RESEARCH AND GUIDANCE FROM HSE

DRIFT Modeling and Sensitivity Analysis of Pressure-liquefied Ammonia Releases

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Research - HSE funded to provide evidence which underpins its policy and regulatory activities
Guidance - freely available to help people comply with health and safety law

Contents

Pressure-liquified ammonia releases

Atmospheric conditions

- Monin-Obukhov length
- Wind speed
- Turbulence levels
- Atm. conditions (P_{atm}, T_{atm})
- Relative humidity

Source conditions

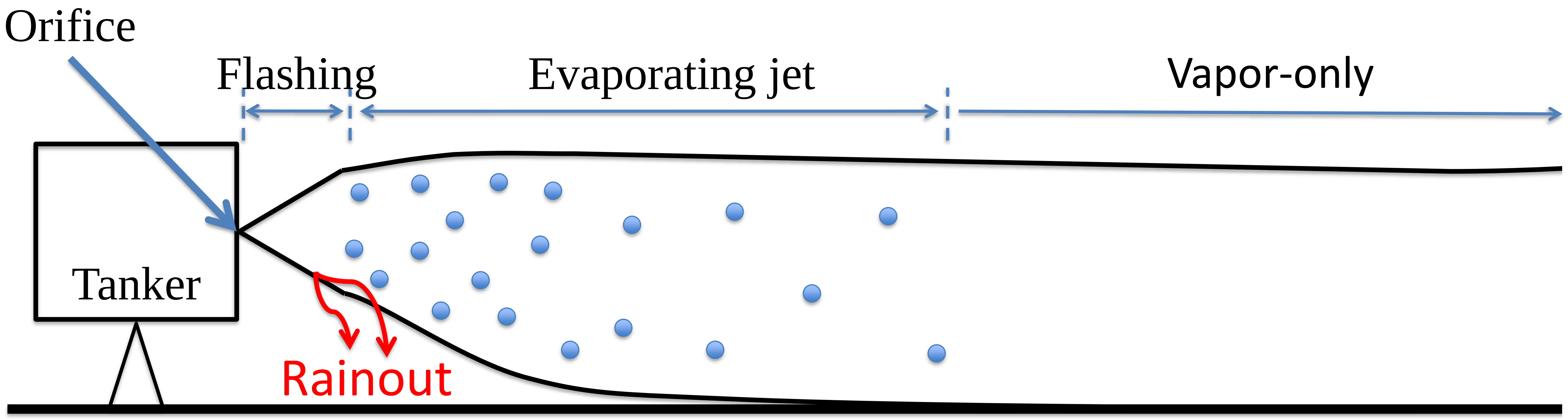
- Orifice geometry
- Orifice conditions (P, T)

