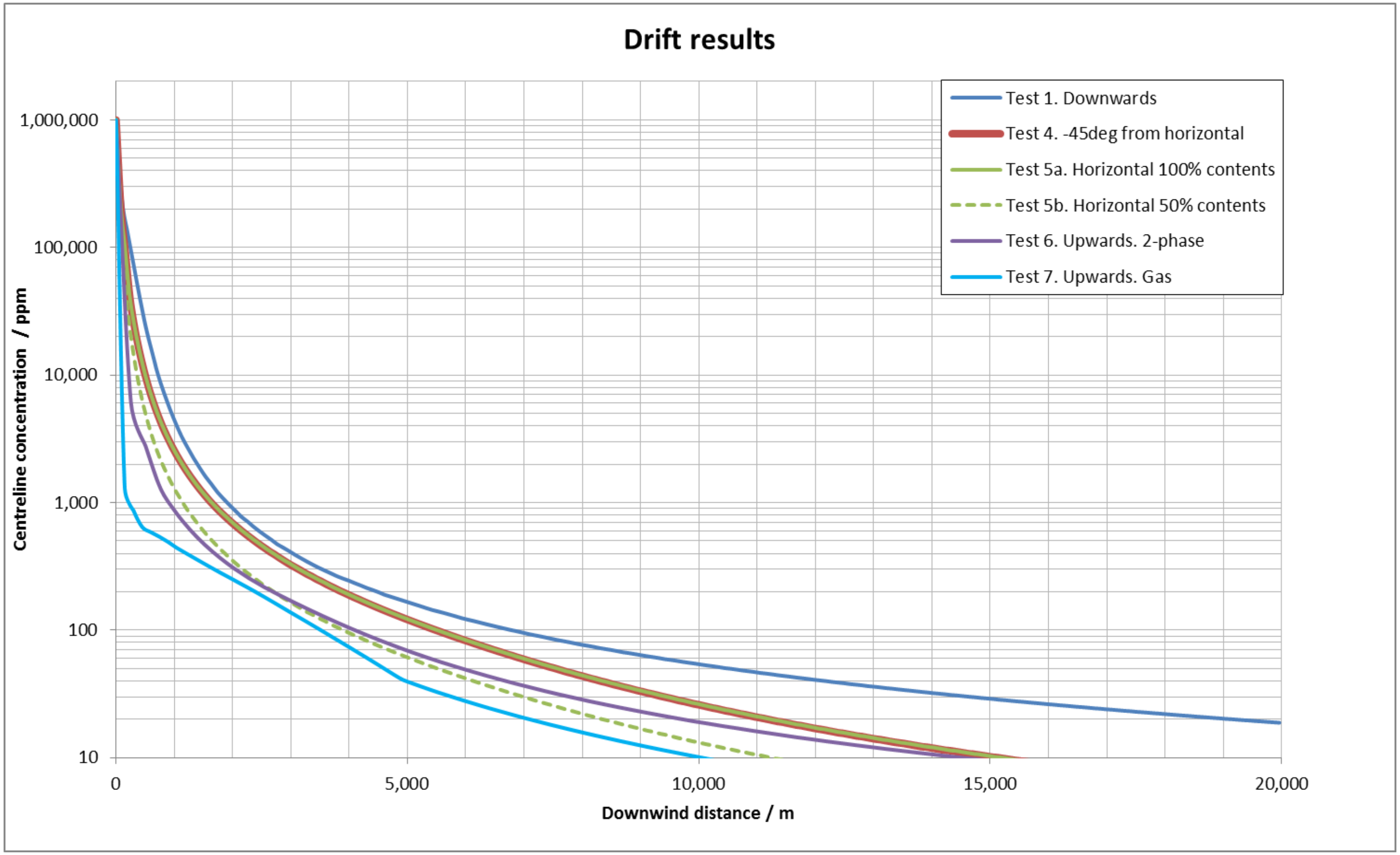


Phast Results Summary



Drift. Centreline concentration, aligned in the wind direction (azimuth of 345 degrees)



Drift. Centreline concentration, aligned in the wind direction (azimuth of 345 degrees)

