HEALTH & SAFETY LABORATORY

Sensitivity Analysis of Dispersion Models for Jet Releases of Dense-Phase Carbon Dioxide

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Content

- Background to CO_2 dispersion
- Objectives
- Global sensitivity analysis
  - Phast
  - GEM
- CFD simulations
- Conclusions
- Future Directions – possible JIP?

Background

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- Rapid development of Carbon, Capture and Storage (CCS) infrastructure planned in next decade

International Energy Agency (IEA): “CCS will play a vital role … to limit global warming, contributing around one-fifth of required emissions reductions in 2050 …around 100 CCS projects would need to be implemented by 2020”

UK Department of Energy and Climate Change (DECC): “Carbon Capture and Storage (CCS) will play a vital role … [in helping halt the rise in global carbon dioxide emissions] ... CCS is the only technology that can turn high carbon fuels into genuinely low carbon electricity.”

Background

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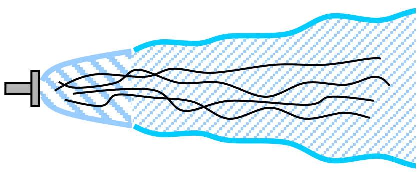
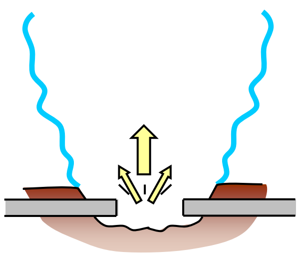
- Need to understand risks posed by pipelines transporting CO_2

Complex Physics

- Two-phase flow



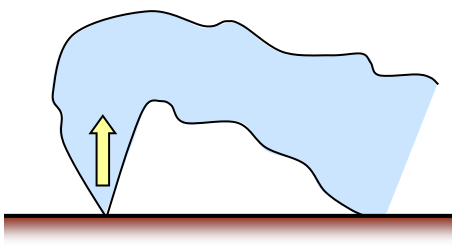
- Craters



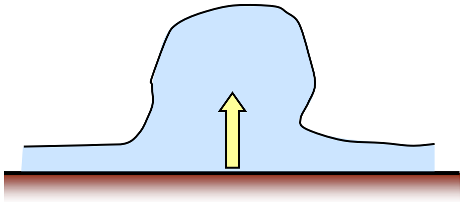
- Deposition of solids
- Humidity effects

Atmospheric B.L.

- Finite wind speed

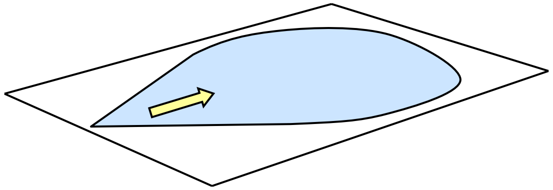


- Low/nil-wind

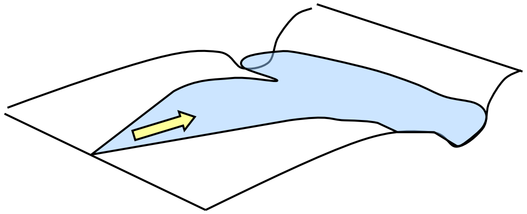


Terrain Effects

- Flat ground



- Topography and obstructions



Objectives

- Which of these inputs (or combinations of inputs) has a significant effect on the dispersion distance?

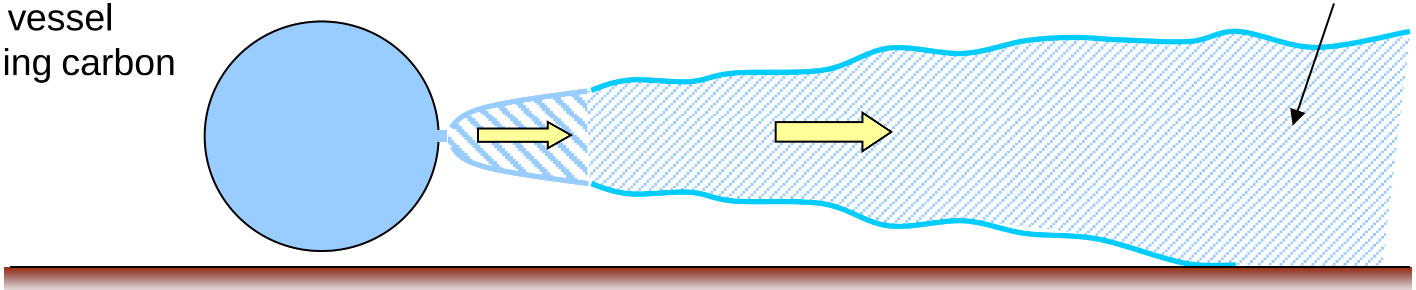
Inputs:

1. Vessel temperature: 5 – 30 ºC
2. Vessel pressure: 100 – 150 barg
3. Orifice size: ½ – 2 inch
4. Wind speed: 0.5 – 50 m/s
5. Ambient humidity: 0 – 100% RH
6. Ground roughness: 0.0001 – 1 m
7. Release height: 0.5 – 3 m

Output of interest:

"Dispersion distance" where concentration reaches 6.9% v/v CO_2

Leak from above-ground vessel containing carbon dioxide



Sensitivity Analysis

- **Option 1: Local sensitivity**:
  - Choose “baseline” case
  - Vary one parameter at a time

- Pros:
  - Conceptually simple and fairly quick

- Cons:
  - How do we choose “baseline” case?
  - No information on interactions between different parameters that vary at the same time

Sensitivity Analysis

- **Option 2: Global Sensitivity**
  - Vary all parameters simultaneously

- Pros:
  - Good coverage of all potential scenarios
  - Includes effects of interactions

- Cons:
  - Costly!
  - Typically requires >10,000 simulations for conventional Monte-Carlo analysis

Sensitivity Analysis

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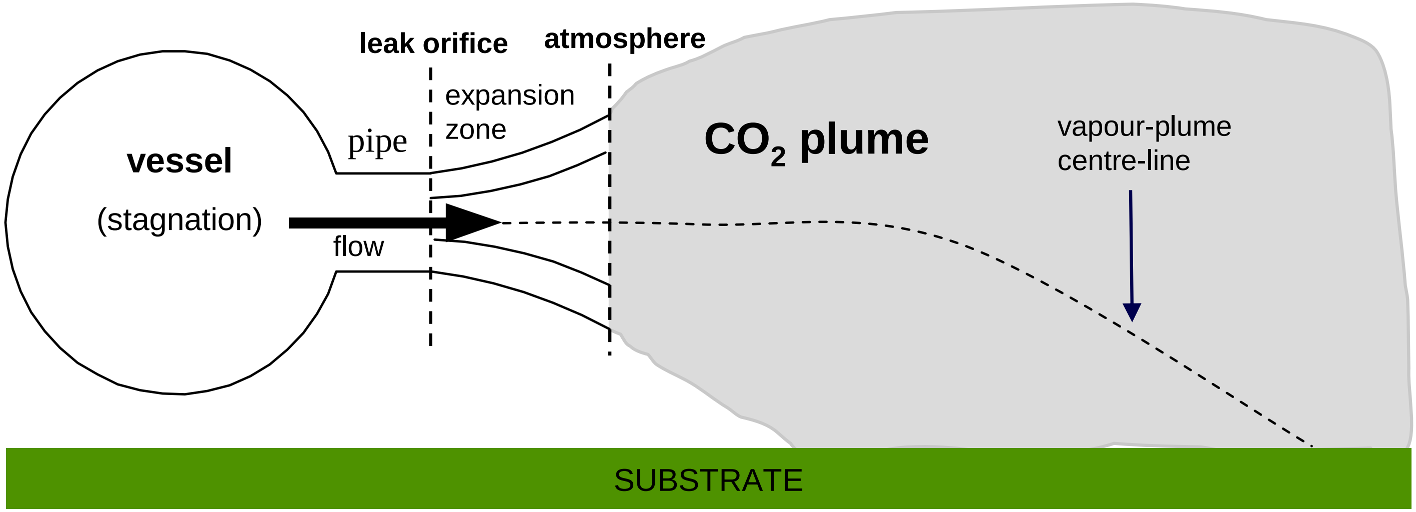
- **Global Sensitivity – the solution?**
  - Construct a *statistical emulator* (i.e. clever curve fit) from the dispersion model output, using a few hundred simulations
  - Run the sensitivity analysis using the emulator
- Pros
  - Fast to run
  - Good coverage and includes effects of interactions
- Cons
  - Need to check emulator provides accurate fit to dispersion model results

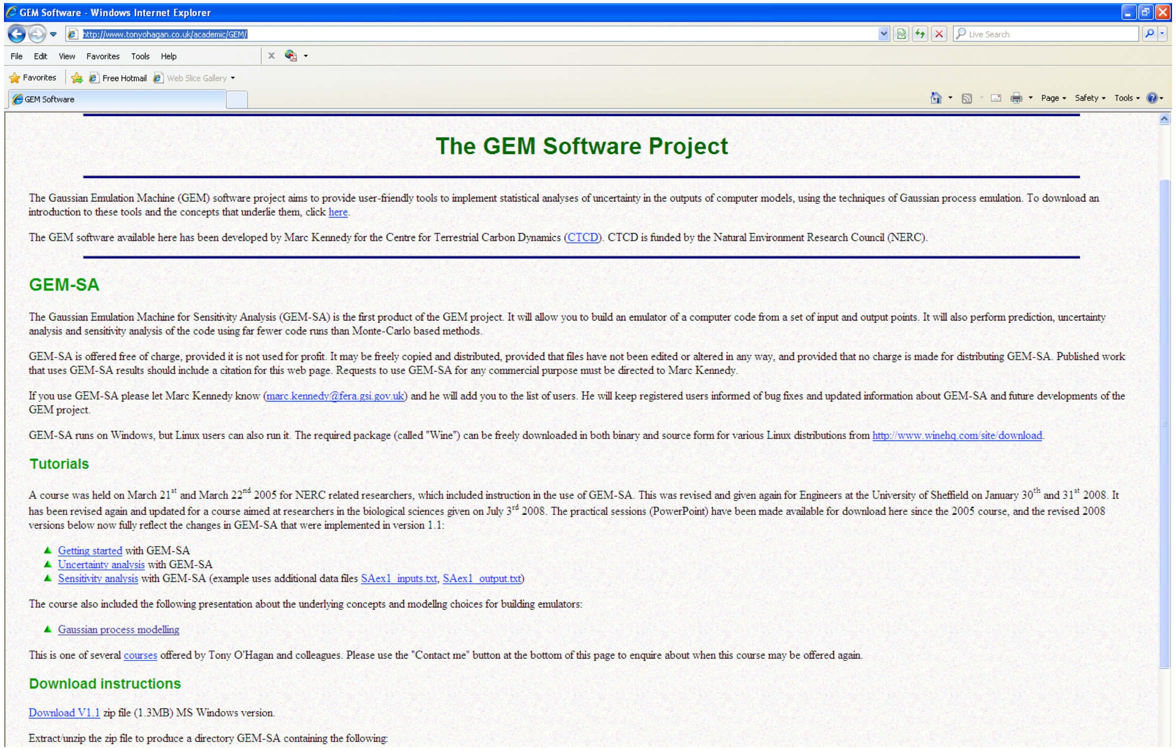
Phast

- Widely used for consequence assessment in process industries
- Integral model: assumes homogenous equilibrium, no rainout, includes humidity effects
- Previously modified to account for solid CO_2 formation
- Validated against CO_2 dispersion experiments

