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

Harmo 18 conference, Bologna, 9–12 October 2017

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

Graham Tickle (GT Science & Software)

Henk Witlox (DNV GL)

Jack Rabbit II Phase 1 (2015)

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

Homeland Security
Science and Technology

Transport Canada

DEFENCE RD DÉFENSE

Release conditions

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

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

Modelling methodology

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

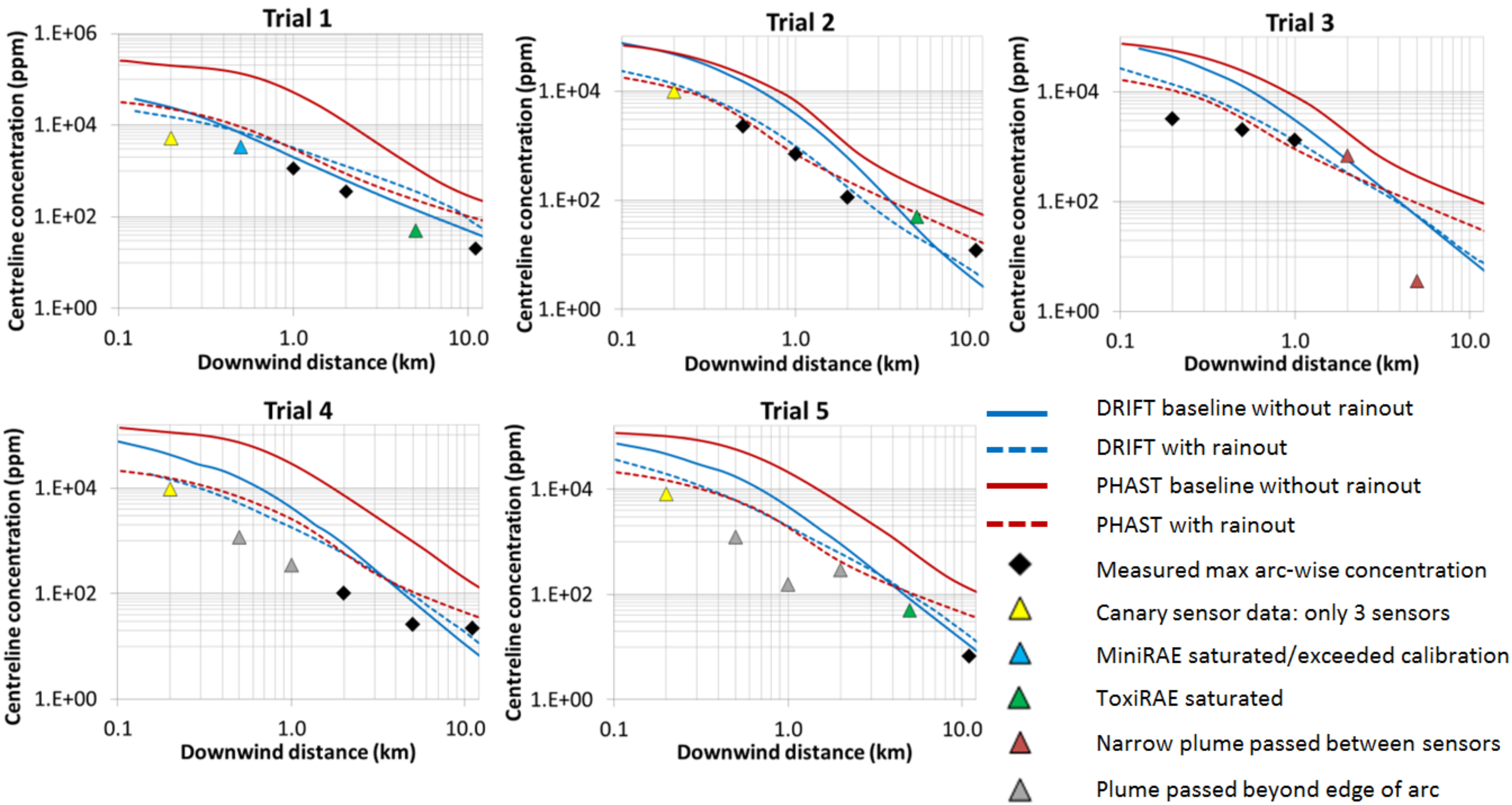
Drift 3.7.2 (ESR Technology)