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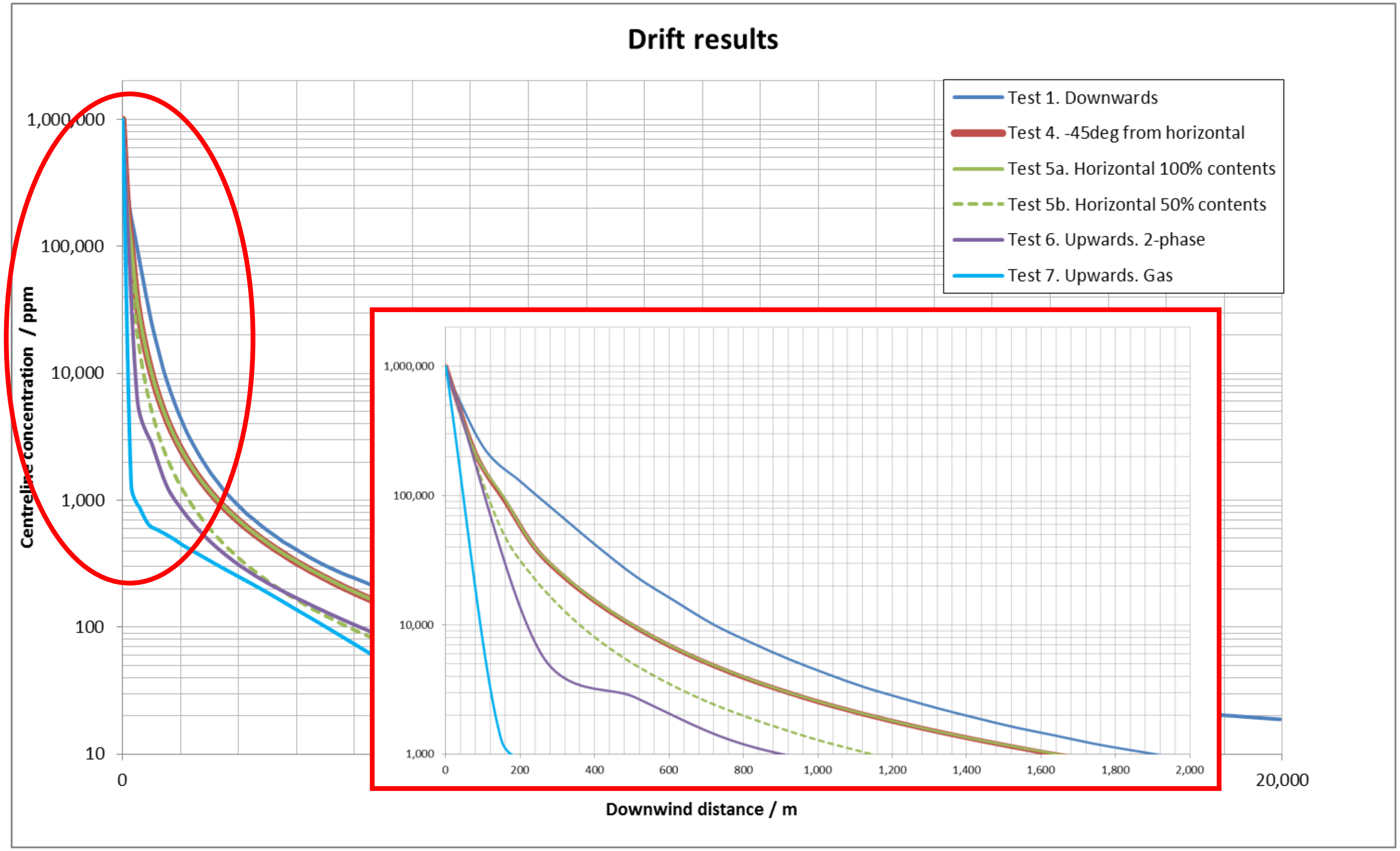
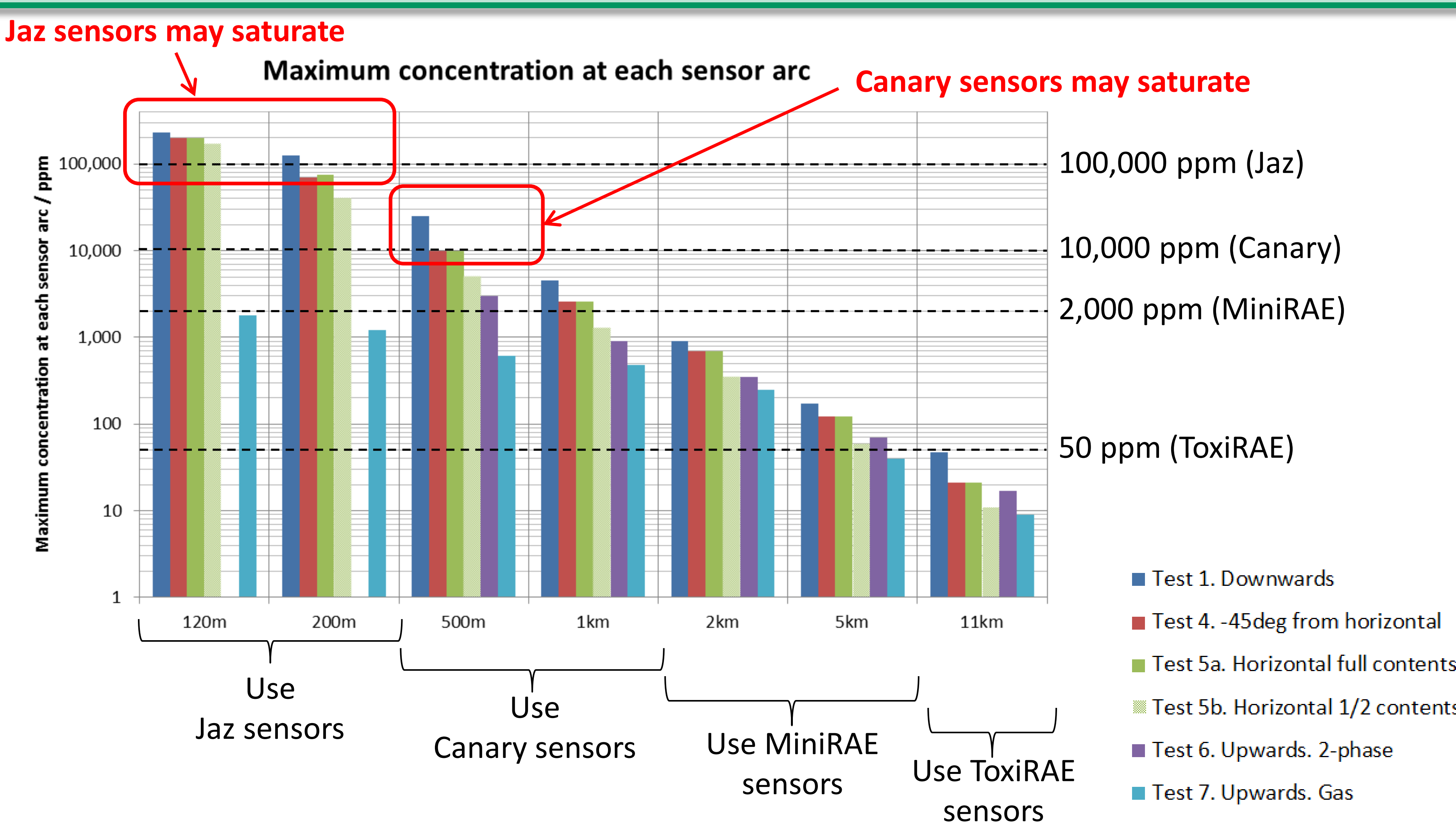