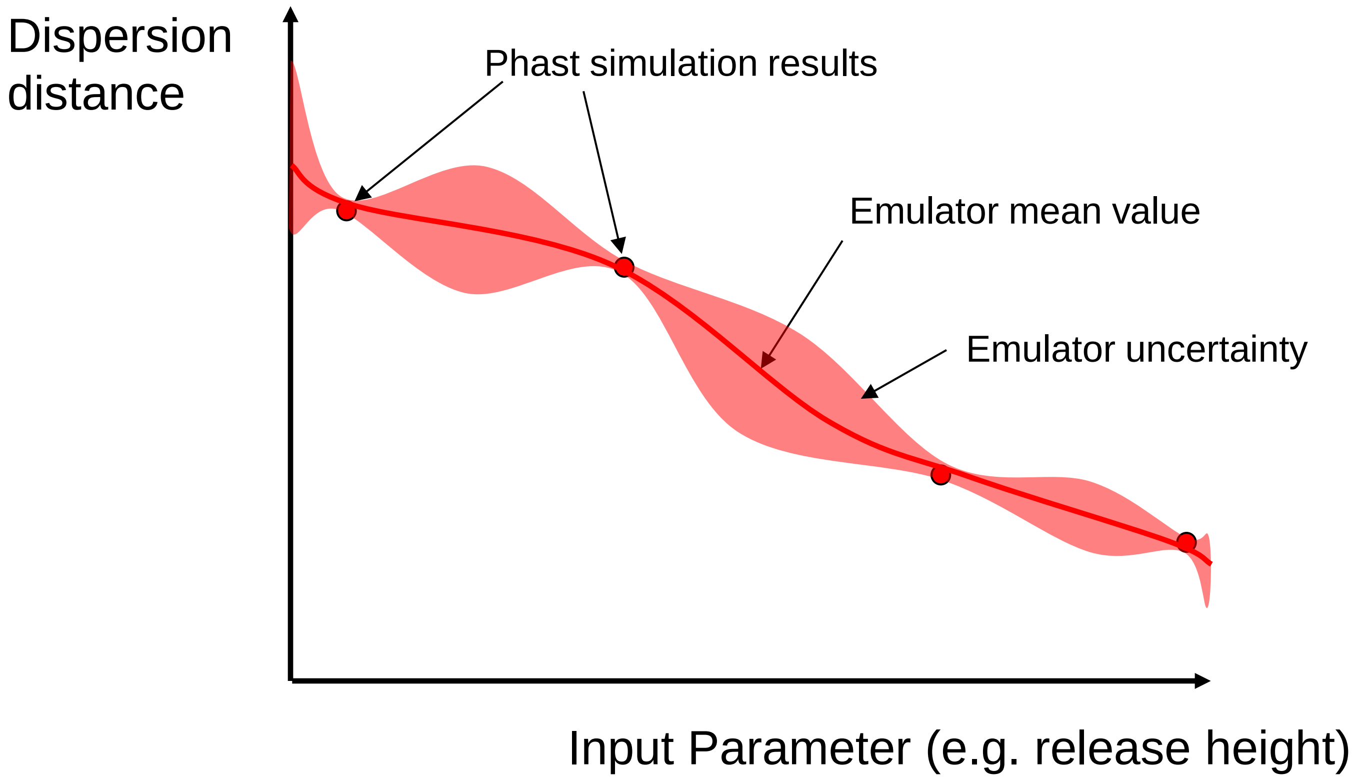


Sensitivity Analysis: GEM

- Gaussian Emulation Machine (GEM)
- Free software (for non-commercial use) developed by Marc Kennedy and colleagues at Sheffield University http://www.tonyohagan.co.uk/academic/GEM/

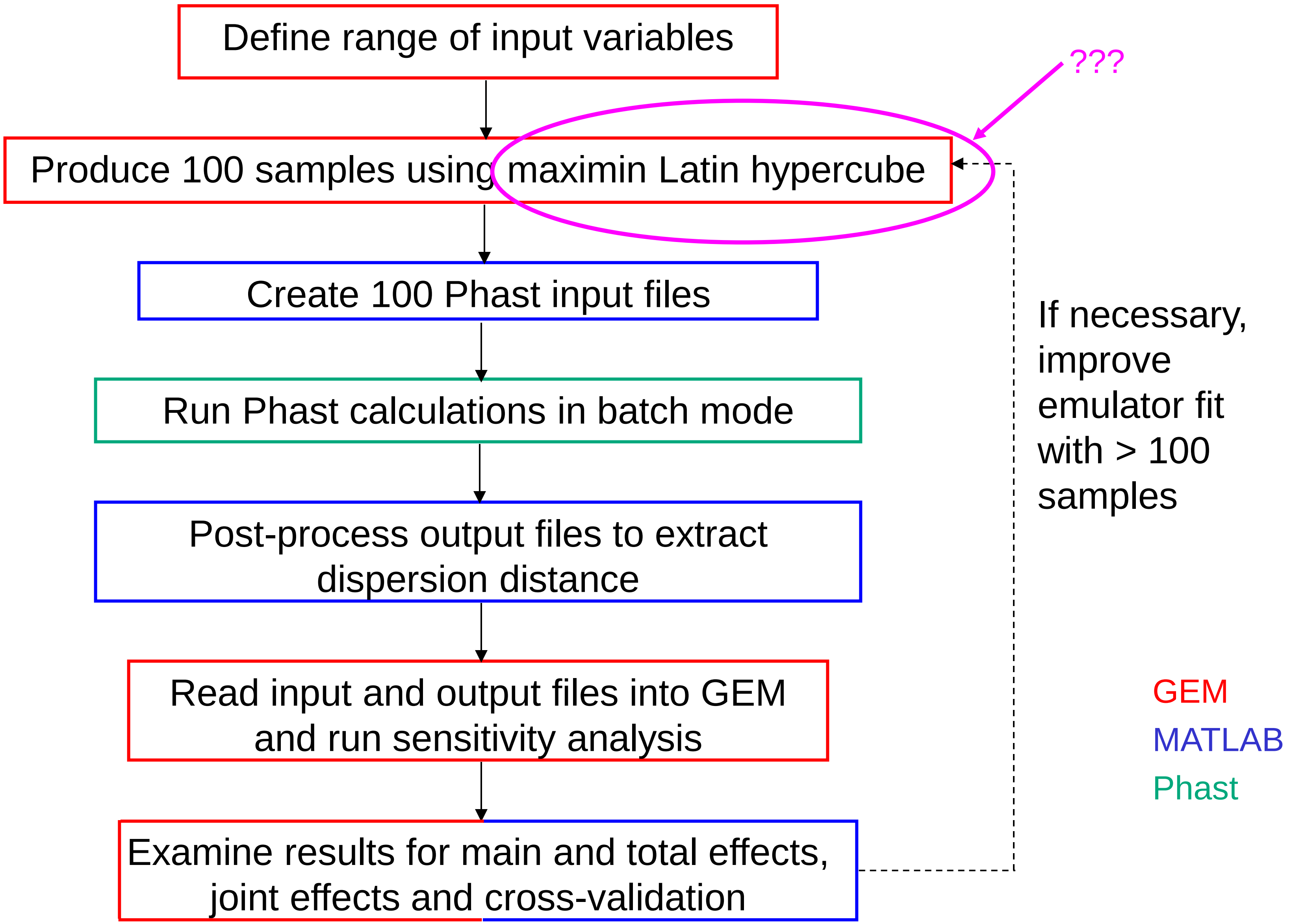


Gaussian Emulator



- Underlying assumption of emulator: output is a homogeneously smooth, continuous function of the input parameters
- Results will be similar if inputs only slightly perturbed – provides significant savings compared to “brute-force” Monte Carlo

Sensitivity Analysis Process



Maximin Latin Hypercube

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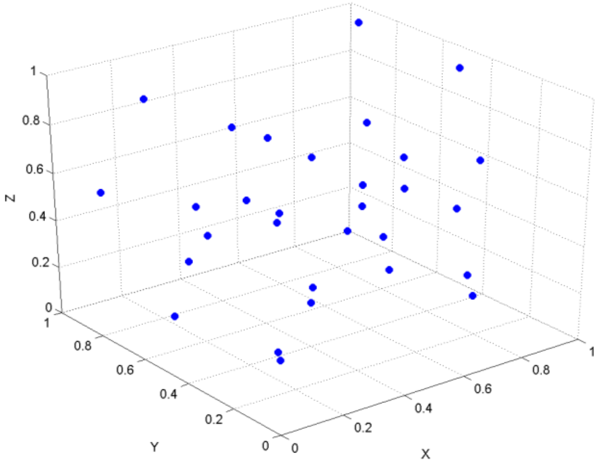
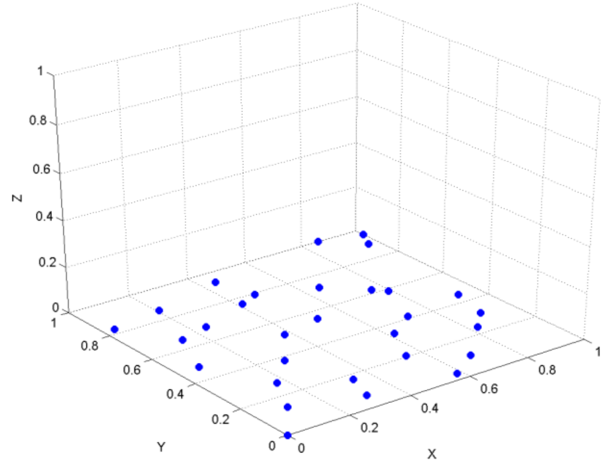
- Example: 3 input variables, 30 samples

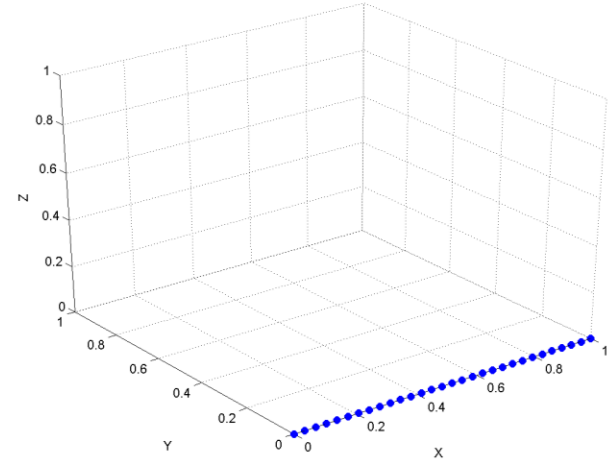
Full 3D sample space



Parameter Z has no effect



Parameters Y and Z have no effect

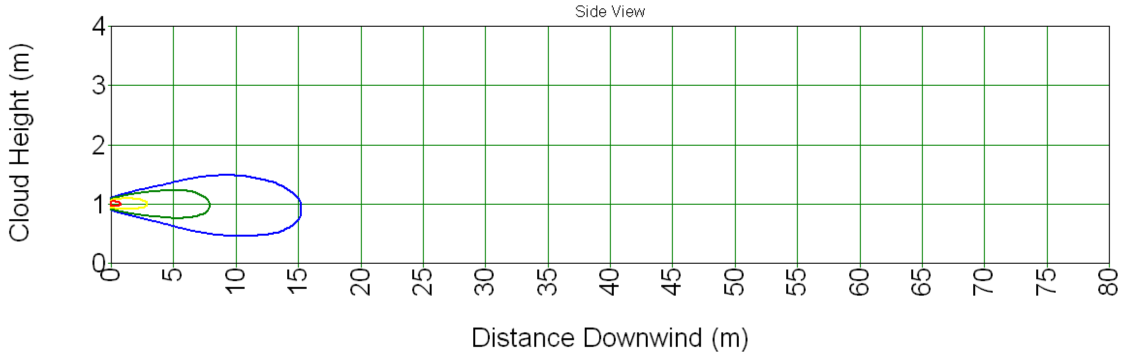


- If Parameters Y and Z had no effect on the results, all 30 samples are equispaced across Parameter X sample space
- Often, just 1 or 2 input parameters dominate model predictions : Latin hypercube maximises coverage from limited number of points