Terrain

- Surface roughness
- Standing water

Misc

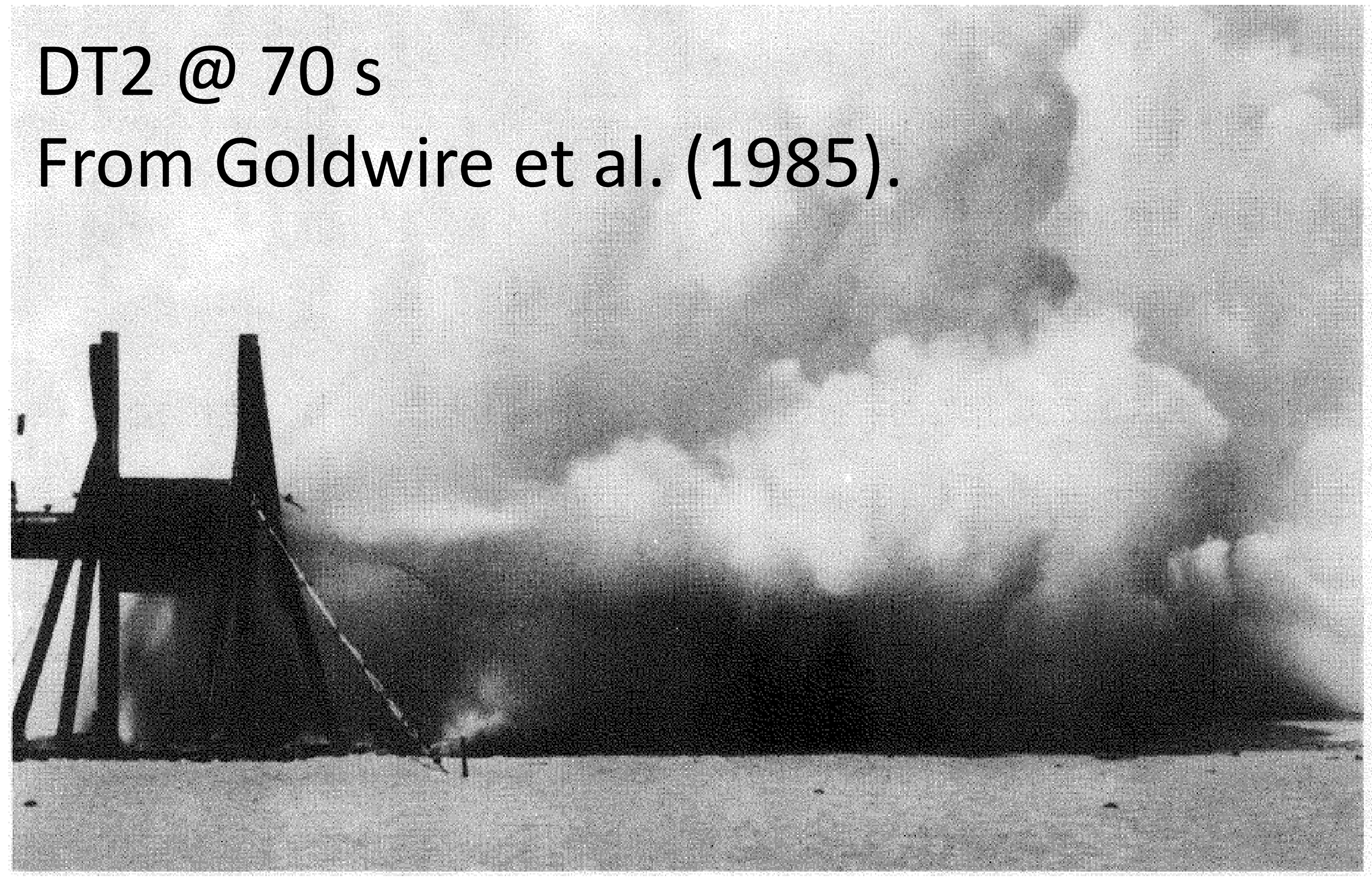
- Rainout



Typical pressure-liquified release.

Desert Tortoise and FLADIS trial description

- The Jack Rabbit III Modelers Working Group (MWG) has been coordinating an international model inter-comparison exercise
- Six pressure-liquefied ammonia release experiments from the Desert Tortoise (1983) and FLADIS (1993-4) trials have been studied
- Modellers provided with set of baseline input parameters



Model input conditions

	DT1	DT2	DT4	FL09	FL16	FL24
Orifice diameter (m)	0.081	0.0945	0.0945	0.0063	0.004	0.0063
Release height (m)	0.79	0.79	0.79	1.5	1.5	1.5
Exit temperature (K)	294.65	293.25	297.25	286.85	290.25	282.6
Exit pressure (bara)	10.1	11.2	11.8	6.93	7.98	5.70
Release rate (kg s^{-1})	80.0	117.0	108.0	0.40	0.27	0.46
Release duration (s)	126	255	381	900	1200	600
Friction velocity (m s^{-1})	0.442	0.339	0.286	0.44	0.41	0.405
Surface roughness (m)	0.003	0.003	0.003	0.04	0.04	0.04
Ambient temperature (K)	301.95	303.55	305.55	288.65	289.65	290.65
Ambient pressure (bara)	0.909	0.909	0.903	1.02	1.02	1.013
Wind speed (m s^{-1})	7.42	5.76	4.51	6.1	4.4	4.9
Monin-Obukhov length (m)	92.7	94.7	45.2	348	138	-77
Relative humidity (%)	13.2	17.5	21.3	86	62	53.6
Rainout mass fraction (%)	5	5	5	0	0	0
Averaging time (s)	80	160	300	600	600	400

Source conditions (Orifice diameter to Release duration)

Atmospheric conditions and terrain (Friction velocity to Relative humidity)

Sensitivity inputs (Wind speed, Monin-Obukhov length, Relative humidity, Rainout mass fraction)