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

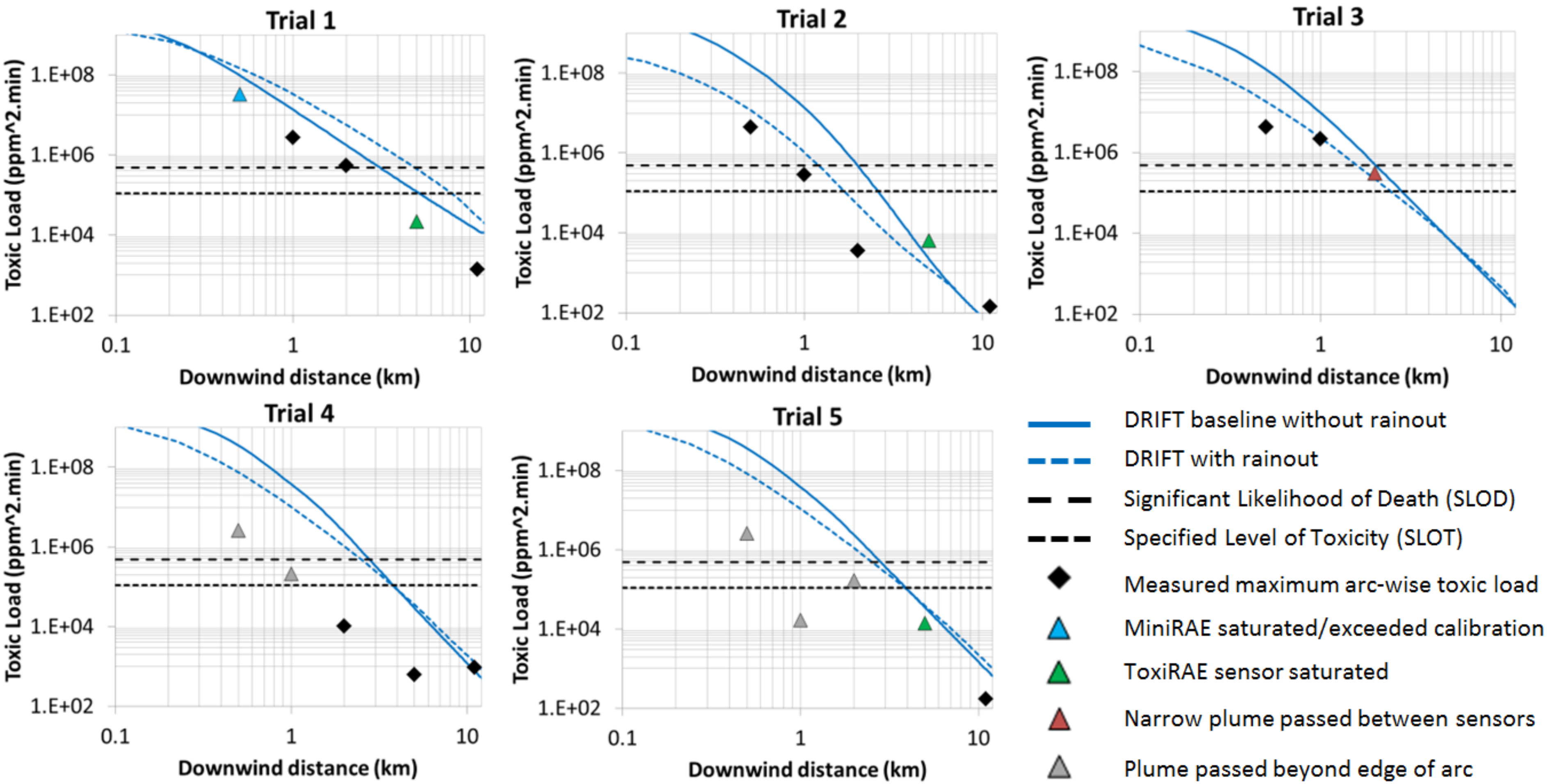
Phast 7.11 (DNV GL)