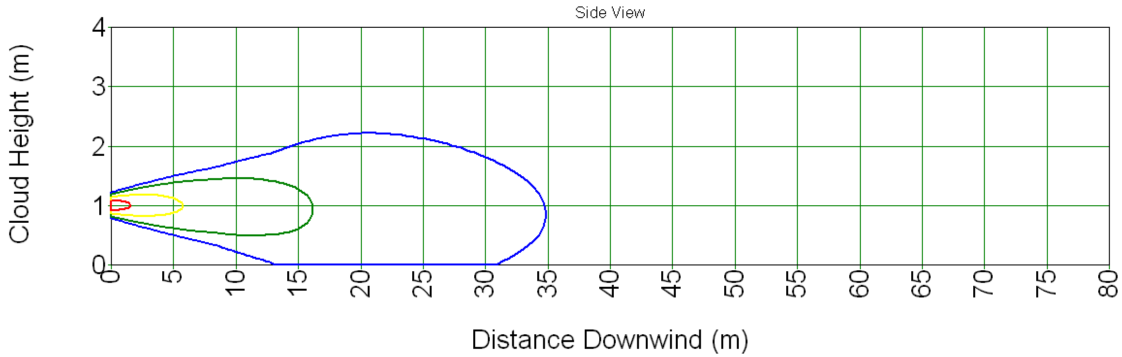
Phast Results

Orifice Diameter

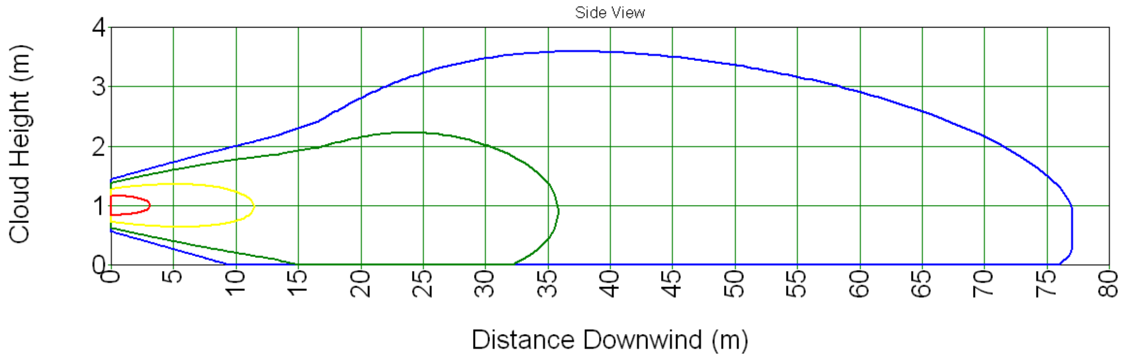
½ inch



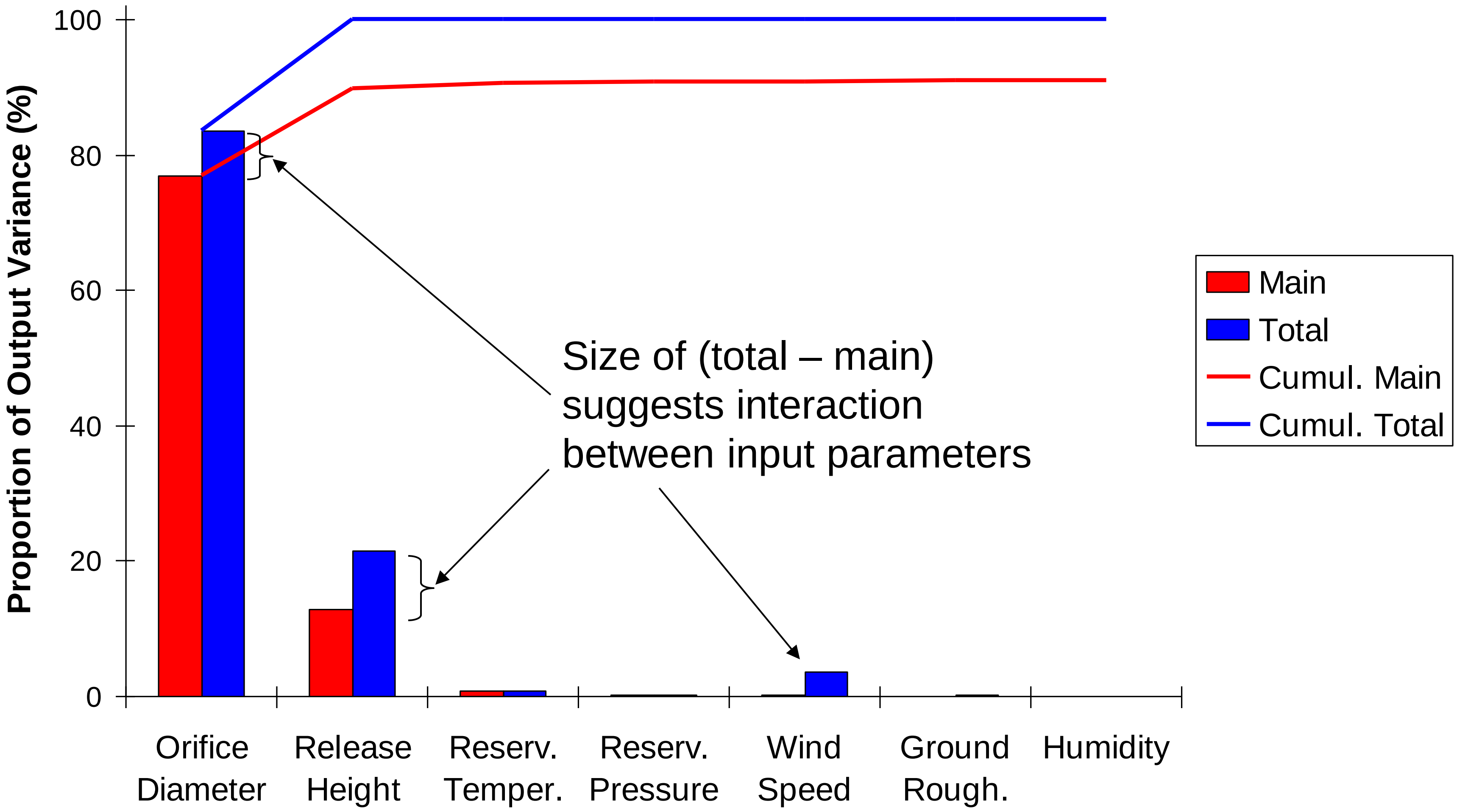
1 inch



2 inch

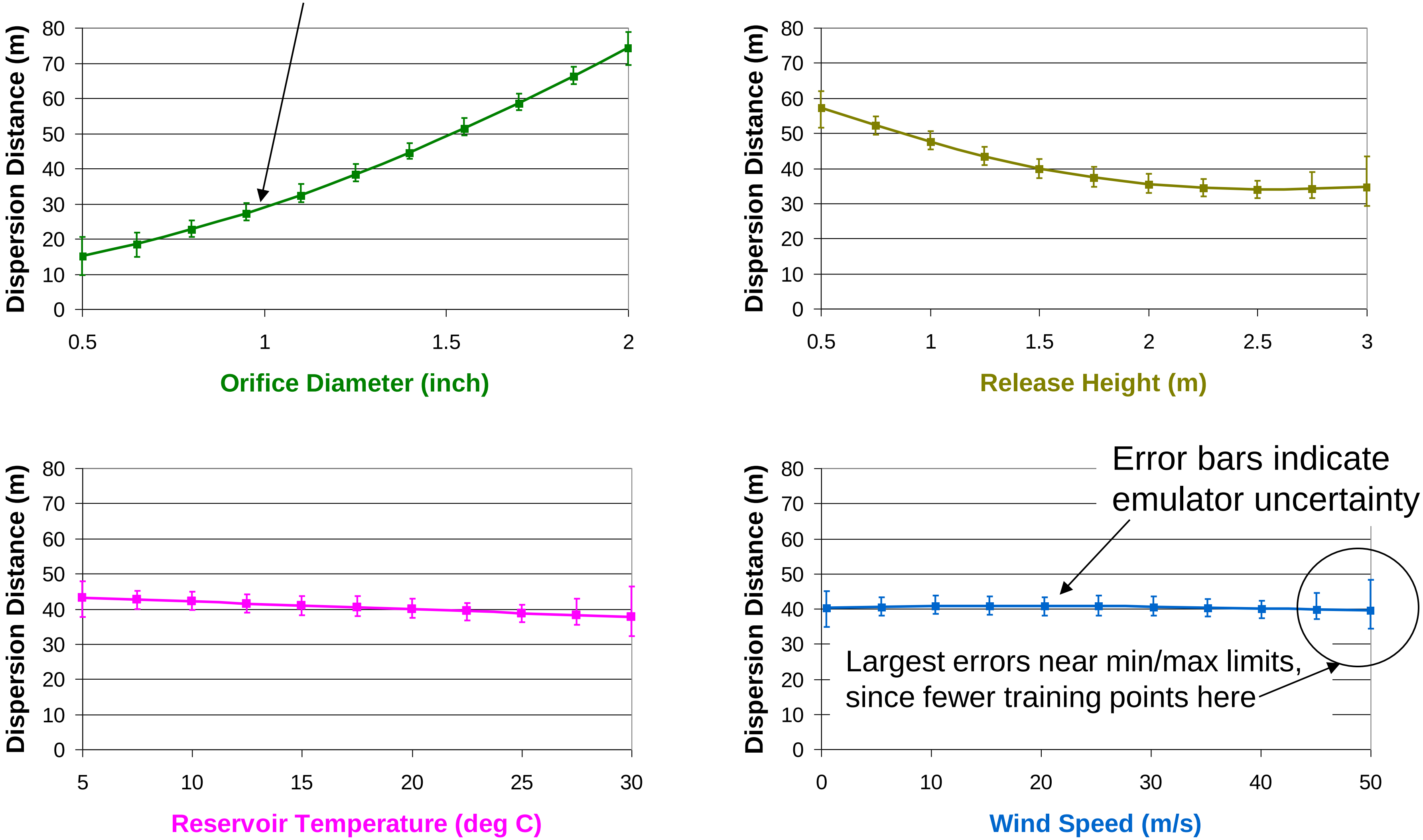


Results: Main + Total Effect



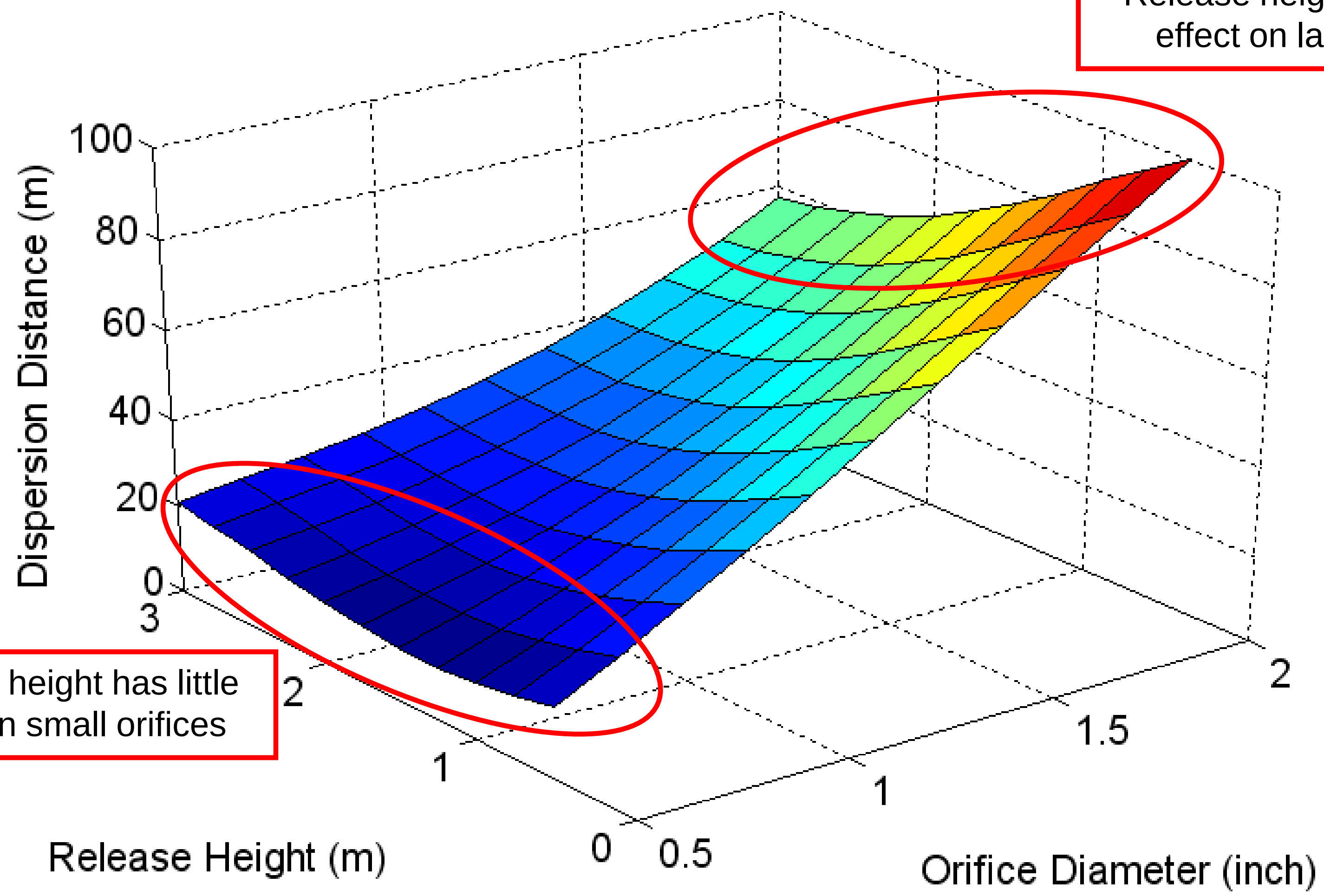
Main Effects

e.g. fix orifice diameter at 1 inch and average over range of all other input parameters



Joint Effects

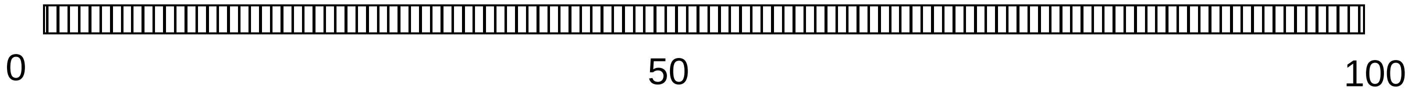
Release height has strong effect on large orifices