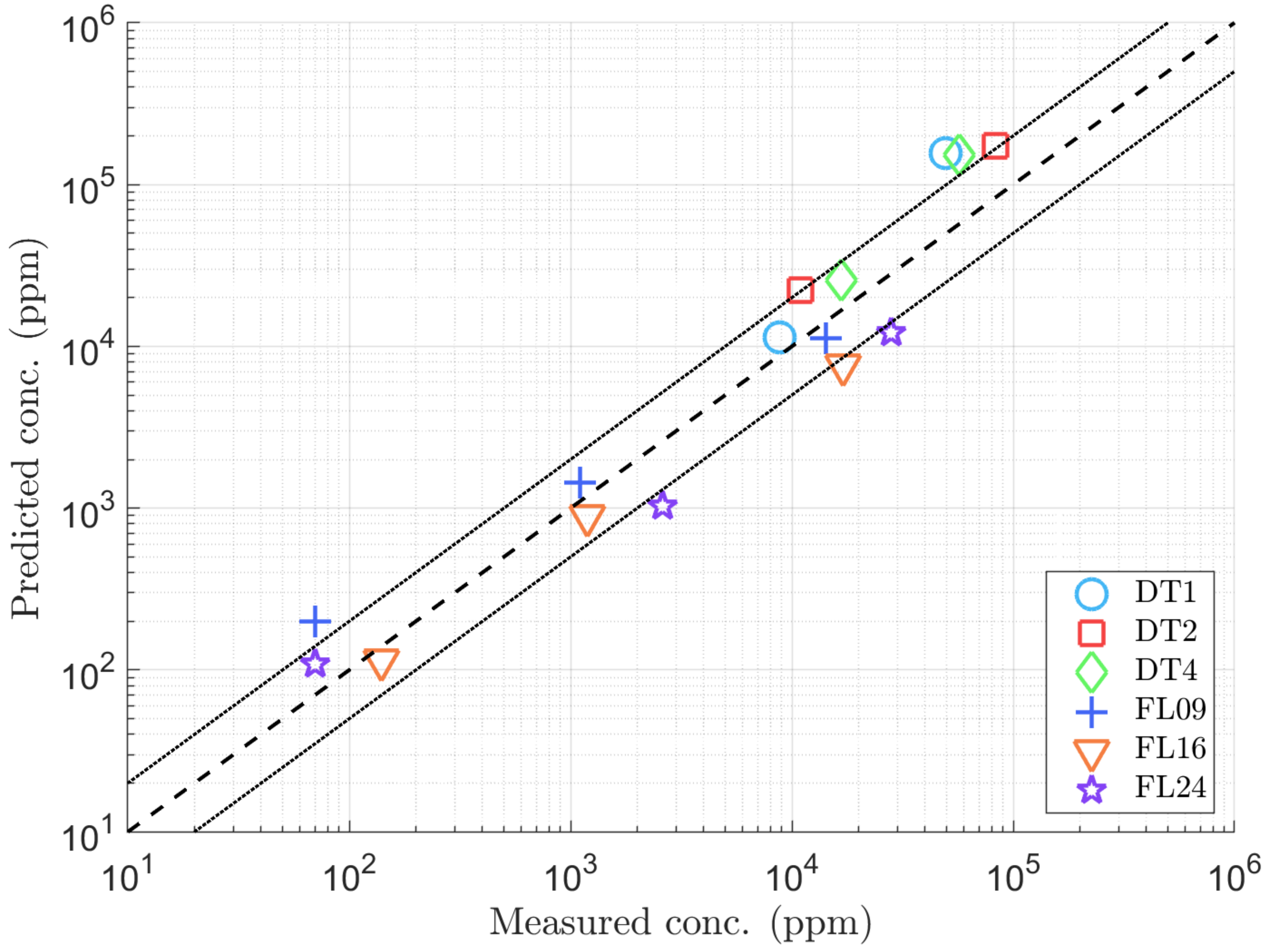
Mostly taken from the SMEDIS database (Carissimo *et al.*, 2001)