Drift Results Summary



Conclusions

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

Disclaimer

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

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

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

Thanks for contributions from:

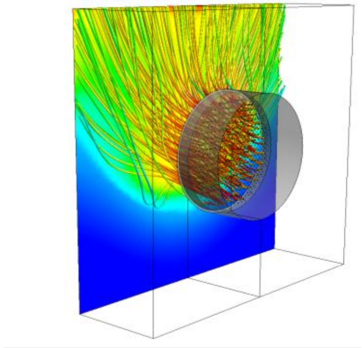
- Simon Gant, Maria Garcia, Rachel Batt (HSL)
- Henk Witlox, Jan Stene (DNV-GL)
- Graham Tickle (GT Science & Software)
- Jack Rabbit II Modelling Working Group

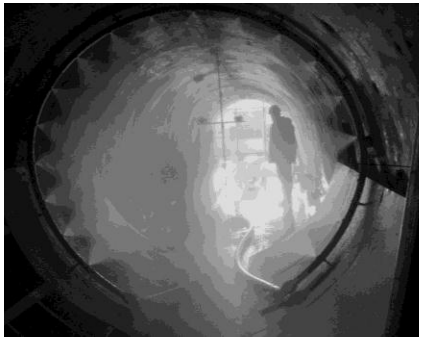
Any questions?

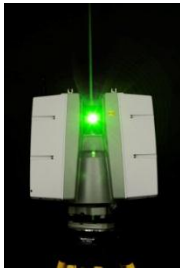
Introduction to HSL

HEALTH & SAFETY LABORATORY

- Multi-disciplinary:
  - Fire and process safety
  - Computational modelling
  - Exposure control
  - Toxicology etc.
- Approx. 400 staff
- 550 acre test site
- Fire galleries and burn hall
- Impact track
- Anechoic chamber
- Thermal test chamber
- Imaging/sampling from UAV



Introduction to HSL

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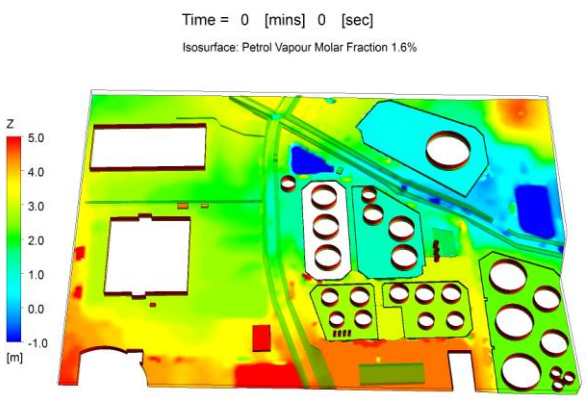
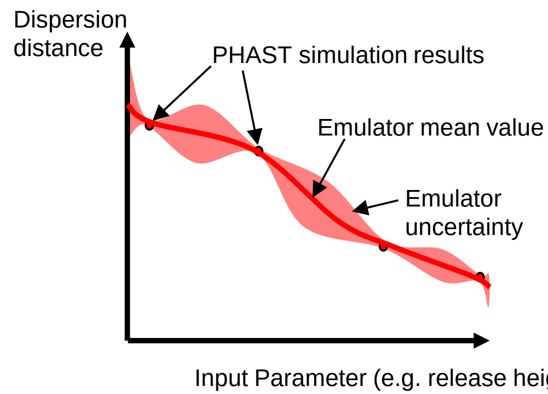
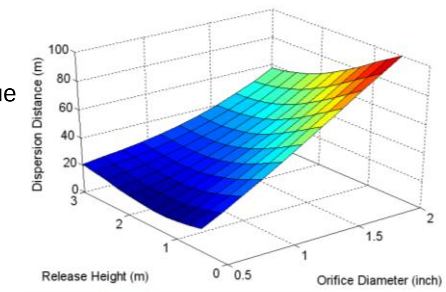
Buncefield Incident Investigation