Release height has little effect on small orifices

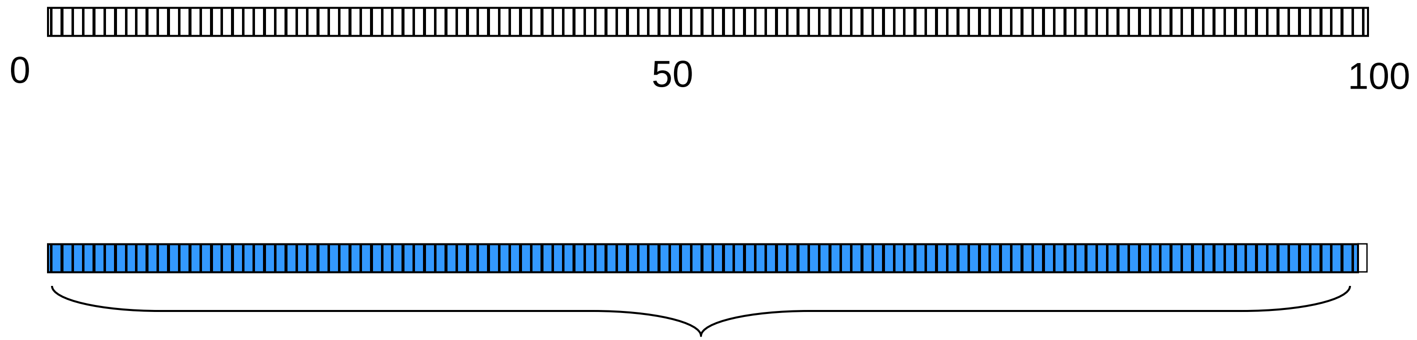
Emulator Cross-Validation

Phast results



Emulator Cross-Validation

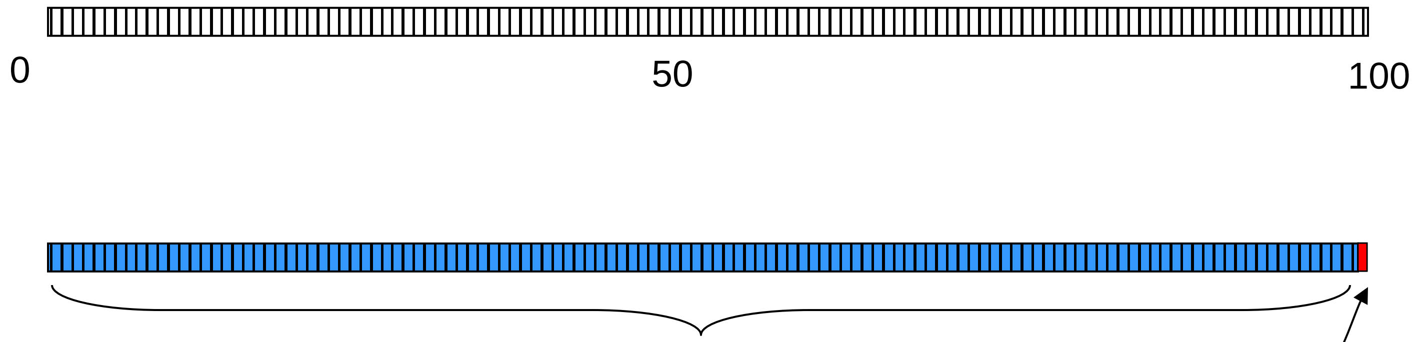
Phast results



Step 1.) Use 99 Phast results to fit emulator

Emulator Cross-Validation

Phast results

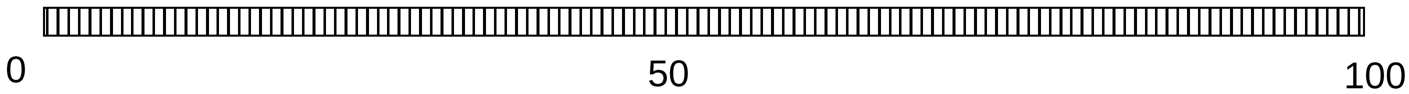


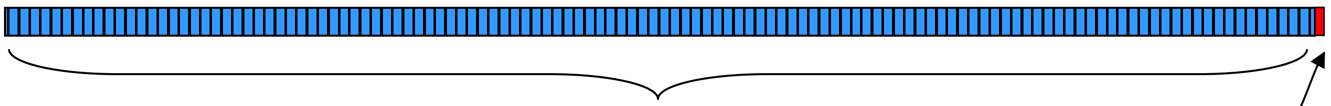
Step 1.) Use 99 Phast results to fit emulator

Step 2.) Use this emulator to predict 100th Phast result

Emulator Cross-Validation

Phast results

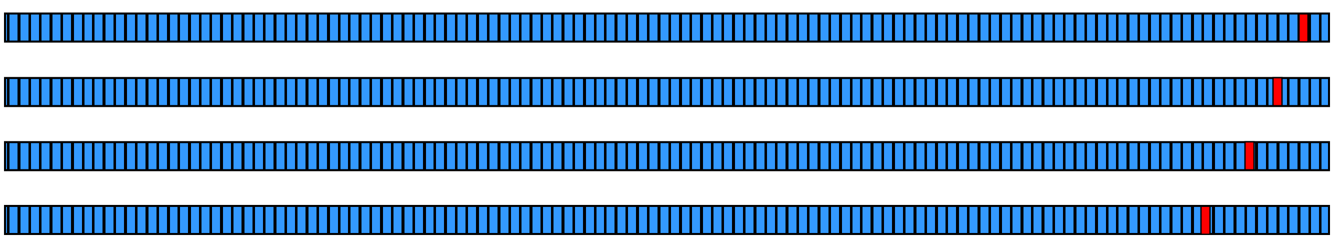




Step 1.) Use 99 Phast results to fit emulator

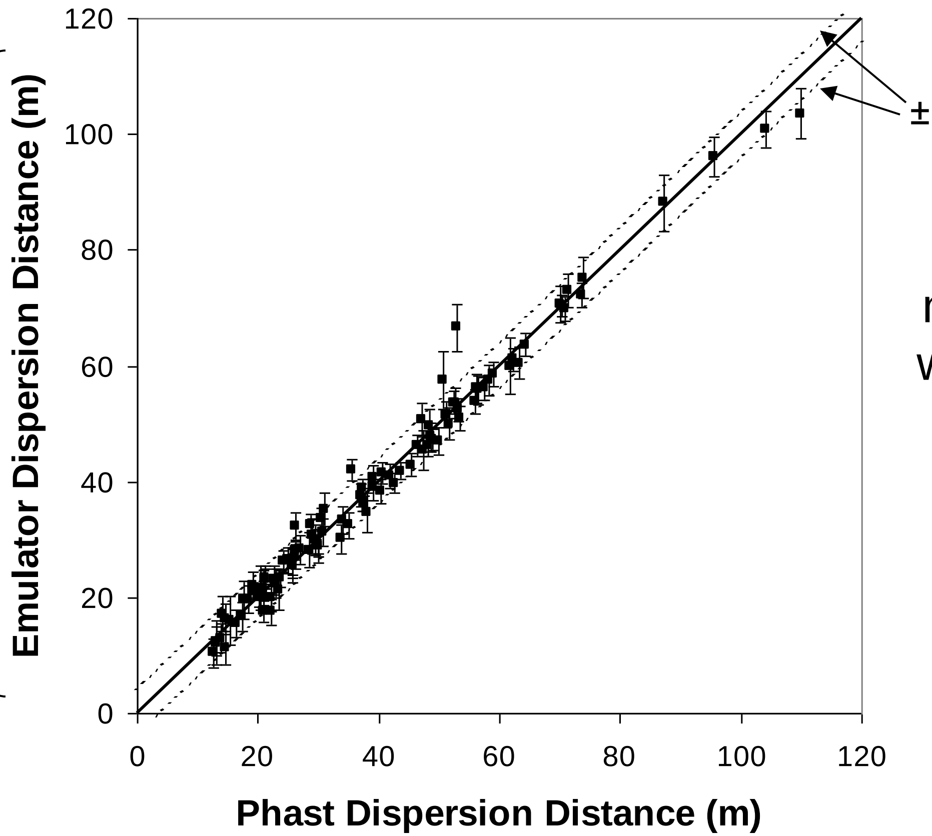
Step 2.) Use this emulator to predict 100th Phast result

Step 3.) Repeat Steps 1 and 2 for each Phast result in turn:



Emulator Cross-Validation

Emulator predictions of Phast results

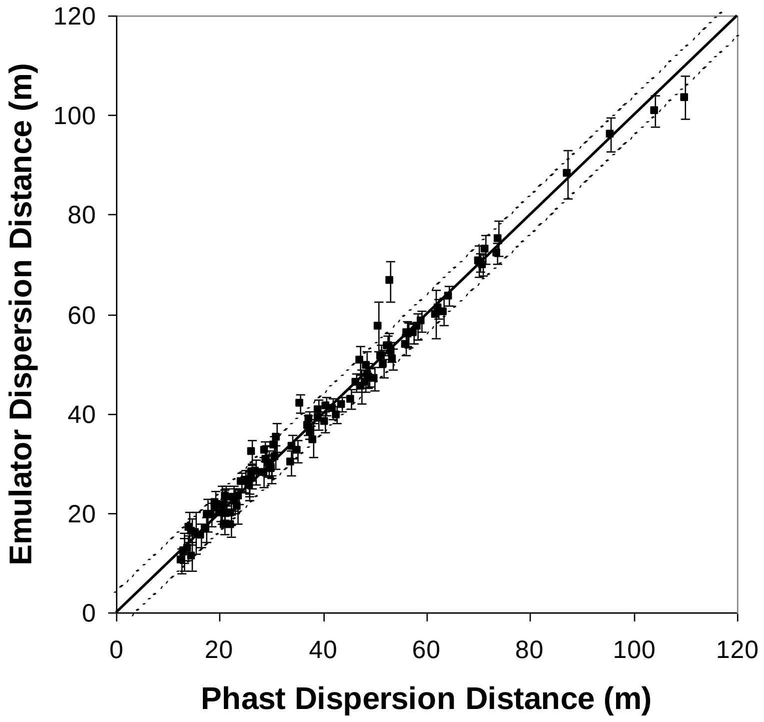


93% of emulator mean predictions within these limits

- Some points are on edge of parameter space and require extrapolation of the emulator – known to produce large errors
- Consequently, results may not converge upon 100% as number of training data points is increased