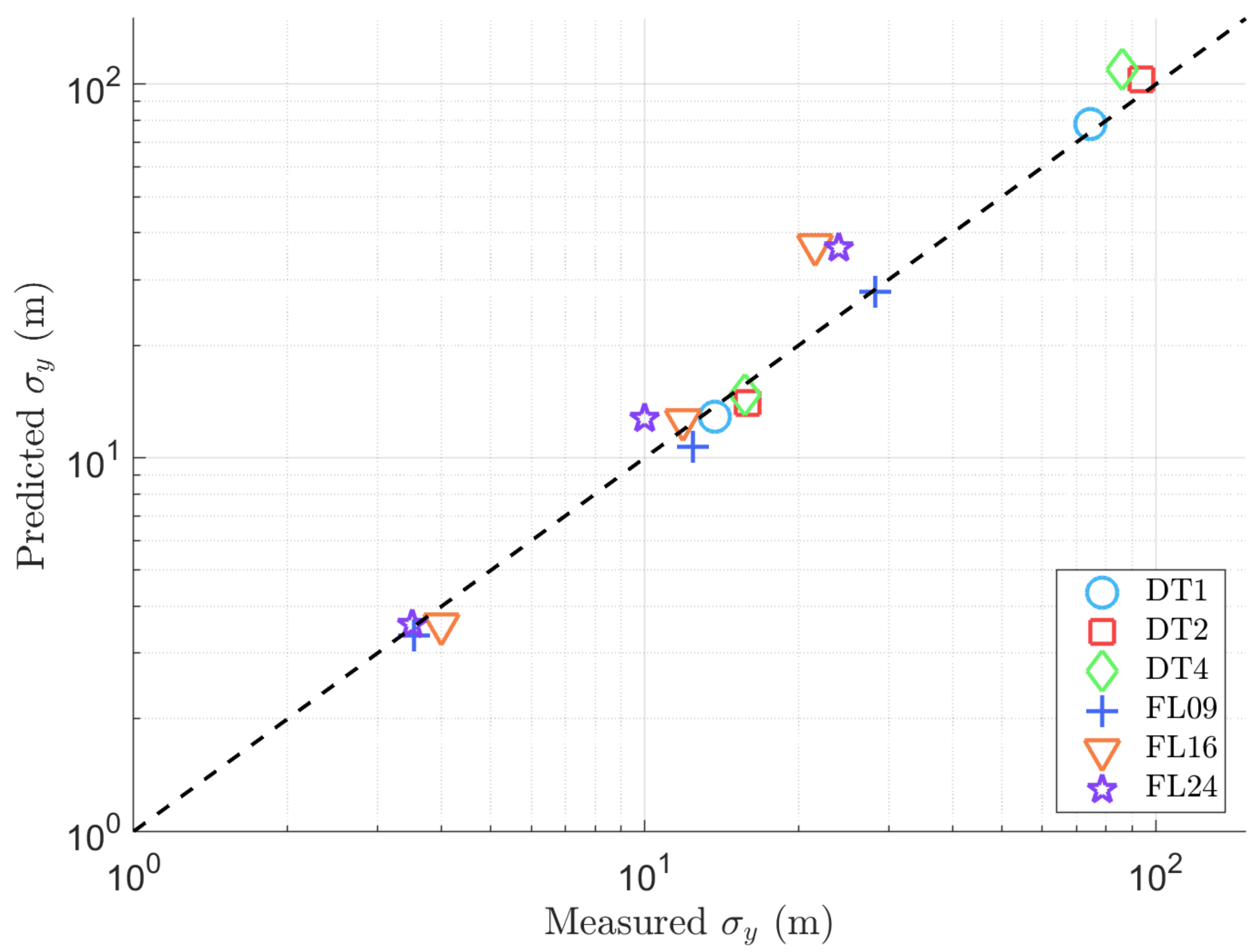
Methodology

- DRIFT v3.7.19 integral model
- Dispersion model, by HSE to model atmospheric dispersion of toxic and flammable substances
- Each run takes < 1 min
- Output: arc-max concentration, cloud shape

Results- comparison with experiment

- Good agreement found with previous experimental results for concentration and cloud width σ_y