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

Comparison of concentration data



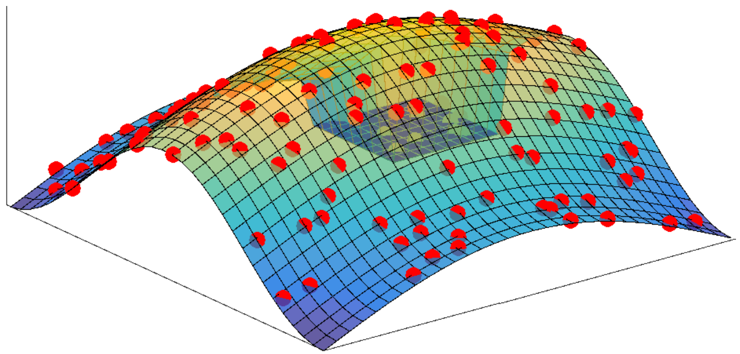
Comparison of Toxic Load data



SLOT/SLOD values available from http://www.hse.gov.uk/chemicals/haztox.htm

Global Sensitivity Analysis using Drift

- Vary all parameters simultaneously



- Benefits
  - Results do not depend on choice of baseline
  - Information provided on interactions between inputs

Range of model inputs and outputs

- Model inputs:
  - Chosen based on Jack Rabbit II experimental ranges and uncertainties:

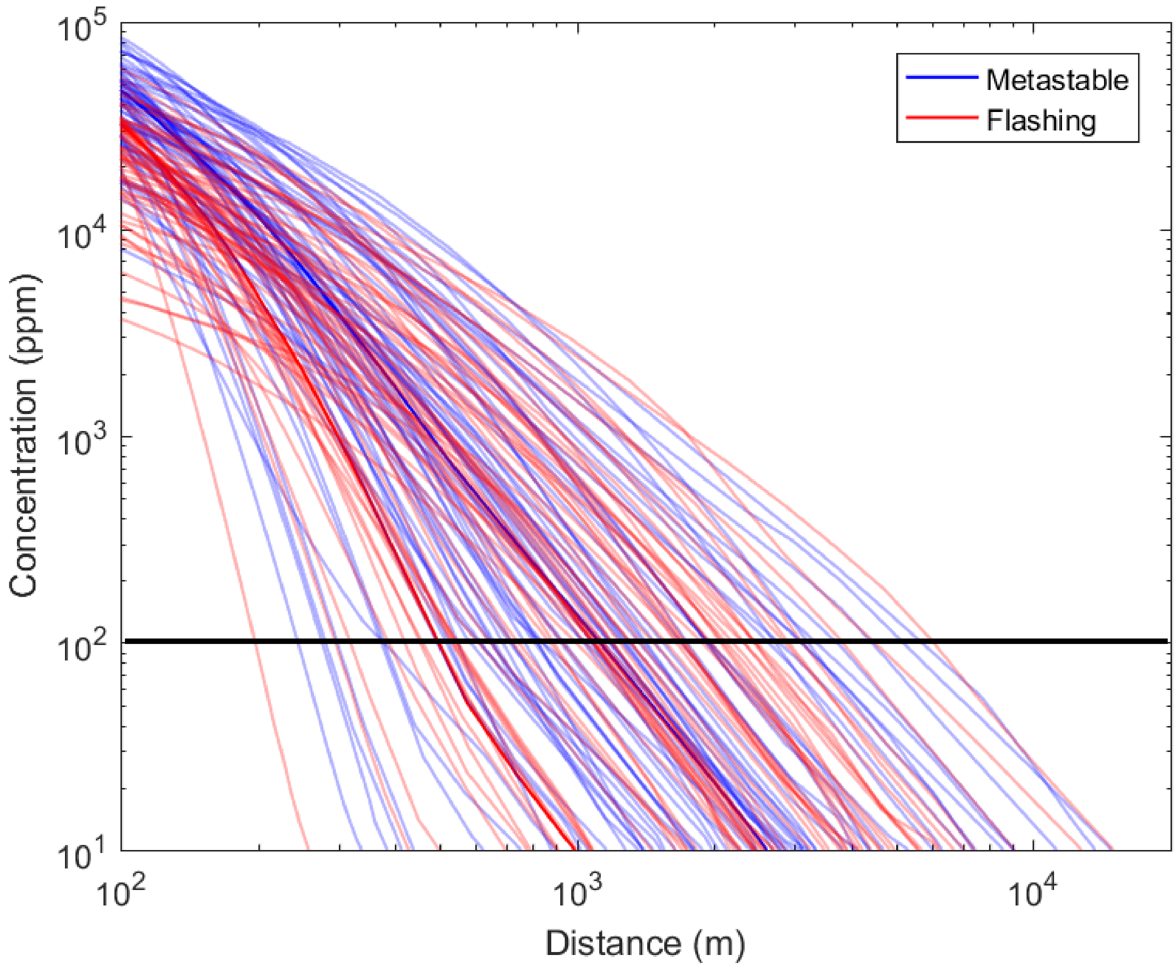
Inventory (kg)	DRIFT Rainout Fraction	Wind Speed at 2m reference height (m s^{-1})	Temperature (K)	1/Monin-Obukhov Length (m^{-1})	Vapour Deposition Velocity (cm s^{-1})
4000	0	1.5	288	-0.12	0
9000	1	5	303	0.08	5