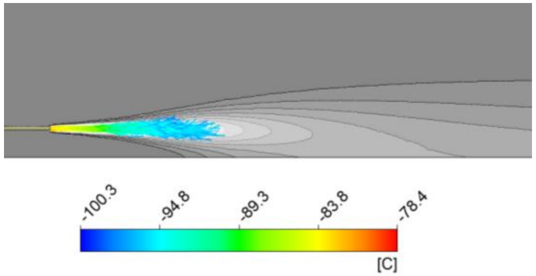


Emulators for global sensitivity analysis

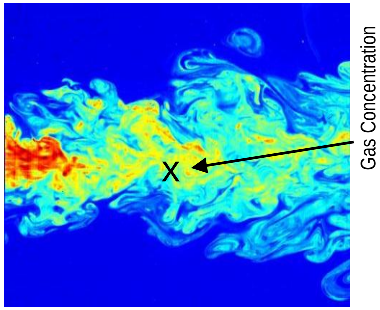




CO_2 two-phase jets



Concentration fluctuations: flammable/toxic



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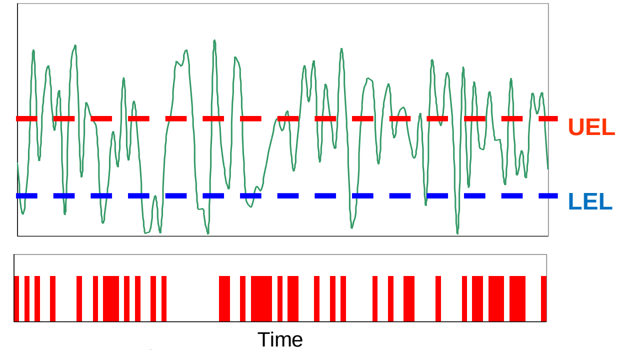
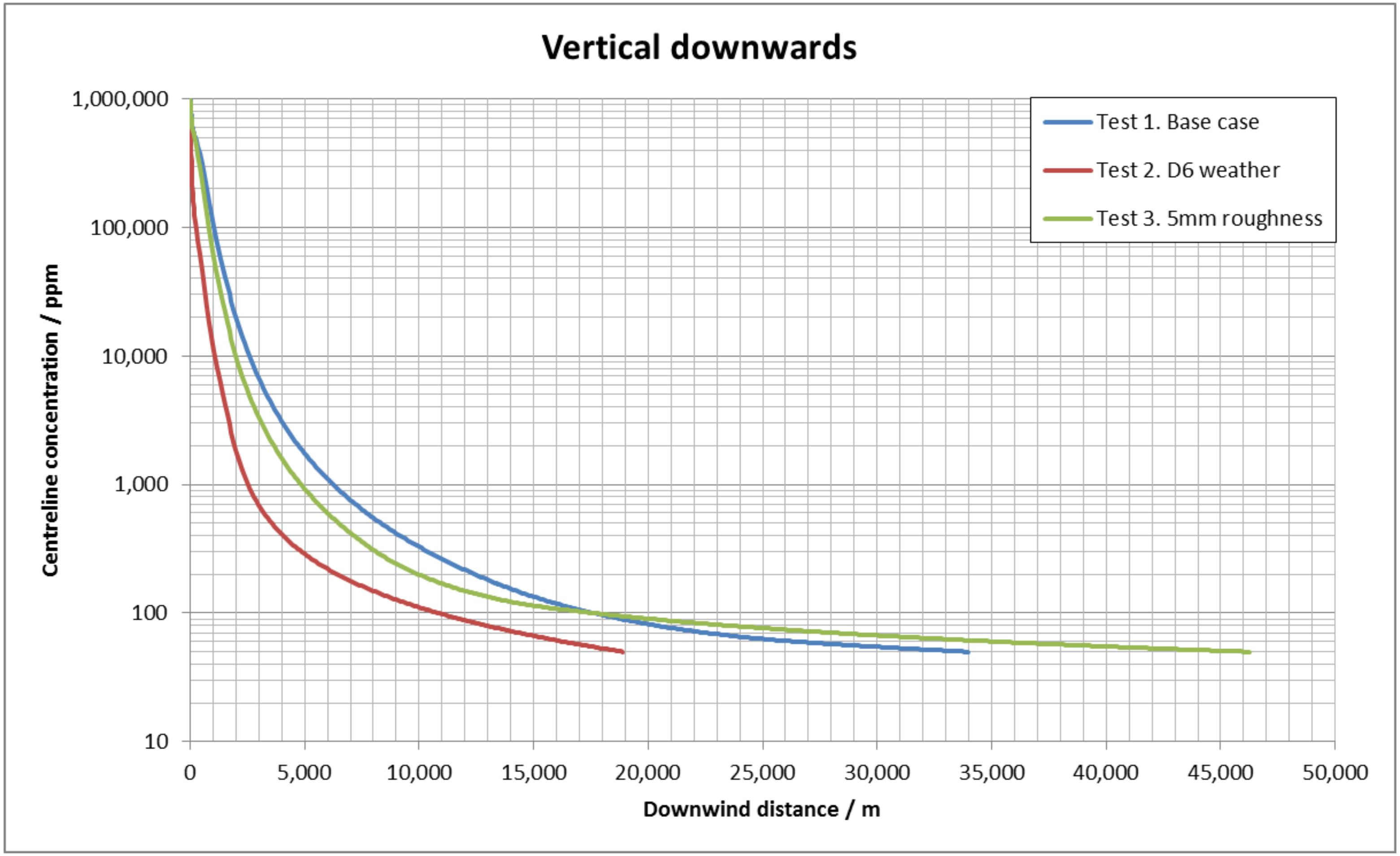