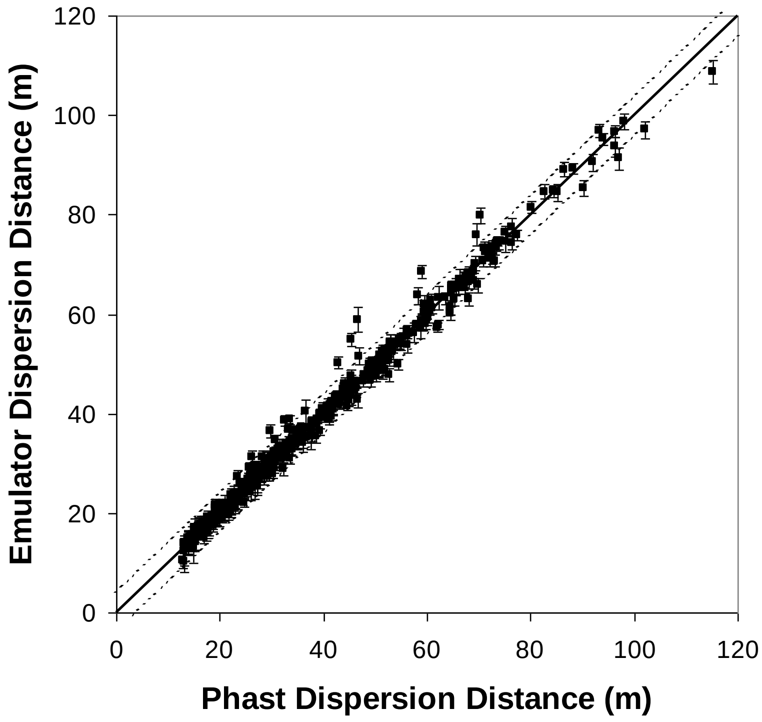
Emulator Cross-Validation

100 Phast training data points



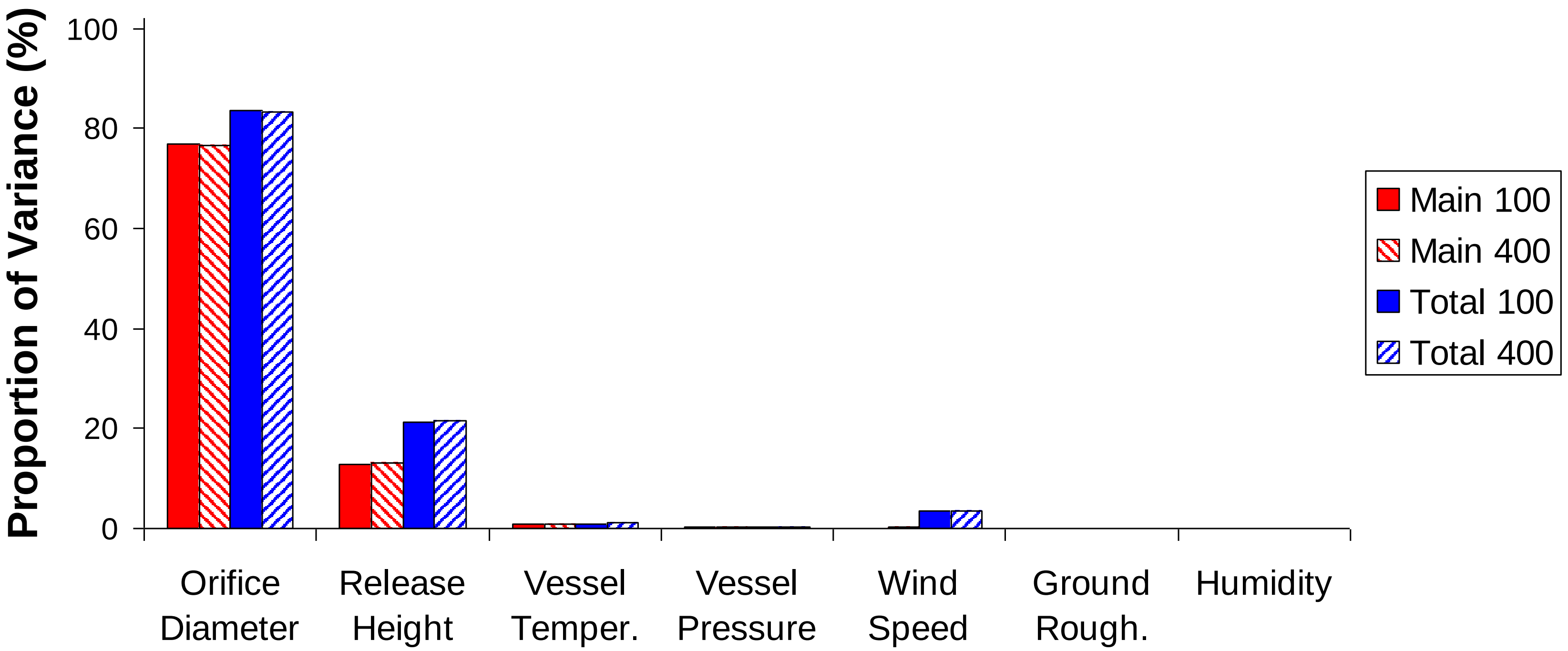
93% within ± 4m

400 Phast training data points



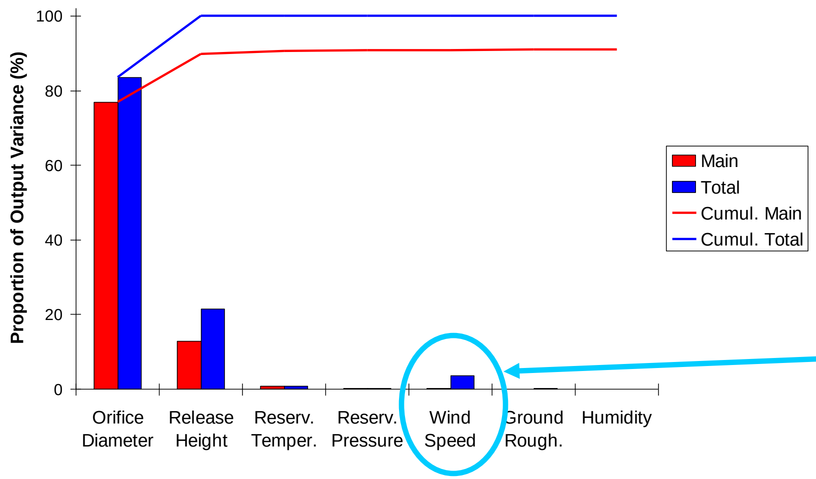
95% within ± 4m

Emulator Cross-Validation



- Increasing number of Phast runs from 100 to 400 does not affect main and total effects
- 100 runs provides acceptable degree of accuracy

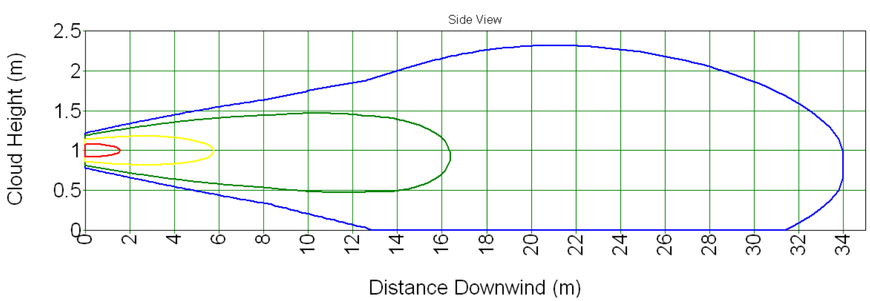
Do results make sense?



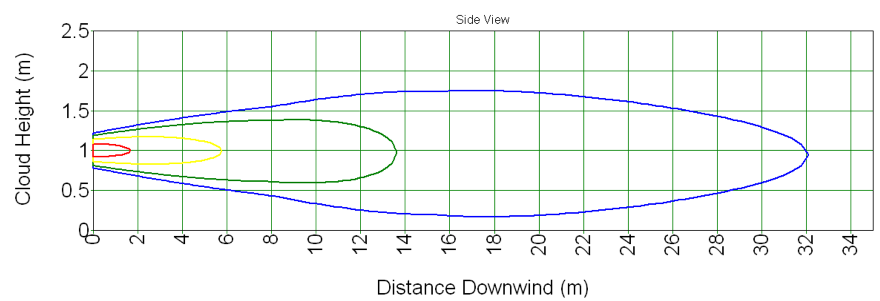
Dispersion distance hardly affected by atmospheric conditions

Even wind speed 0.5 – 50 m/s ?!

0.5 m/s wind



50 m/s wind



Plume Behaviour

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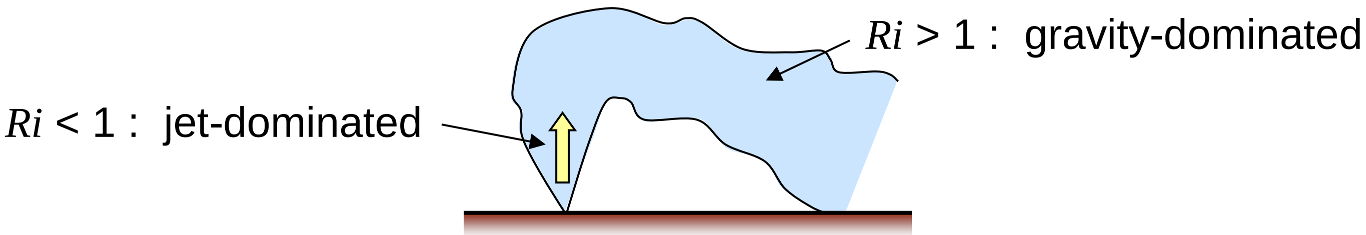
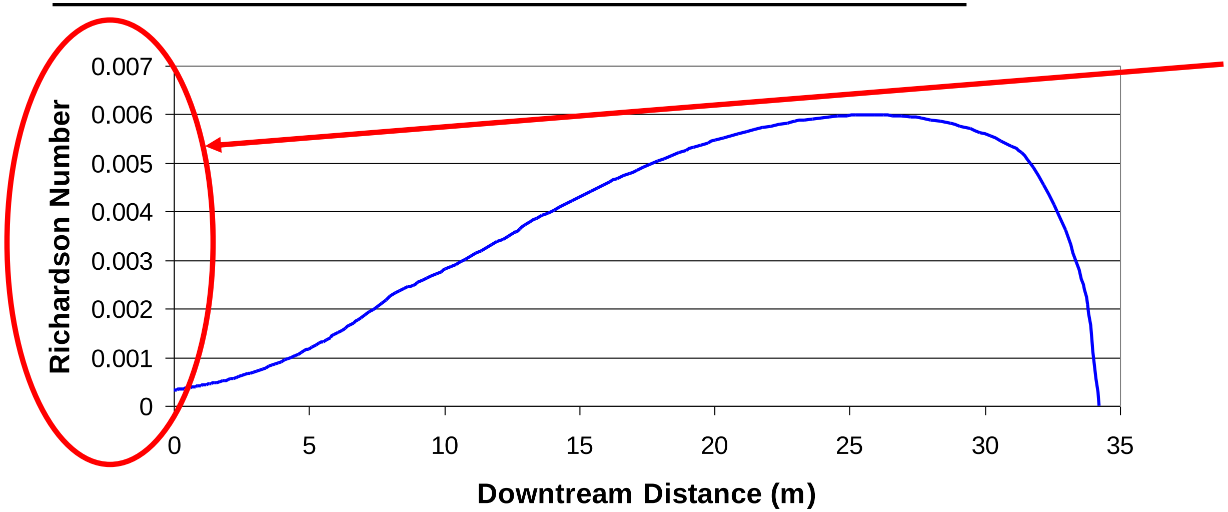
- Plume behaviour characterised by Richardson Number

$$Ri = \frac{gL}{U^2}\frac{\Delta\rho}{\rho} = \frac{\text{Gravity forces}}{\text{Inertia forces}}$$



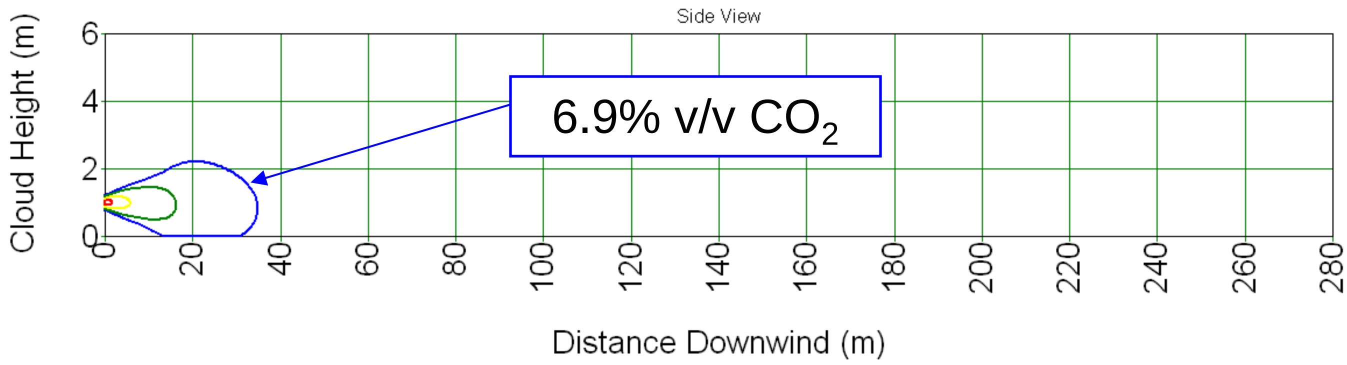
Phast results for 1-inch orifice with 0.5 m/s wind:

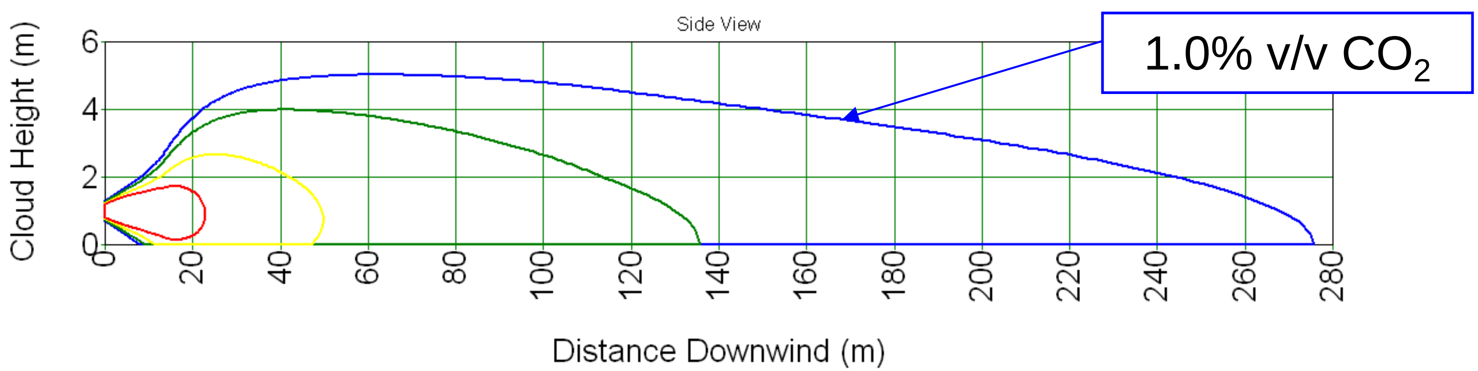


Plume behaviour is governed by jet momentum

Wind Speed Effects

Defining the edge of cloud using a lower concentration:

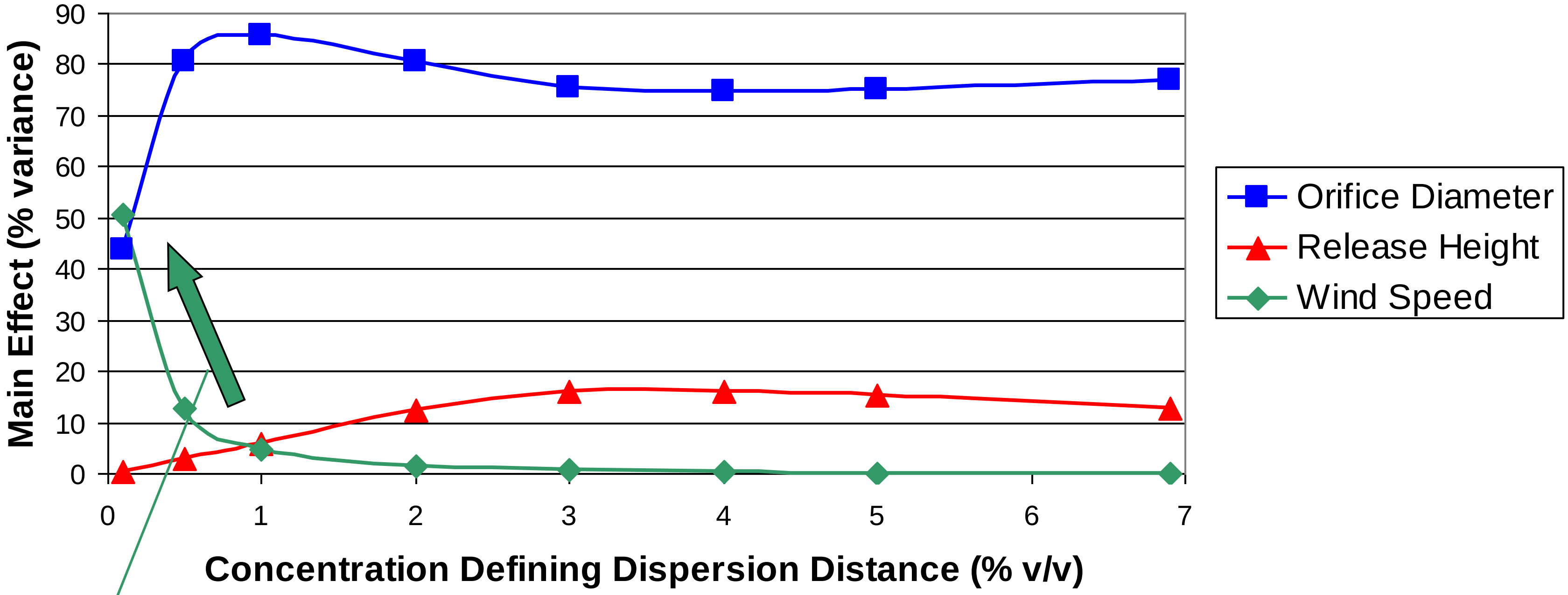




- Same model inputs in each case
- At lower concentrations, plume is more influenced by environment

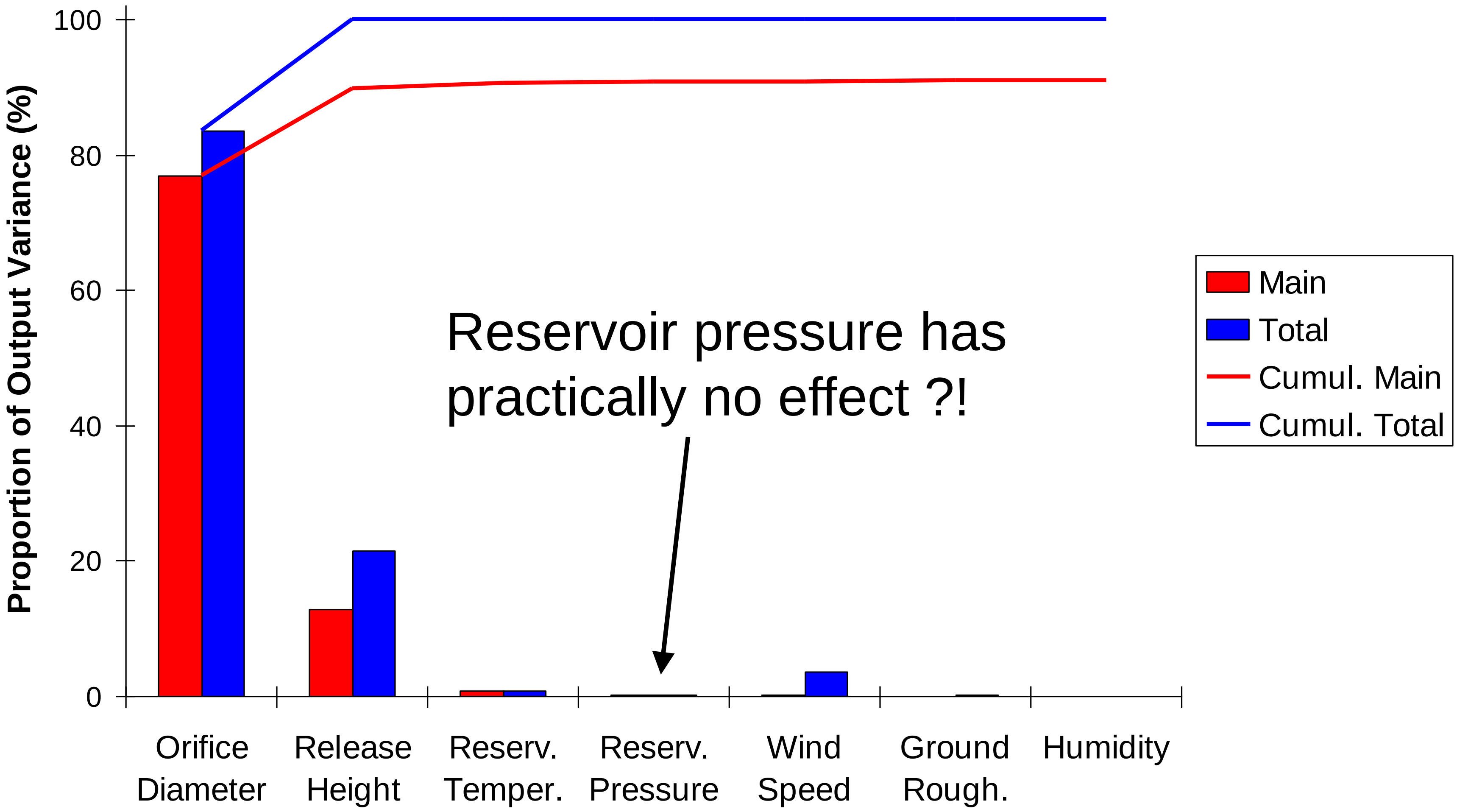
Wind Speed Effects

- Repeated sensitivity analysis with different model output



At concentrations below 1% CO_2, the wind speed has a significant effect

Effect of Reservoir Pressure



Effect of Reservoir Pressure

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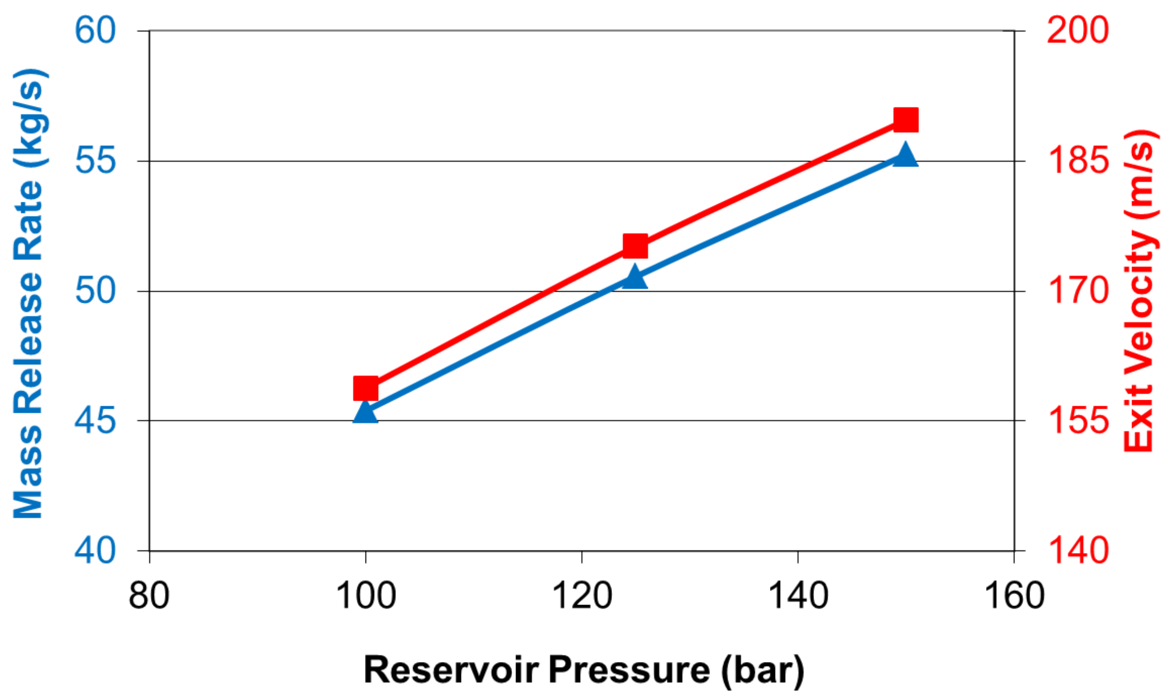
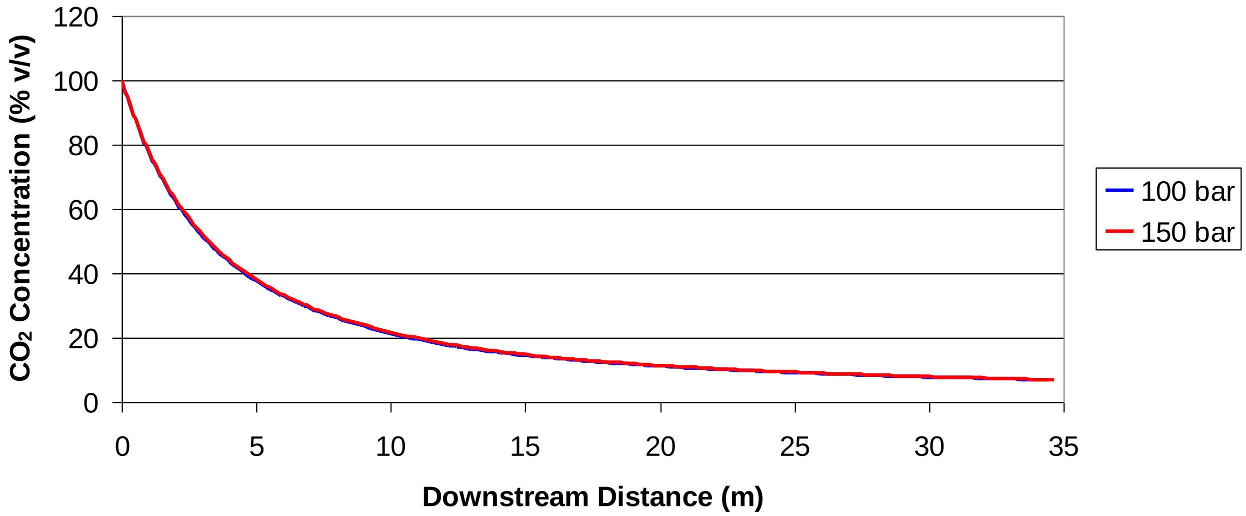
Increasing "Reservoir Pressure" has competing effects:

- Increases flow rate : higher concentrations
- Increases momentum : lower concentrations (due to more jet entrainment)



Effect of Reservoir Pressure

- **Net result**: pressure has little effect on dispersion distance



- Similar to behaviour observed in sub-sonic gas jets
- Impinging CO_2 jets may exhibit different behaviour, e.g. craters?

Strengths of Emulators

- Fast results for global sensitivity analysis!
  - 7 variable model inputs
  - Just 100 Phast runs
  - < 30 mins computing time (inc. Phast runs)
- Improved understanding:
  - Main and total effects
  - Average effect of each parameter
  - Joint effects of two parameters
- Cross-validation tests on sample size are simple and quick

Weaknesses of Emulators

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- Underlying mathematics are complex

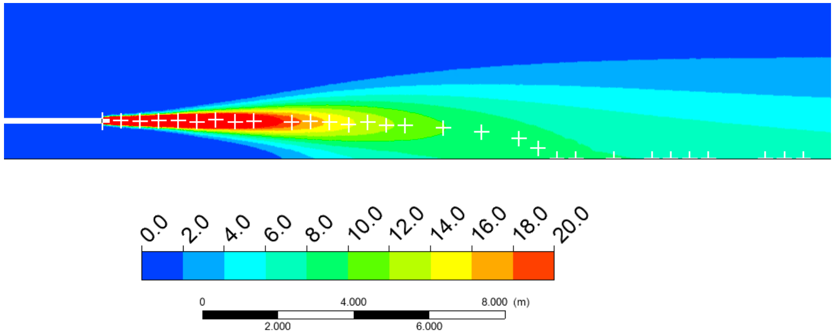
- Further work needed to account for:
  - Steps in model output
    - e.g. from input on/off switches
  - Non-uniform or normal distributions of model inputs
    - e.g. log-normal wind speed distribution

… but these can be handled by using Monte-Carlo sampling of the emulator

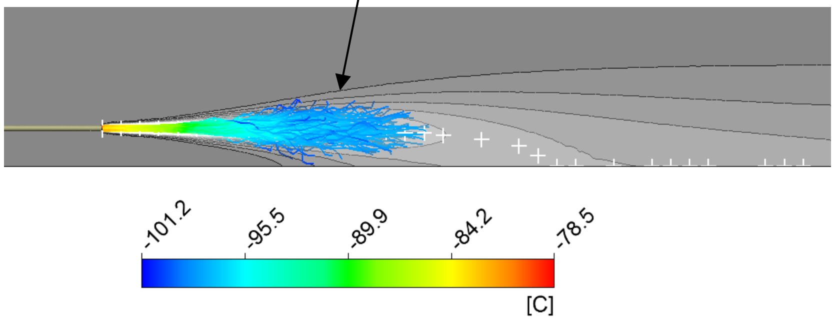
ANSYS-CFX

Lagrangian model tracks particles and their sublimation (does not assume homogeneous equilibrium)