  - Flashing or metastable release
- Model output: Distance to 100 ppm concentration

Global Sensitivity Analysis method

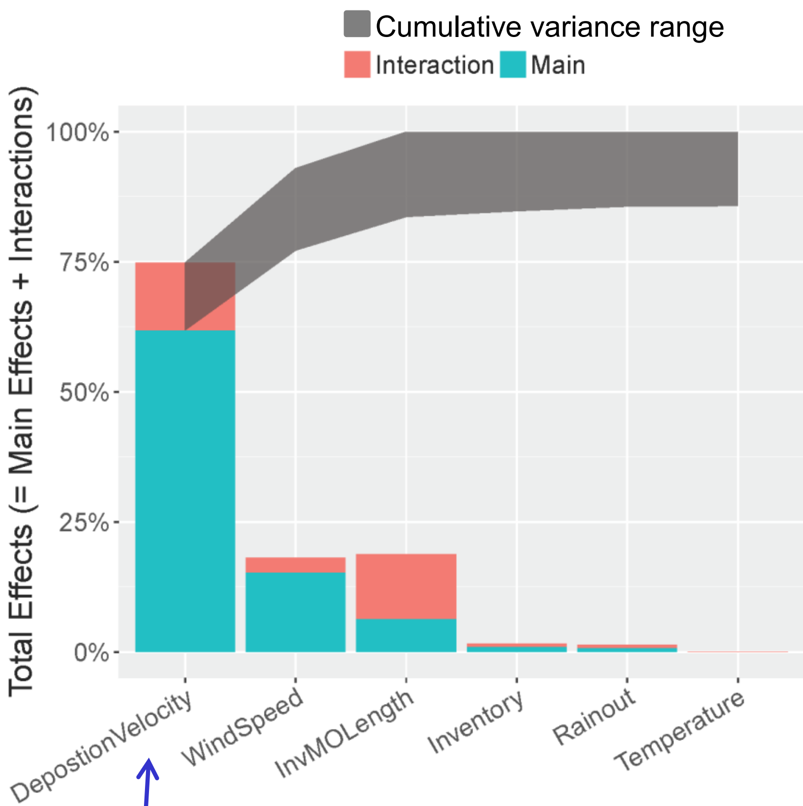
- Gaussian Emulation Machine (GEM) software
  - https://www.tonyohagan.co.uk/academic/GEM/
- Emulator constructed from 127 Drift simulations
  - Sobol' sequence sampling method
    - 64 with metastable release
    - 63 with flashing release
- Cross-validation checks performed to ensure emulator produces a good fit to the Drift results
- Sensitivity analysis results:
  - Which inputs affect the outputs? (Variance: main and total effects)
  - How do the inputs affect the outputs? (Mean-based analysis)