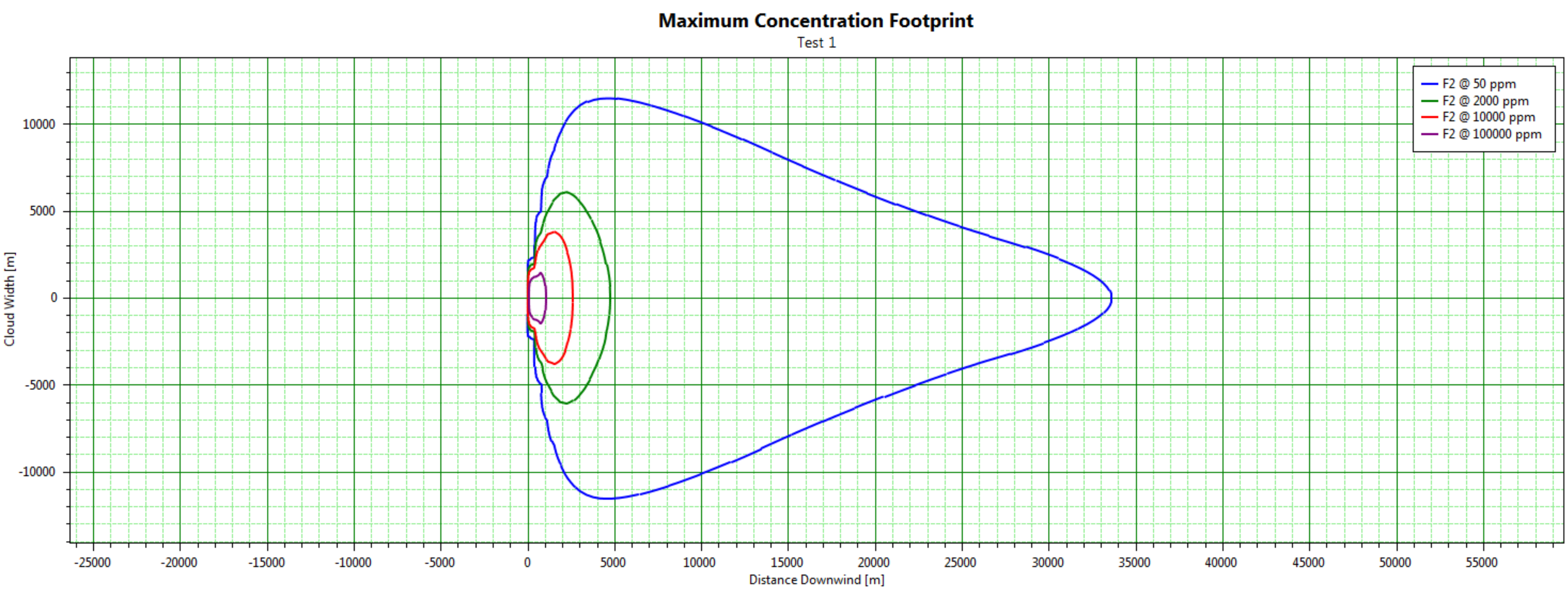
Flammable?

Phast. Vertical downwards

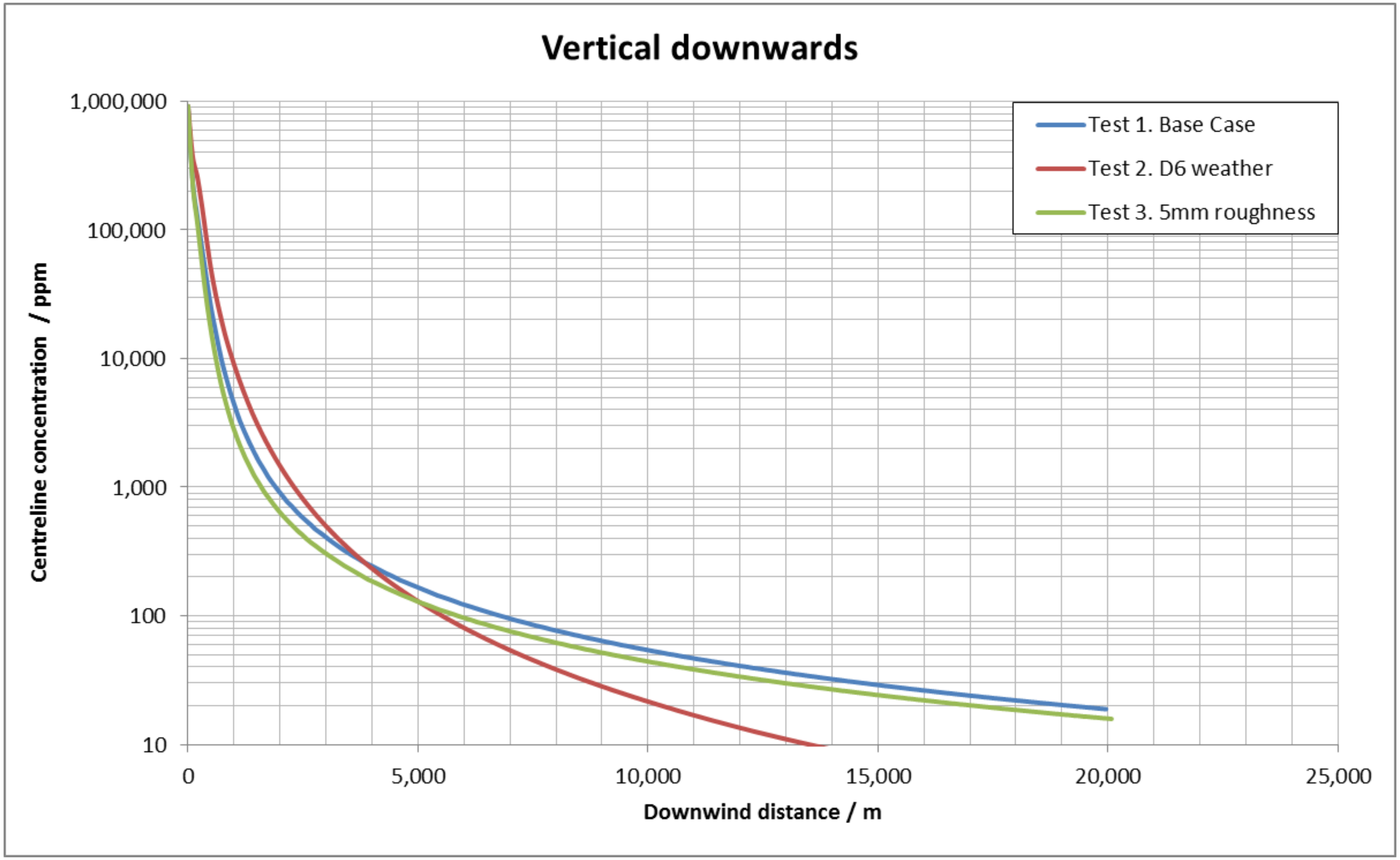


Phast. Vertical downwards (Test 1)