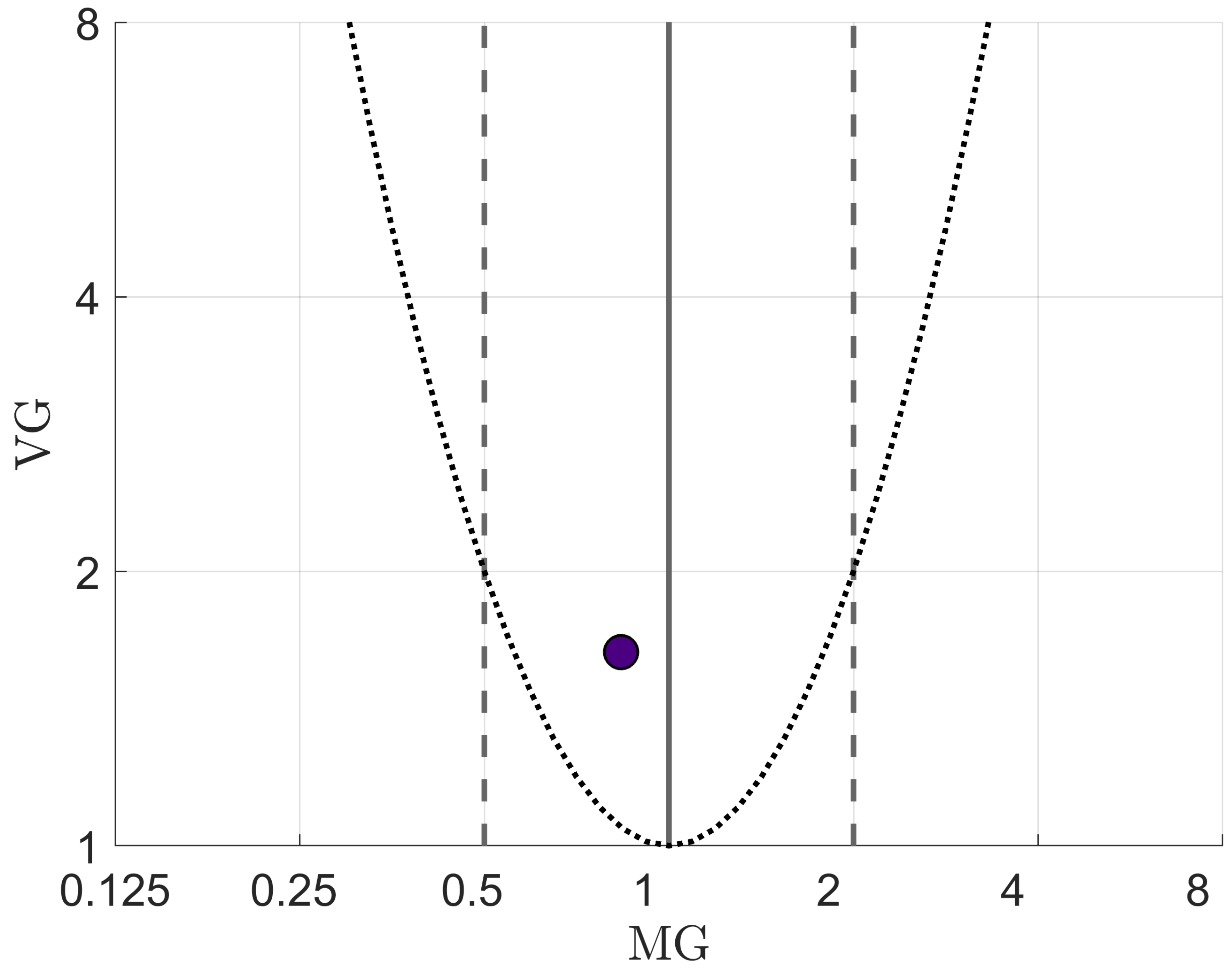




Results- comparison with experiment

- Model evaluation statistics, MG, VG, FAC2

Measure	Formula	Value
Geometric Mean Bias (MG)	$\exp\left[\langle \ln\left(C_0 C_p^{-1}\right)\rangle\right]$	0.83
Geometric Variance (VG)	$\exp\left[\langle \ln\left(C_0 C_p^{-1}\right)^2\rangle\right]$	1.63
Fraction within a factor of 2 (FAC2)	$0.5 \le C_p C_o^{-1} \le 2$	0.47