Drift results used to build emulator

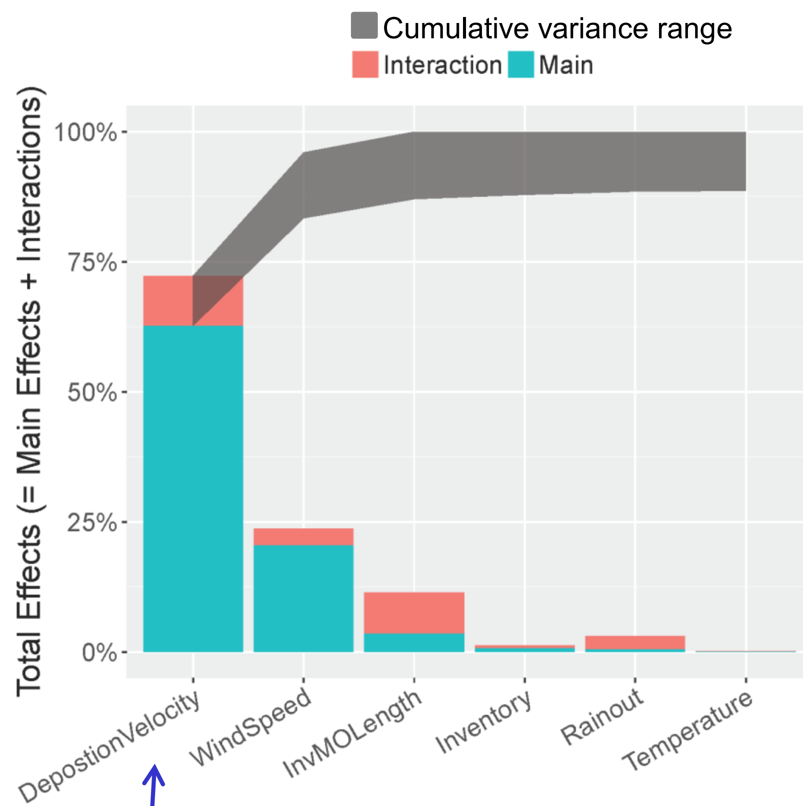


Sensitivity analysis based on predicted distance to 100 ppm concentration

Main and total effects on Lowry Plot



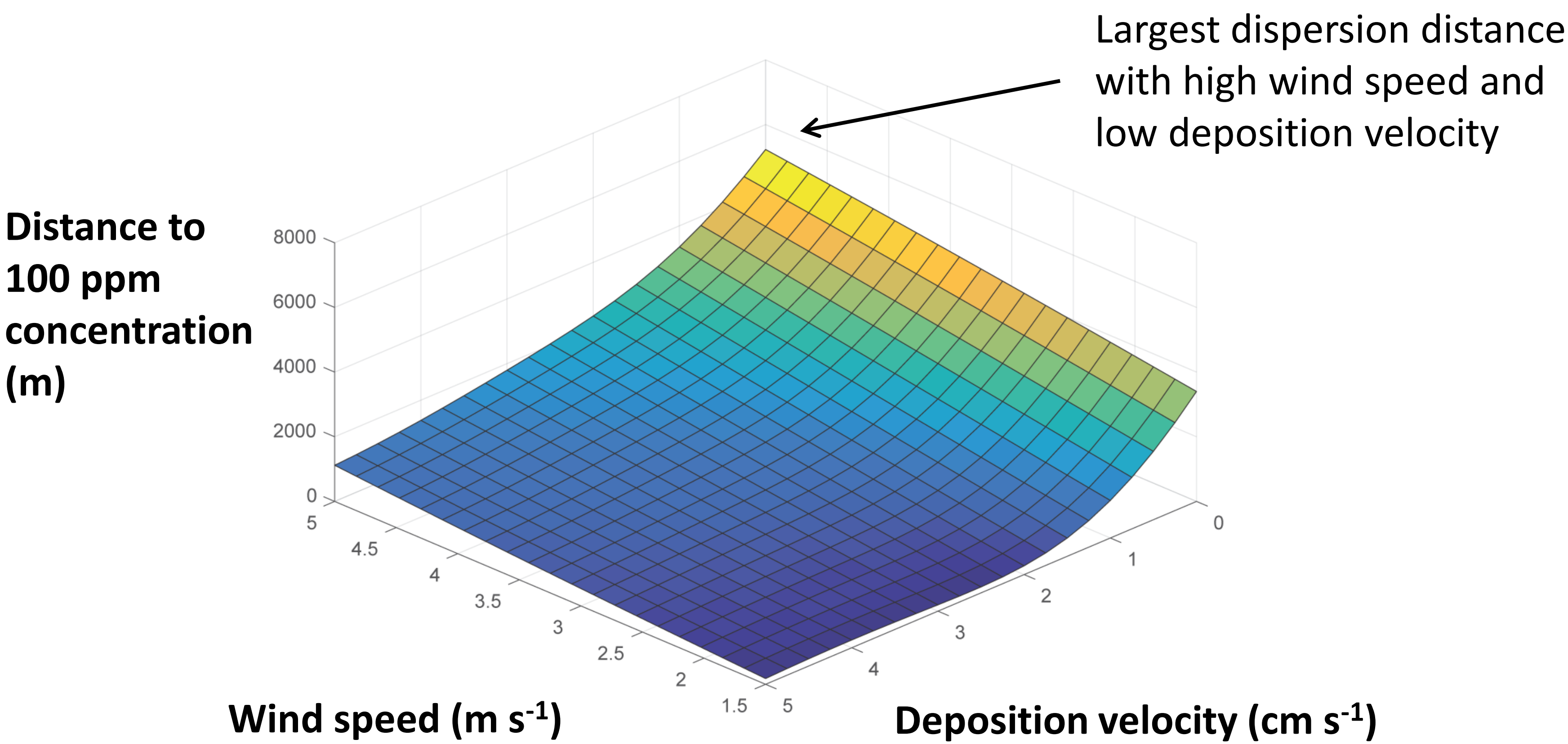
Metastable



Flashing