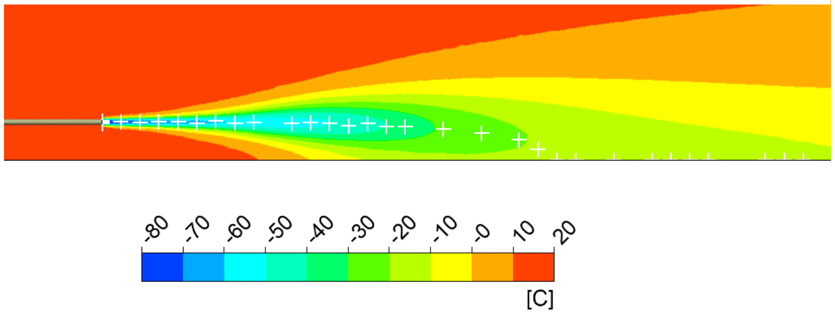
CO_2 Gas Concentration (% vol/vol)



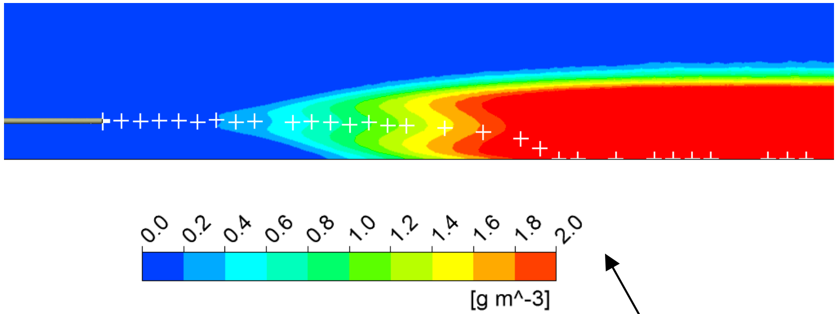
CO_2 Particle Temperature (deg C)



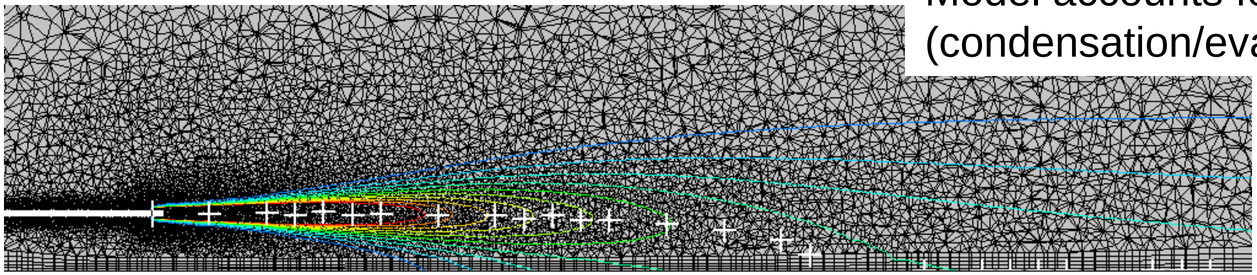
Gas Temperature (deg C)



Water Droplet Concentration (g/m^3)

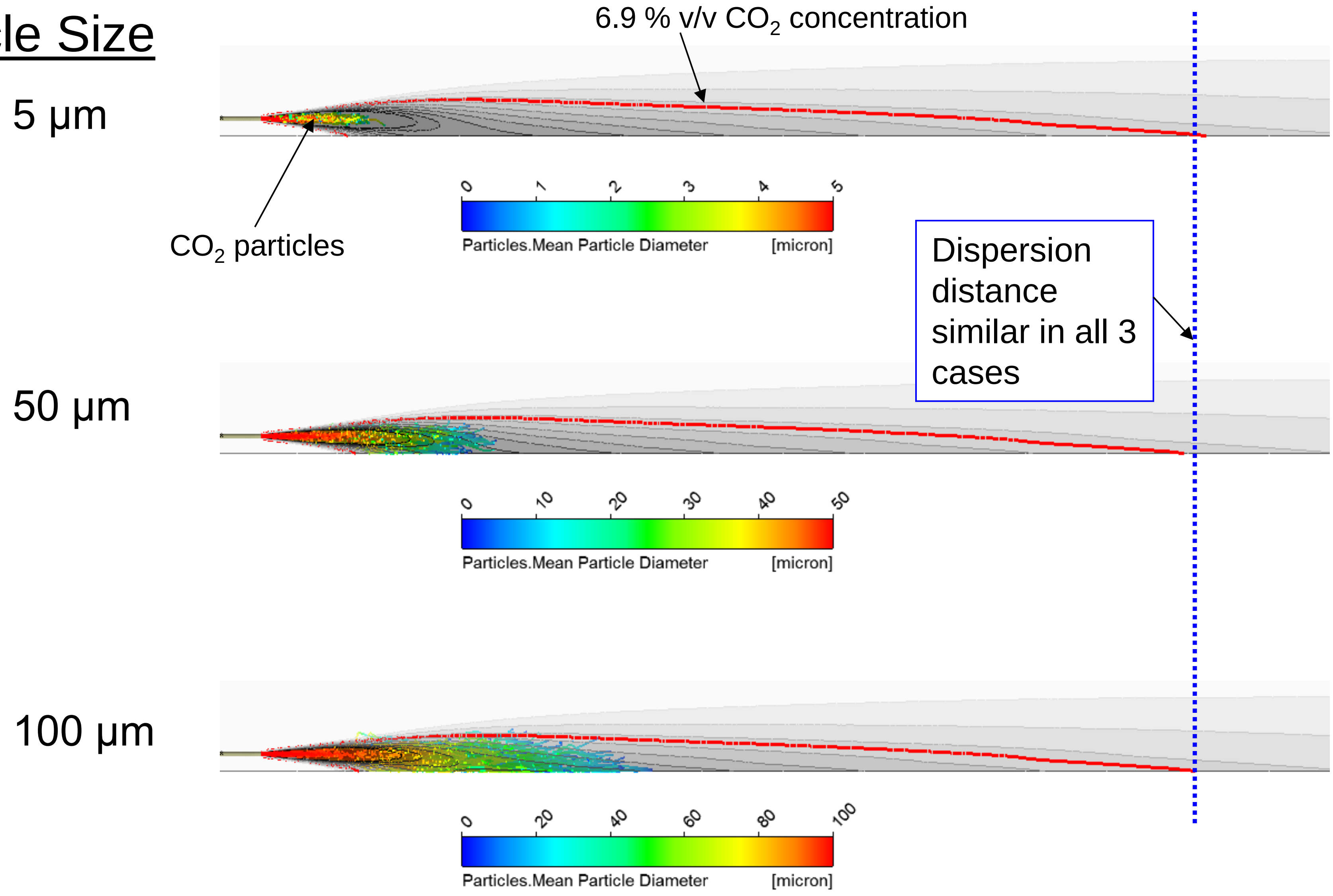


Model accounts for humidity effects (condensation/evaporation)



CFD Results

Particle Size



CFD Results

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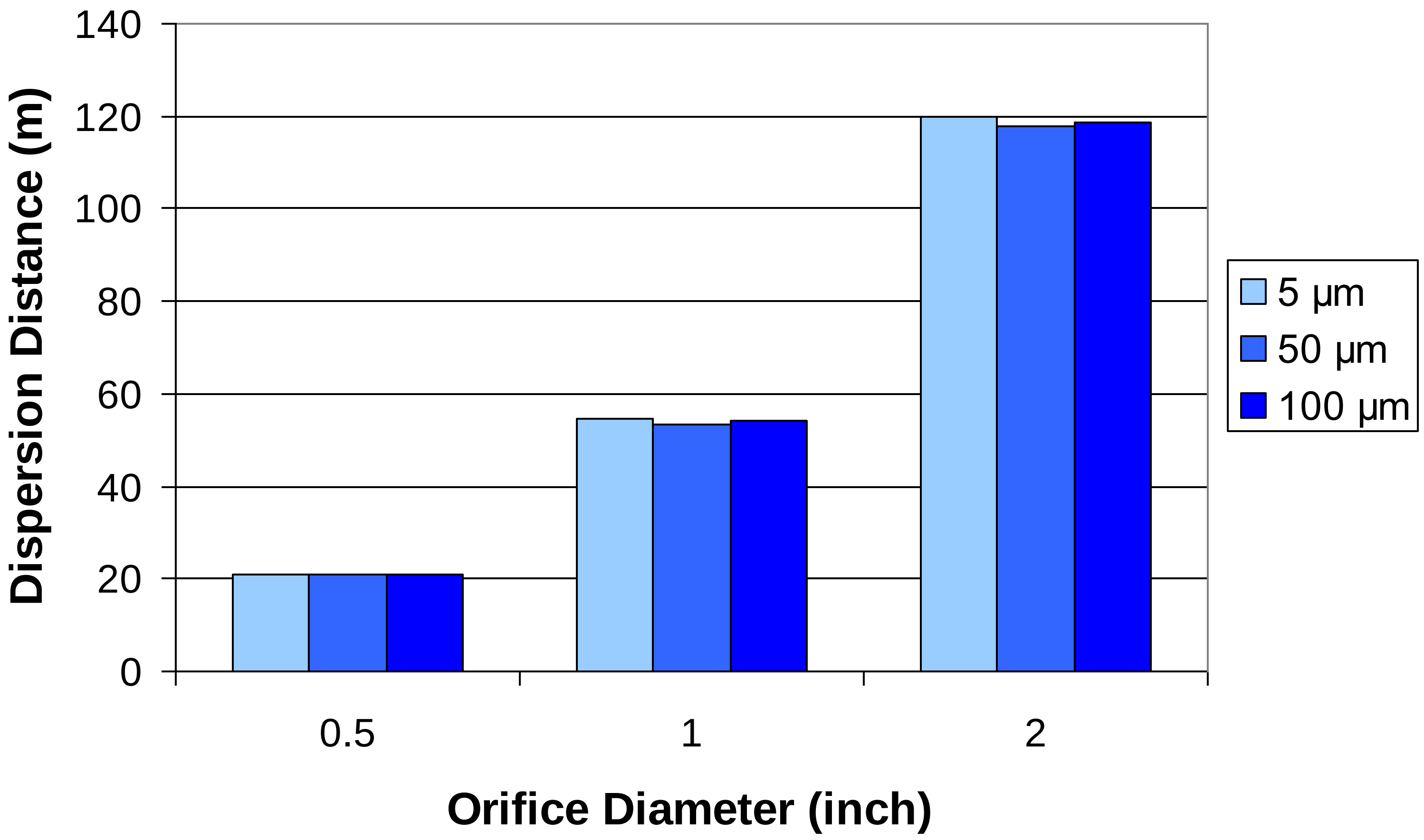
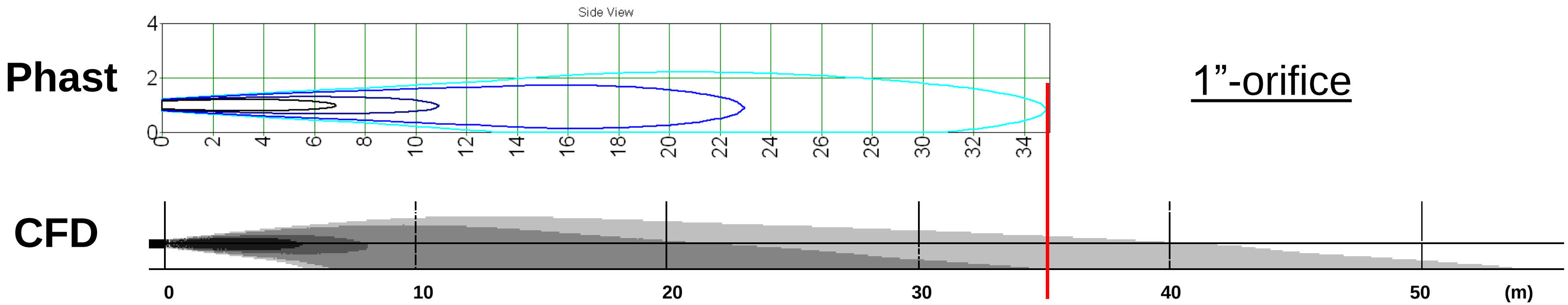
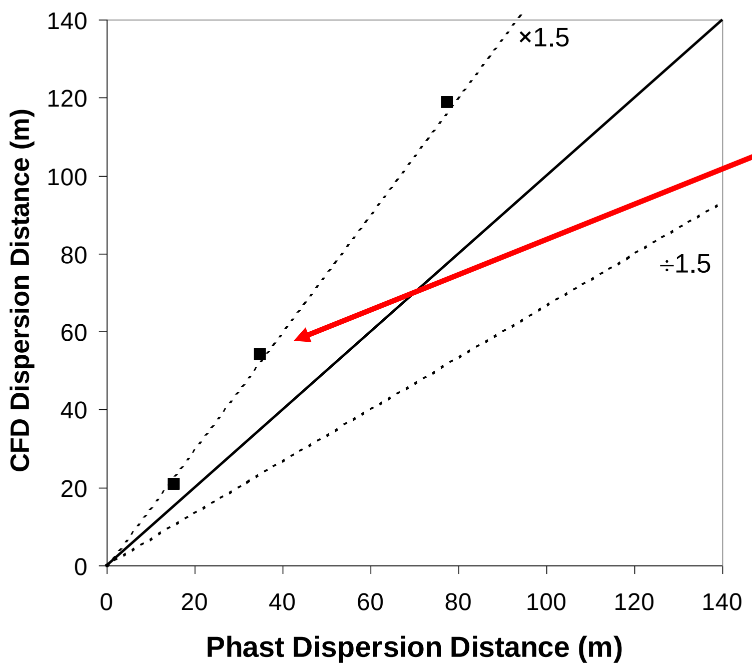
- Similar results for orifice diameters 0.5” – 2”