Sensitivity runs- methodology

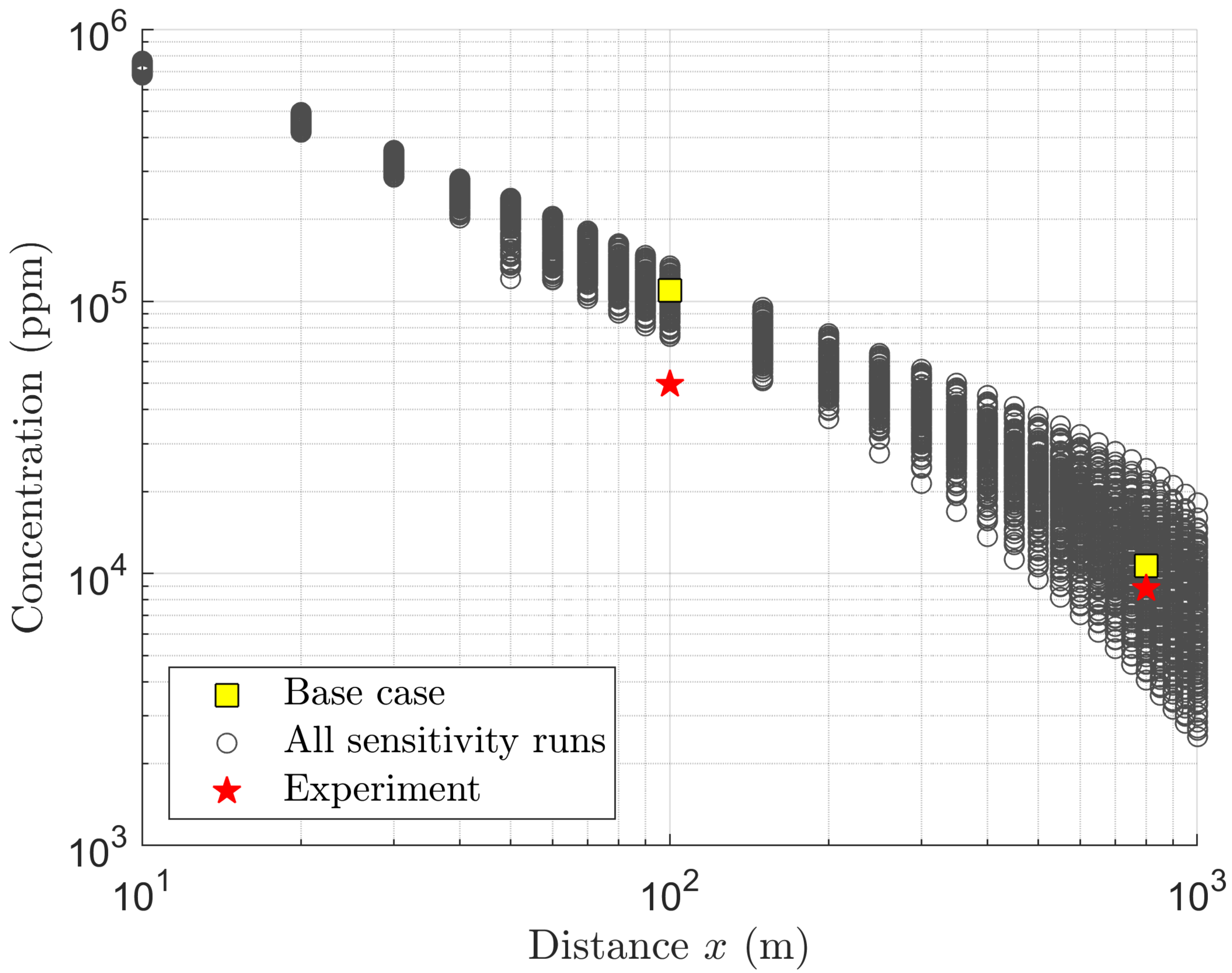
- DT1 chosen for further analysis, due to its similarity with future JRIII experimental releases
- Parameters varied: liquid rainout, wind speed, Monin-Obukhov length, relative humidity
- Total of 150 DRIFT runs carried out, feeding into a Gaussian process emulator to perform a global sensitivity analysis

Input parameter	Min	Max
Wind speed (m s^{-1})	2	6
Inverse Monin-Obukhov length (m^{-1})	-0.07	0.01
Relative humidity (%)	5	60
Rainout mass fraction (%)	0	40