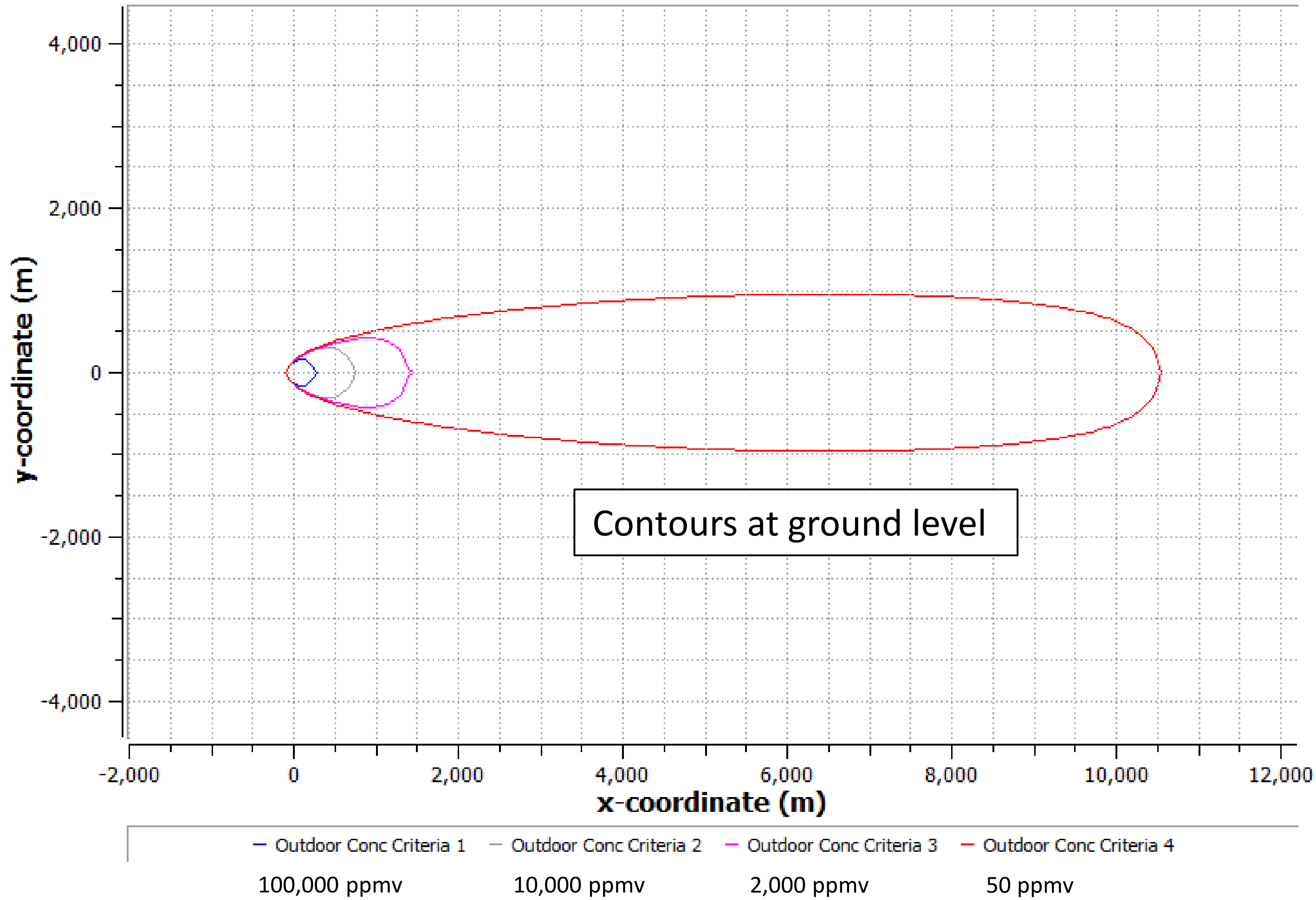
Contours at ground level



Drift. Vertical downwards

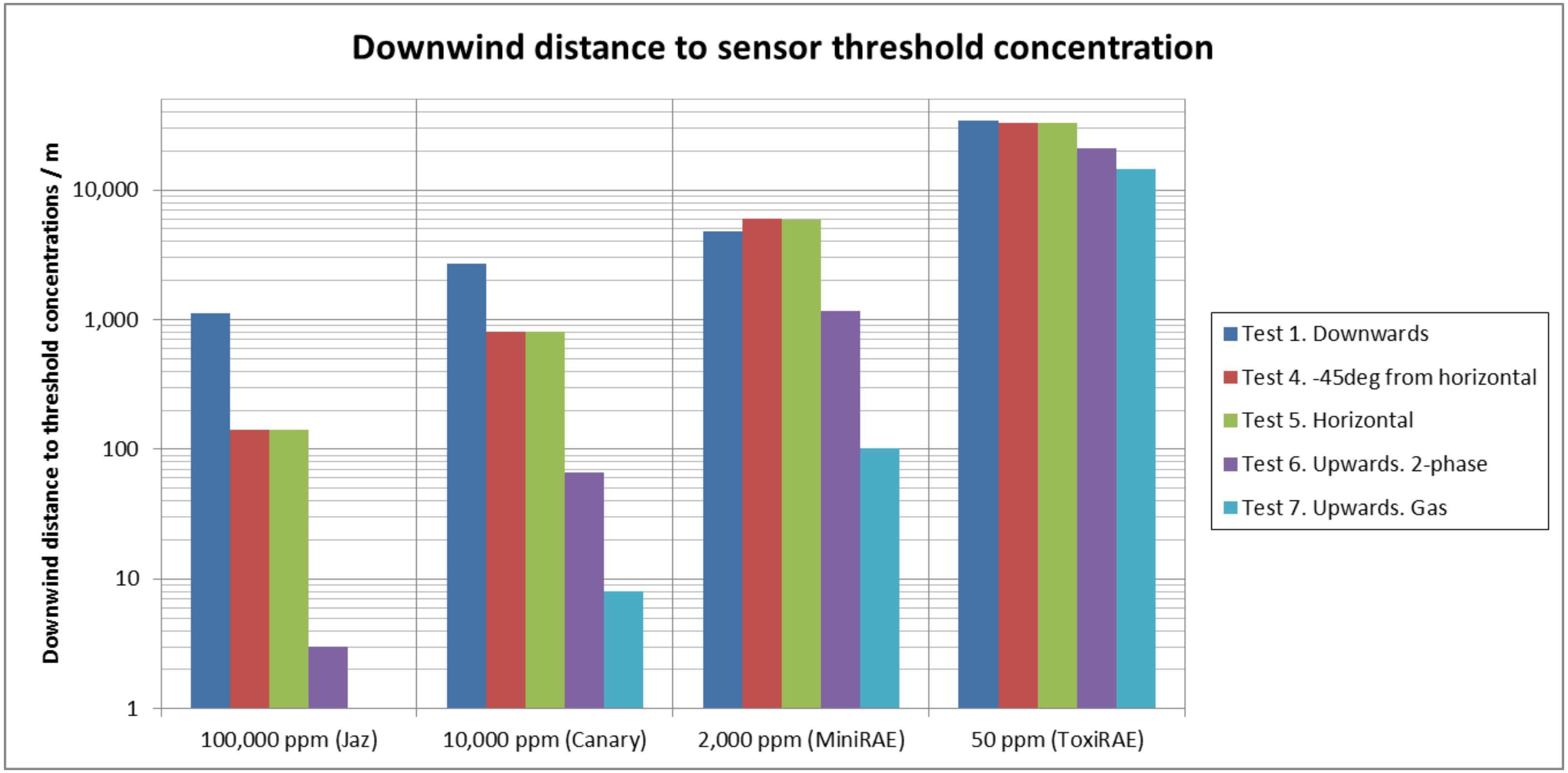


Drift. Vertical downwards (Test 1)