Deposition velocity has the strongest effect on the results

Surface plot showing physical effects



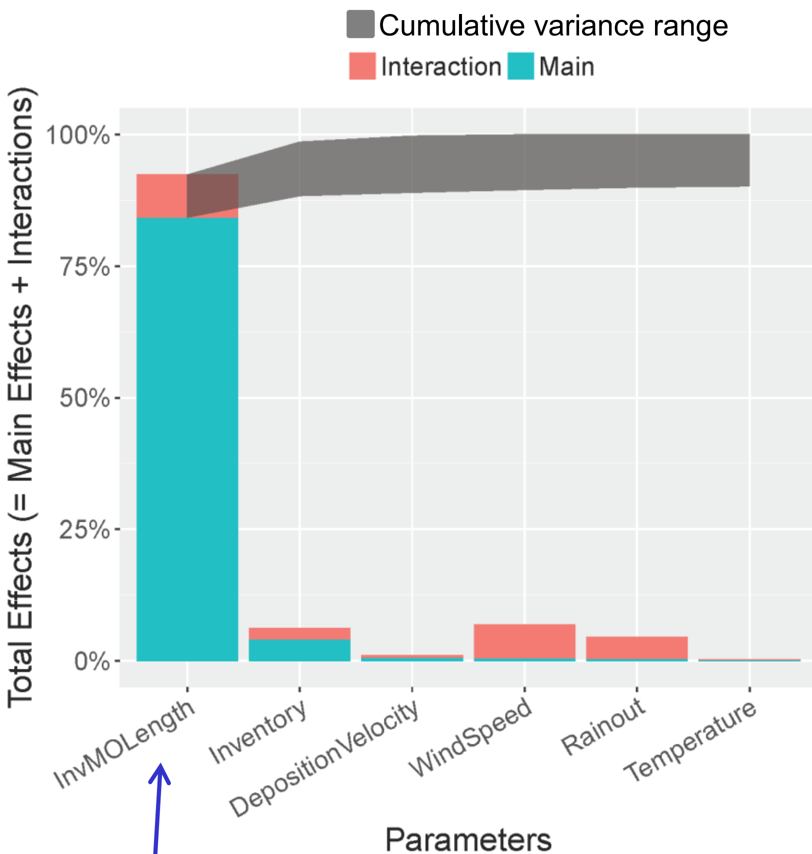
Range of model inputs and outputs

- Model inputs:
  - Chosen based on Jack Rabbit II experimental ranges and uncertainties:

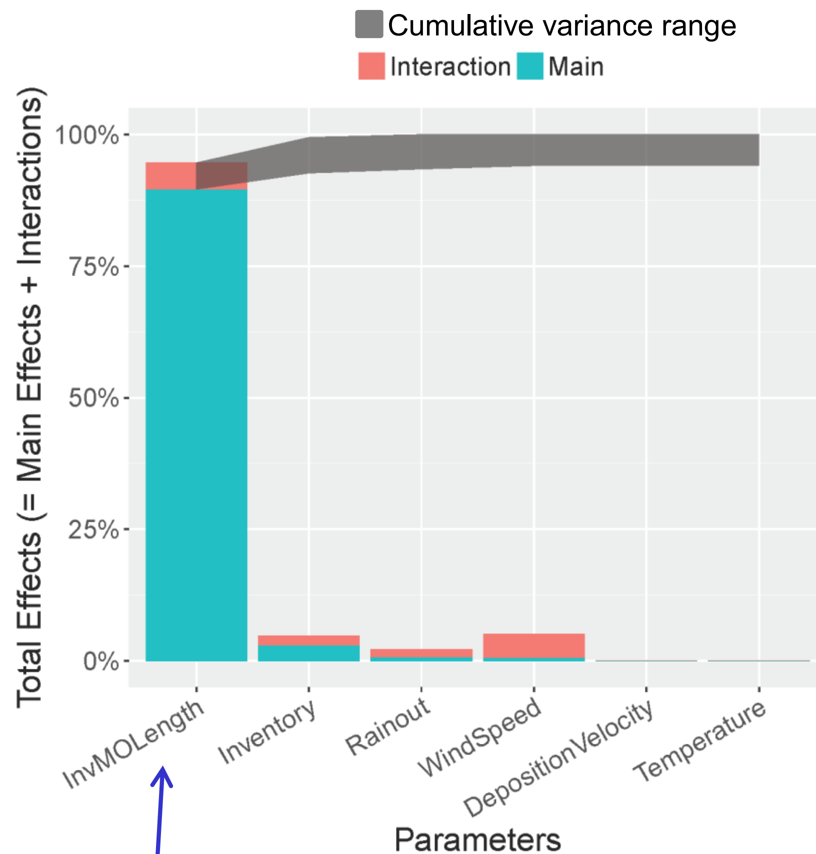
Inventory (kg)	DRIFT Rainout Fraction	Wind Speed at 2m reference height (m s^{-1})	Temperature (K)	1/Monin-Obukhov Length (m^{-1})	Vapour Deposition Velocity (cm s^{-1})
4000	0	1.5	288	-0.12	0
9000	1	5	303	0.08	~~5~~ 0.05

  - Flashing or metastable release
- Model output: Distance to 100 ppm concentration

Deposition velocity range: 0 – 0.05 cm s^{-1}



Metastable



Flashing

Atmospheric stability has the strongest effect on the results

Discussion

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

Discussion

- Inventory probably had little effect here because:
  - 6-inch hole diameter was used in all cases
  - Maximum flow rate remained almost constant (the release duration changed as the inventory changed)
    - Could look at a range of hole sizes to examine any effects of different flow rates
- Catastrophic releases may exhibit different behaviour
- Results from global sensitivity analysis depend on:
  - Defined ranges of the input parameters
  - Choice of model output (in this case, downwind distance to 100 ppm)

Summary

- Drift and Phast models in best agreement with the experimental data when they accounted for rainout, but tended to over-predict concentrations to a greater extent when rainout was ignored
- Global sensitivity analysis using Drift showed that dry deposition could have a dominating effect on the predicted concentrations of these trials if a high deposition velocity of 5 cm s^{-1} was assumed
- However, 5 cm s^{-1} is probably far too high a value for Dugway and further analysis using a lower dry deposition value of 0.05 cm s^{-1} showed that atmospheric stability (Inverse Monin-Obukhov length) had a dominating effect in that case, with deposition having practically no effect
- Further work on dry deposition is required to understand reasonable modelling assumptions and inputs for chlorine releases

Acknowledgements

- The authors would like to express their sincere thanks to the organisations responsible for funding and managing the Jack Rabbit II trials (primarily U.S. Department of Homeland Security and U.S. Defence Threat Reduction Agency) and the MWG coordinators and participants

- In particular to: Richard Babarsky, John Boyd, Andy Byrnes, Joseph Chang, Shannon Fox, Steven Herring, Steven Hanna, Kevin Luong, John Magerko, Thomas Mazzola, Ronald Meris, Nathan Platt, Thomas Spicer, Jeffry Urban and Jeffrey Weil

Disclaimer

GT Science & Software contributed towards the work on Drift, and DNV GL Software contributed towards the work on Phast, but the Drift and Phast simulations presented in this paper were performed by HSE and have not been independently checked by the software developers.

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