Sensitivity runs- all plots

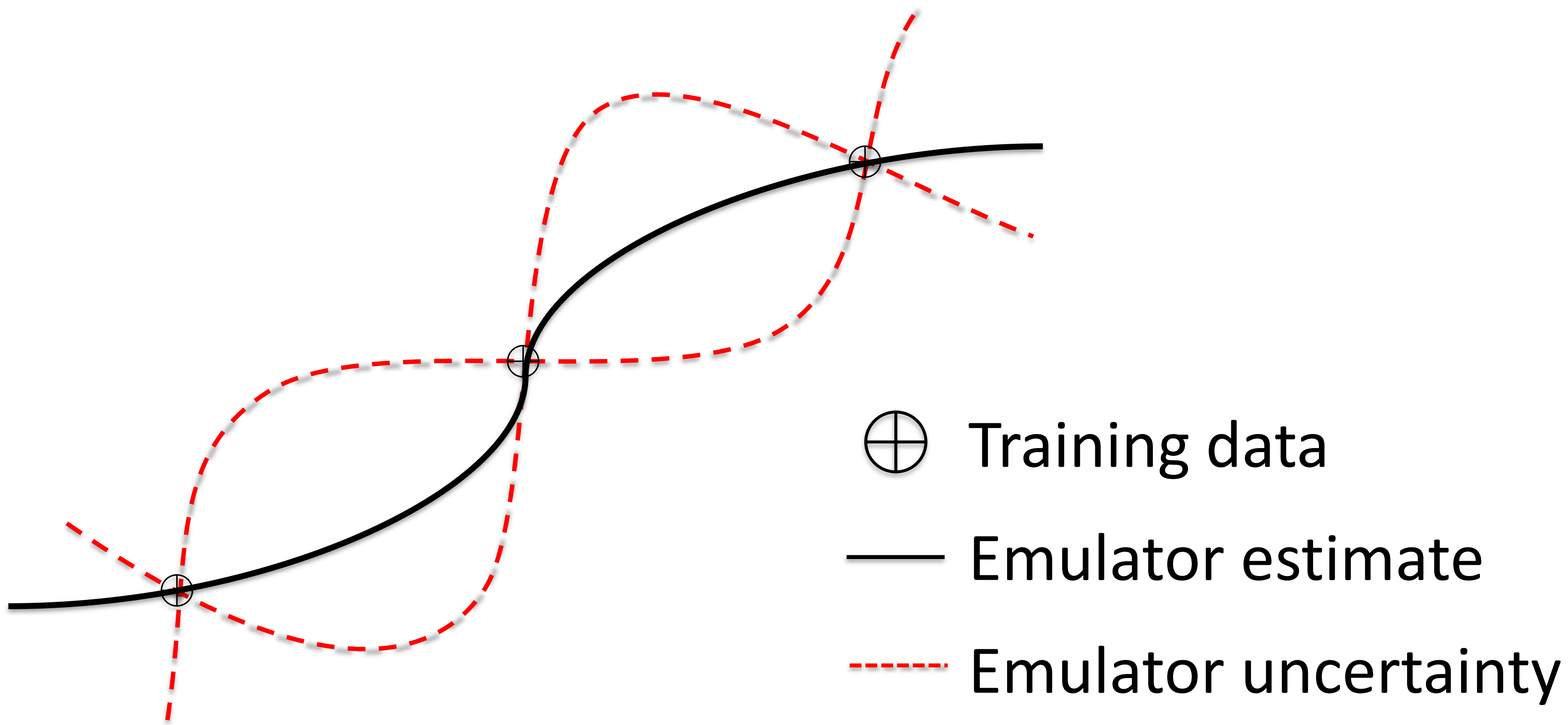
- All 150 profiles are plotted to visualize the range of model outputs.

- Over-prediction at 100 (m).
- Further downstream at 800 m, concentration results are closer to experimental results.
- Increase in spread of concentration at 50 m coincides with the cloud reaching the ground.