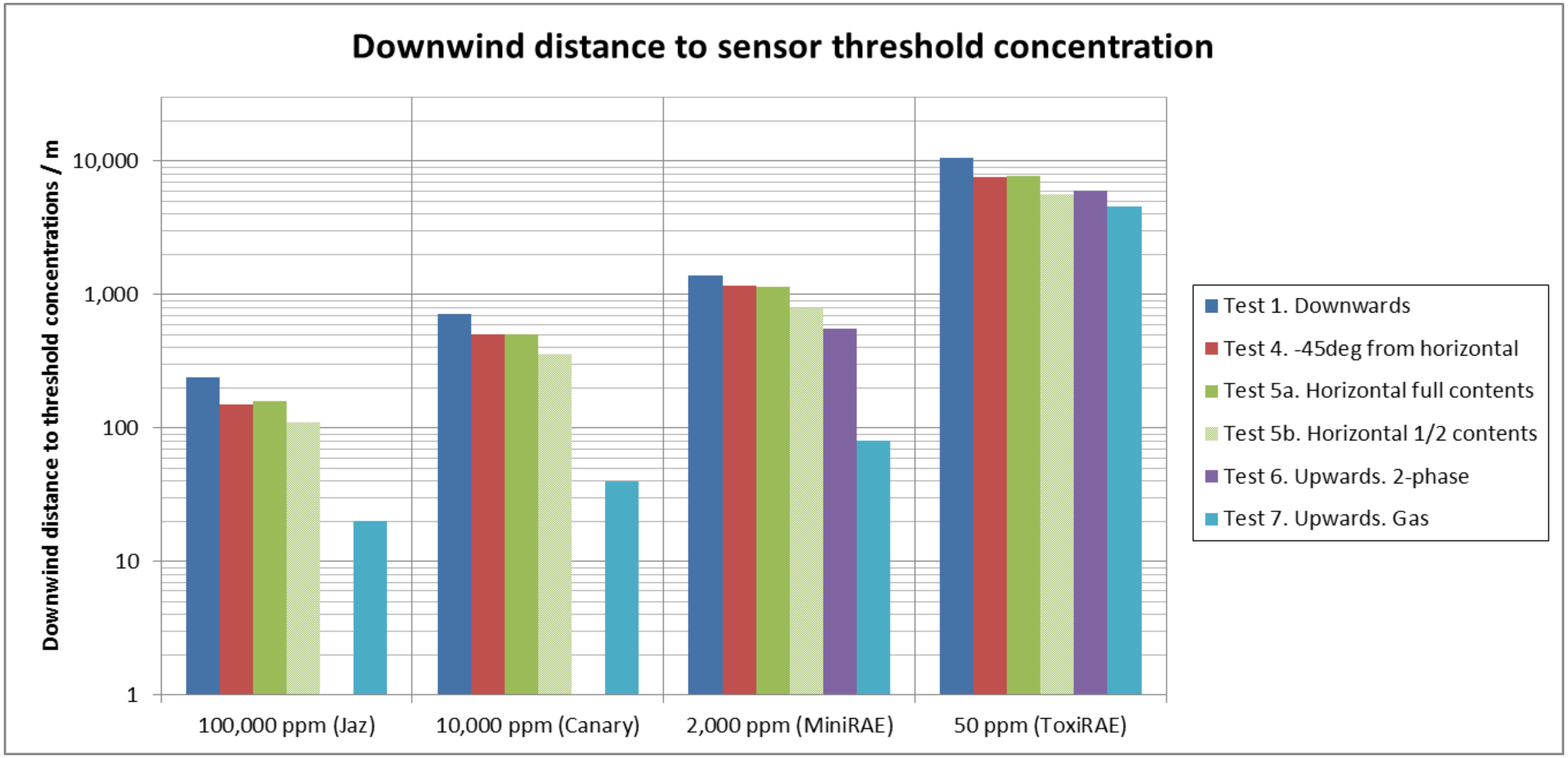
Phast Results Summary

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



Drift Results Summary

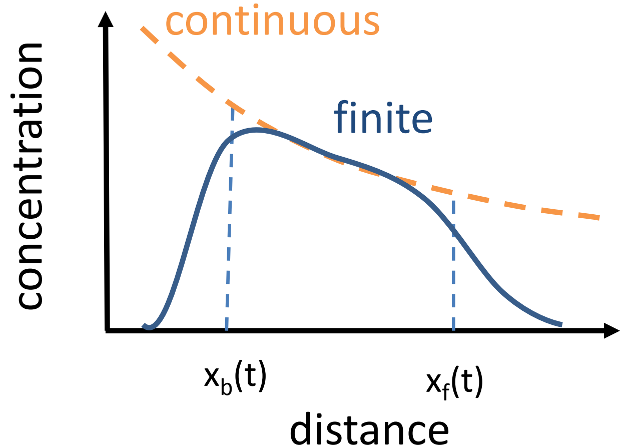
- Main question: will sensors reach saturation (maximum) concentration and not record useful data?



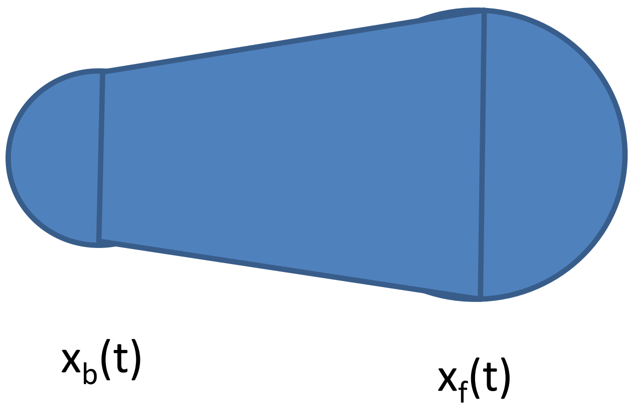
PHAST Model

- Equation-of-state
  - **Default PHAST EOS** since it provides more accurate liquid density for chlorine from DIPPR than SRK or Peng-Robinson EOS
- Orifice flow
  - **Meta-stable liquid** since it gives higher mass flow rate than flashing in the orifice
  - **Compressible flow** since it gives slightly higher mass flow rate than Bernoulli
- Jet expansion to atmospheric pressure
  - **Conservation of Momentum** model: more accurate velocity than isentropic model
- Droplet Size Model
  - **DNV Phase III JIP model**: appropriate for use with Conservation of Momentum jet expansion model (choice has no effect on dispersion results)
- Averaging time