CFD – Phast Comparison

- CFD plume shows more wedge-shaped side profile





CFD dispersion distances are ~50% larger than Phast

Conclusions

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- Global sensitivity analysis can be used for practical consequence modelling at low cost using an emulator
- Its results are useful to help understand model behaviour and identify important model input parameters
- This can be used to:
  - Concentrate efforts on important parameters (measure them to reduce the uncertainty in the model predictions?)
  - Reduce number of simulations
- In the case studied here: orifice size and release height were the most important inputs
- Size of the particle in the range 5 – 100 μm had little effect

Future Work

- Joint Industry Project or partnership on sensitivity/uncertainty of consequence models:
  - Short course on sensitivity/uncertainty analysis for process safety engineers
  - Develop software tools to integrate methods in consequence models (integral models, CFD etc.)
  - Apply different methods to practical engineering test cases
  - Develop best practice guidance

- Questions to address:
  - How to incorporate input distributions, e.g. weather data, and on/off input parameters?
  - Can we use emulators for consequence models and Bayesian methods for failure frequencies to improve risk assessments?
  - Can we estimate uncertainty in results from risk assessments?

Grazie mille!

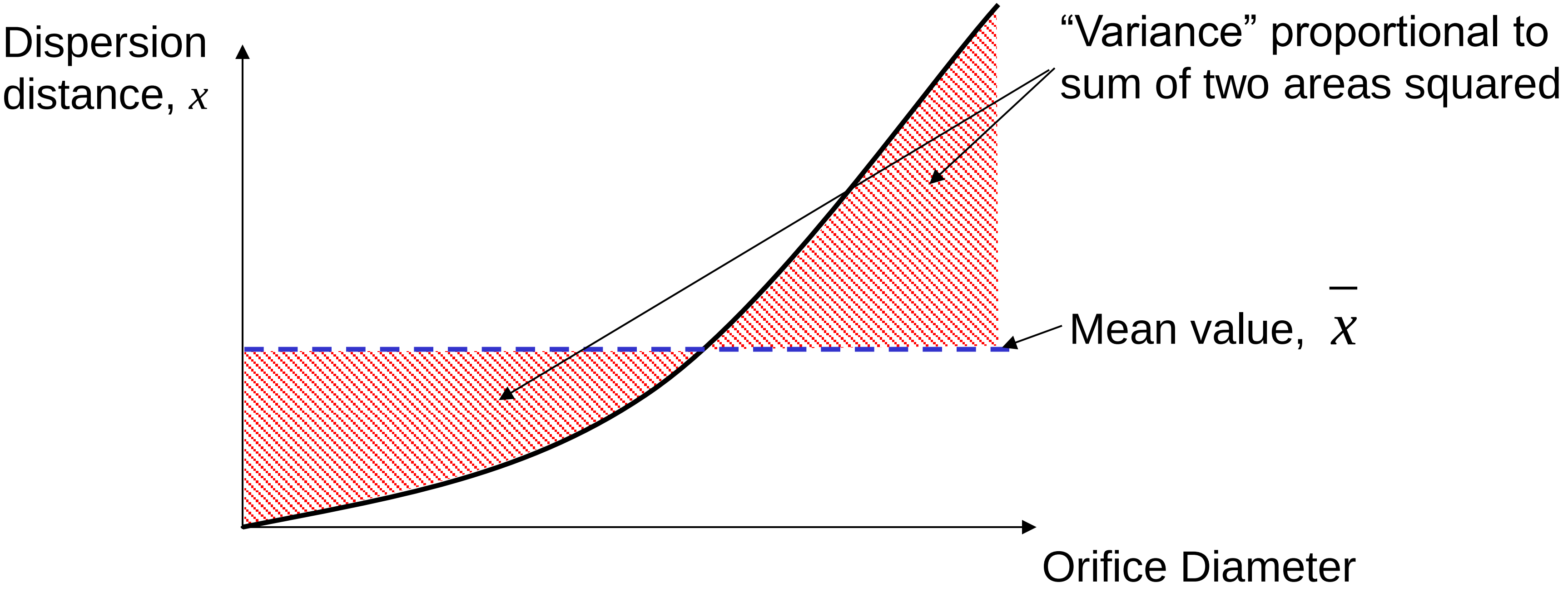
P.S. See me if you would like a demonstration of GEM

Variance-Based Sensitivity Analysis

- What is "variance"?

$$Var = \sigma^2 = \frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2$$

An indication of how much a parameter varies about the mean



- If an input produces a large amount of variance in the dispersion distance, it has a significant effect

Variance-Based Sensitivity Analysis

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- **Main Effect** of Parameter *A*:
  - The amount of variance that would be removed from the total output variance if we learnt of the true value of *A*

$$S_x = \frac{V(E(Y|P_x))}{V_y}$$

- **Total Effect** of Parameter *A*:
  - The amount of variance that would remain unexplained if the values of all other parameters except *A* were known, and the variance was produced only by varying *A*

$$ST_x = 1 - \frac{V(E(Y|P_{-x}))}{V_y}$$

Mean

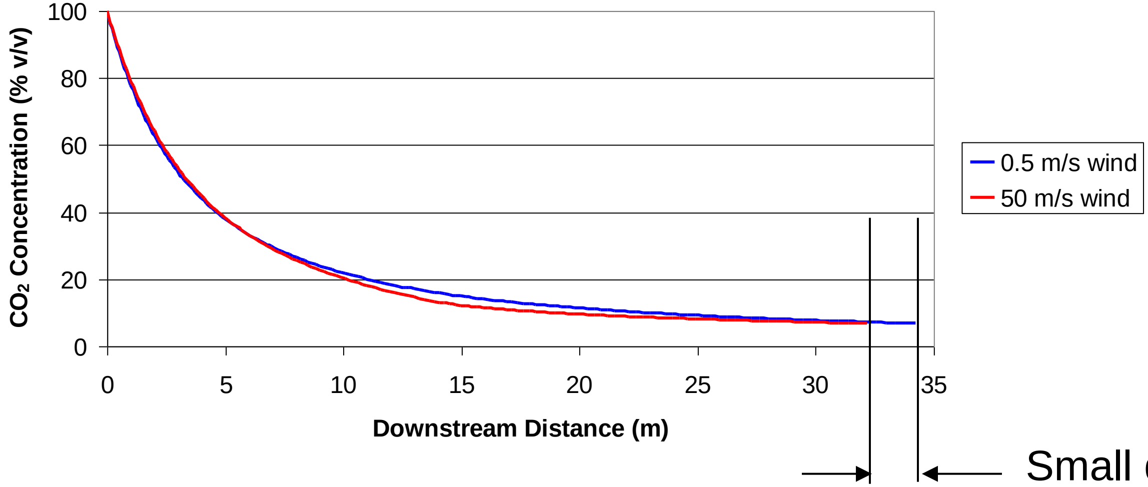
$$f(x_1, x_2, x_3) = f_0 + f_1(x_1) + f_2(x_2) + f_3(x_3) + f_{12}(x_1, x_2) + f_{13}(x_1, x_3) + f_{23}(x_2, x_3) + f_{123}(x_1, x_2, x_3)$$

Main Effect for x_1

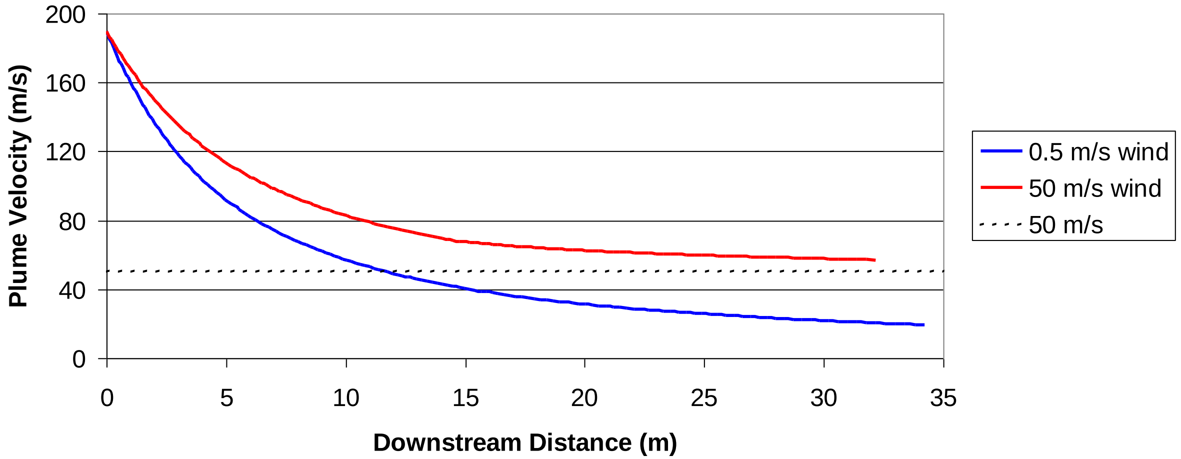
Total Effect for x_1

Effect of Wind Speed

- Phast results for 1 inch orifice with 0.5 and 50 m/s wind:



Small difference in dispersion distance



What are we interested in?

HEALTH & SAFETY LABORATORY

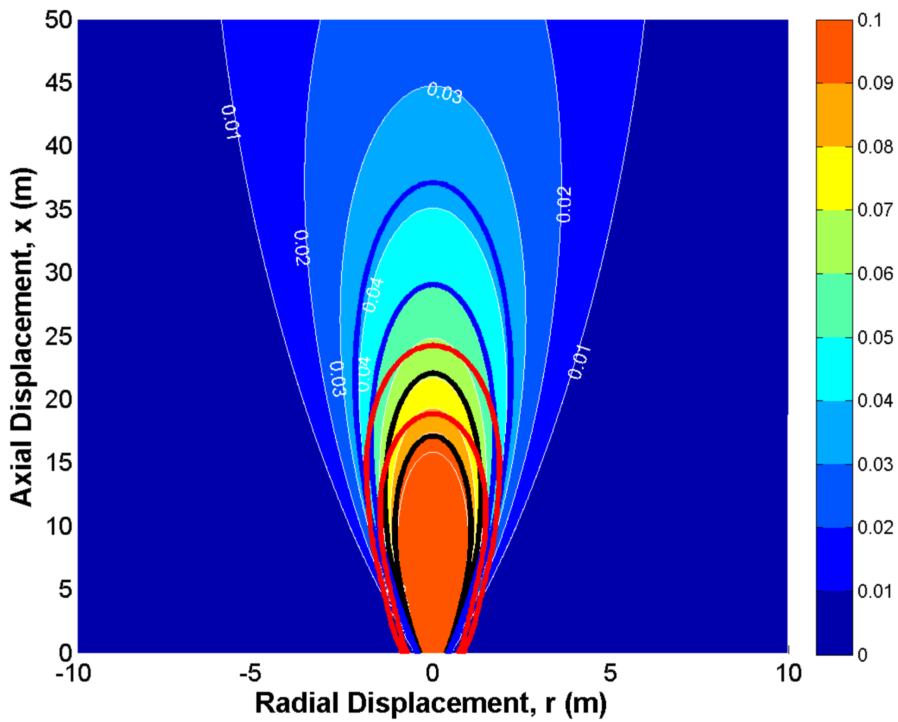
- Cloud extent based on HSE contours of Toxic Load:
  - Specific Level of Toxicity (SLOT)
  - Significant likelihood of Death (SLOD)

$$TL = \int C^8 dt$$

	SLOT	SLOD
DTL (ppm^n.min)	1.5×10^{40}	1.5×10^{41}
Exposure duration	30 min	30 min
Conc. (% v/v CO_2) assuming no fluctuations	6.9	9.2
Conc. (% v/v CO_2) with factor of two fluctuations	3.7	5.0

- In comparison, NIOSH IDLH = 4% v/v CO_2

Concentration Fluctuations



- CO_2 jet : diameter 0.5m and exit velocity 50 m/s.
- Coloured contours show the CO_2 gas concentration
- Three sets of curves show the SLOT and SLOD calculated using different toxic load models
- Gant and Kelsey "Accounting for the effect of concentration fluctuations for gaseous releases of carbon dioxide" J. Loss Prev. Proc. Ind., 25 (1), p52-59, 2012