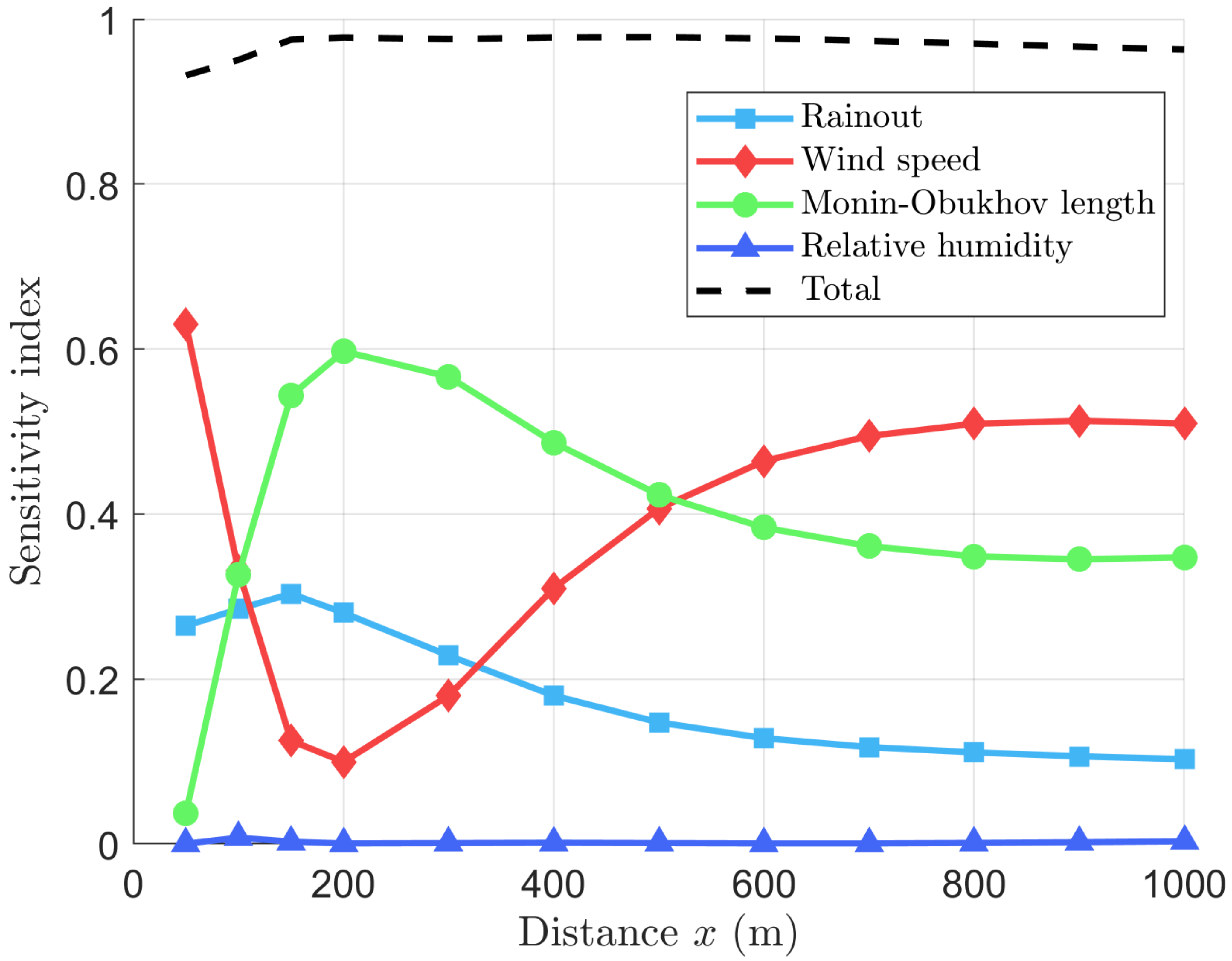


Fitting a Gaussian emulator

- Statistical analysis of $N = 150$ runs carried out using GEM (Gaussian emulator machine)
- Emulator identifies inputs that have a significant influence on downwind concentration
- GEM run for a number of positions along the downwind position x



Gaussian emulator- results



- Sensitivity index plotted as a function of downwind distance x
- 4 input parameters depend on x
- Relative humidity has little influence – could be taken out of future analysis?
- Monin-Obukhov length dominates output at 200 m
- Wind speed dominates further downwind

Conclusions

- Predicted concentrations from DRIFT dispersion model in good agreement with measurements from the Desert Tortoise and FLADIS trials
- Sensitivity analysis showed that:
  - Predicted concentrations are strongly affected by wind speed and atmospheric stability
  - Rainout has a modest effect, which decreases with distance downwind
  - Humidity has very little effect on predicted concentrations
- Running multiple simulations improves understanding of model and input uncertainty
- Could be useful to repeat sensitivity analysis when designing future Jack Rabbit III experiments, to understand potential impact of uncertain and/or variable test conditions

Acknowledgements

Thank you

Any questions?

- The contents of this presentation, including any opinions and/or conclusions expressed, are those of the authors alone and do not necessarily reflect HSE policy