  - **18.75 s** : i.e. no time averaging in PHAST, in order to match short averaging time of sensors and predict peak concentrations

DRIFT Finite-Duration Model



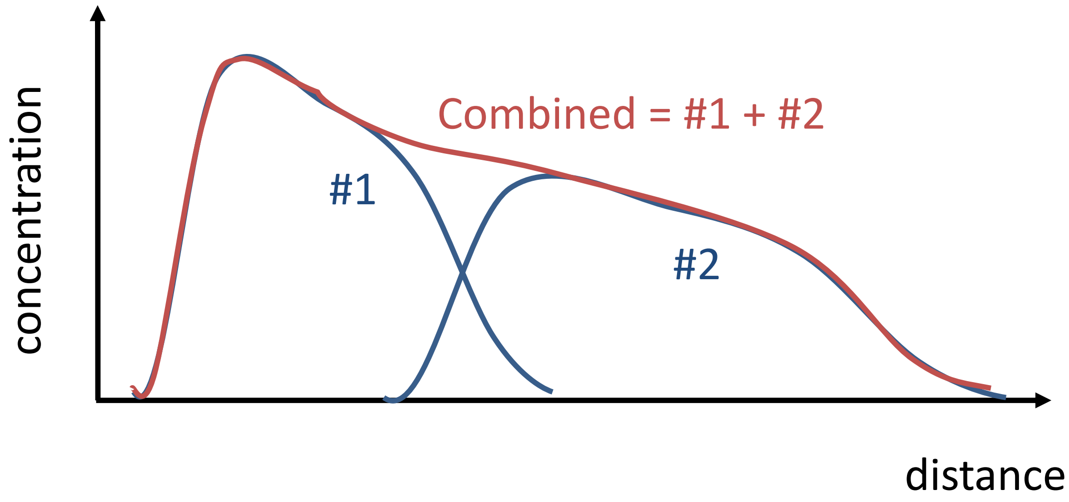
Centreline Concentration



Cloud Shape

DRIFT Time-Varying Model

- Split into finite-duration segments
- Add concentrations



DRIFT Modelling Assumptions (1)

- Aerosol modelling
  - Flash expansion of superheated liquid in jet phase
  - Vaporisation based upon homogeneous equilibrium
  - Liquid chlorine assumed to form ideal solution with condensed water
- Low-momentum area source
  - Neglects jet entrainment after impingement, but accounts for gravity spreading (and gravity driven edge entrainment)
- Finite-duration dispersion model includes
  - Along-wind and across-wind spreading of the cloud (gravity and passive)
  - Shear leaning of the cloud when passive

DRIFT Modelling Assumptions (2)

- Terrain
  - Horizontal flat ground

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