

Content

- Background to CO₂ dispersion
- Objectives
- Global sensitivity analysis
 - Phast
 - GEM
- CFD simulations
- Conclusions
- Future Directions – possible JIP?

Background

- 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.”

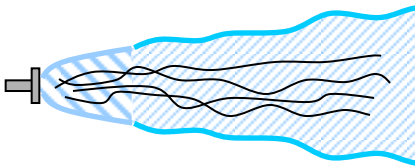


Background

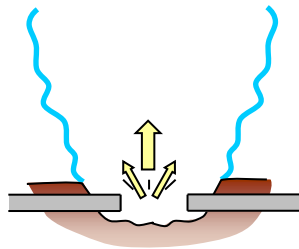
- Need to understand risks posed by pipelines transporting CO₂

Complex Physics

- Two-phase flow



- Craters

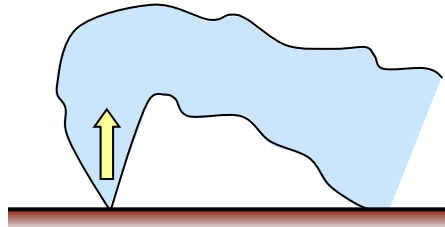


- Deposition of solids

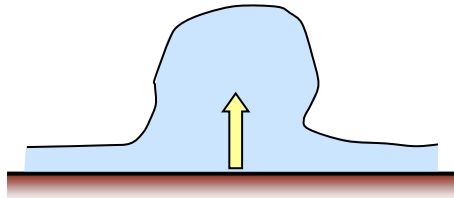
- Humidity effects

Atmospheric B.L.

- Finite wind speed

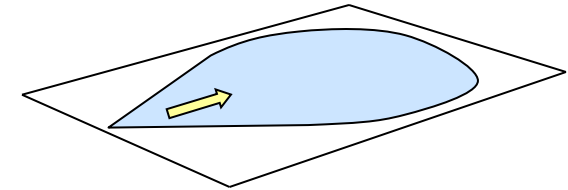


- Low/nil-wind

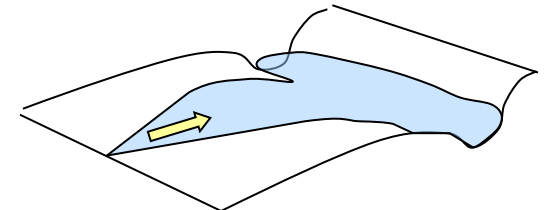


Terrain Effects

- Flat ground



- Topography and obstructions



Objectives

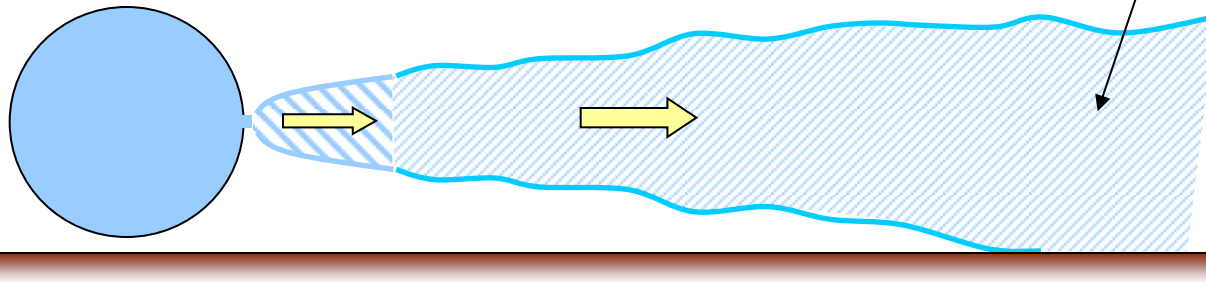
- Which of these inputs (or combinations of inputs) has a significant effect on the dispersion distance?

Inputs:

1. Vessel temperature: 5 – 30 °C
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

Leak from above-ground vessel containing carbon dioxide



Output of interest:

“Dispersion distance” where concentration reaches 6.9% v/v CO₂

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

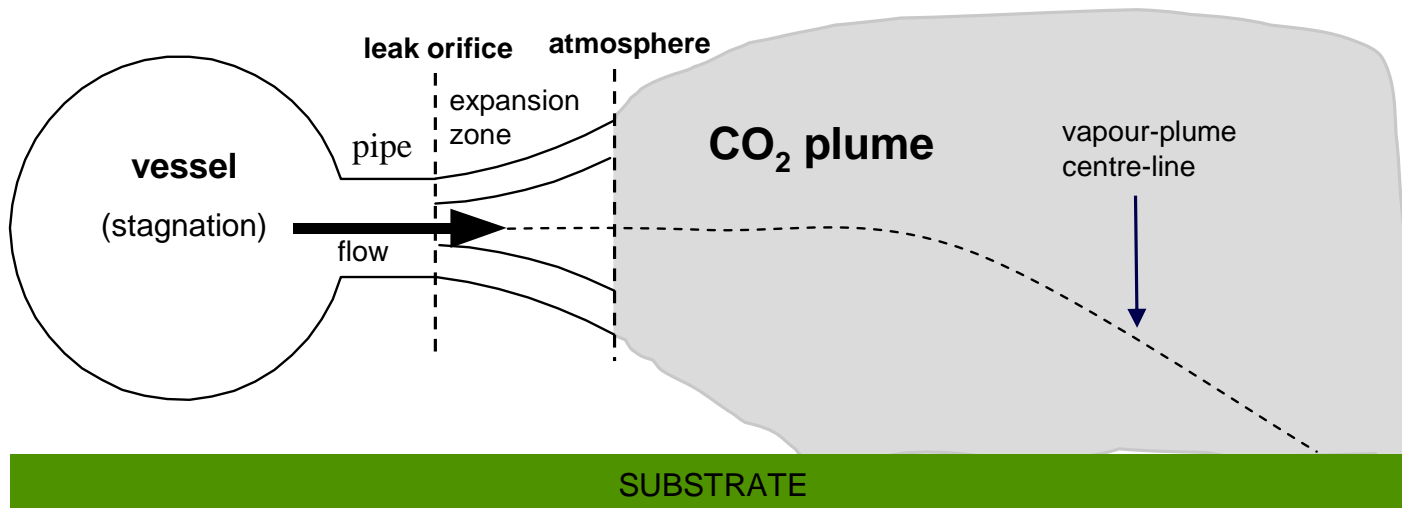
- **Option 2: Global Sensitivity**
 - Vary all parameters simultaneously
- **Pros:**
 - Good coverage of all potential scenarios
 - Includes effects of interactions
- **Cons:**
 - Costly!
 - Typically requires >10,000 simulations for conventional Monte-Carlo analysis

Sensitivity Analysis

- **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 CO₂ formation
- Validated against CO₂ 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/>



The screenshot shows a web browser window titled "GEM Software - Windows Internet Explorer". The address bar shows the URL <http://www.tonyohagan.co.uk/academic/GEM/>. The page content includes:

The GEM Software Project

The Gaussian Emulation Machine (GEM) software project aims to provide user-friendly tools to implement statistical analyses of uncertainty in the outputs of computer models, using the techniques of Gaussian process emulation. To download an introduction to these tools and the concepts that underlie them, click [here](#).

The GEM software available here has been developed by Marc Kennedy for the Centre for Terrestrial Carbon Dynamics (CTCD). CTCD is funded by the Natural Environment Research Council (NERC).

GEM-SA

The Gaussian Emulation Machine for Sensitivity Analysis (GEM-SA) is the first product of the GEM project. It will allow you to build an emulator of a computer code from a set of input and output points. It will also perform prediction, uncertainty analysis and sensitivity analysis of the code using far fewer code runs than Monte-Carlo based methods.

GEM-SA is offered free of charge, provided it is not used for profit. It may be freely copied and distributed, provided that files have not been edited or altered in any way, and provided that no charge is made for distributing GEM-SA. Published work that uses GEM-SA results should include a citation for this web page. Requests to use GEM-SA for any commercial purpose must be directed to Marc Kennedy.

If you use GEM-SA please let Marc Kennedy know (marc.kennedy@fera.gov.uk) and he will add you to the list of users. He will keep registered users informed of bug fixes and updated information about GEM-SA and future developments of the GEM project.

GEM-SA runs on Windows, but Linux users can also run it. The required package (called "Wine") can be freely downloaded in both binary and source form for various Linux distributions from <http://www.winehq.com/site/download>.

Tutorials

A course was held on March 21st and March 22nd 2005 for NERC related researchers, which included instruction in the use of GEM-SA. This was revised and given again for Engineers at the University of Sheffield on January 30th and 31st 2008. It has been revised again and updated for a course aimed at researchers in the biological sciences given on July 3rd 2008. The practical sessions (PowerPoint) have been made available for download here since the 2005 course, and the revised 2008 versions below now fully reflect the changes in GEM-SA that were implemented in version 1.1:

- ▲ [Getting started](#) with GEM-SA
- ▲ [Uncertainty analysis](#) with GEM-SA
- ▲ [Sensitivity analysis](#) with GEM-SA (example uses additional data files [SAex1_inputs.txt](#), [SAex1_output.txt](#))

The course also included the following presentation about the underlying concepts and modelling choices for building emulators:

- ▲ [Gaussian process modelling](#)

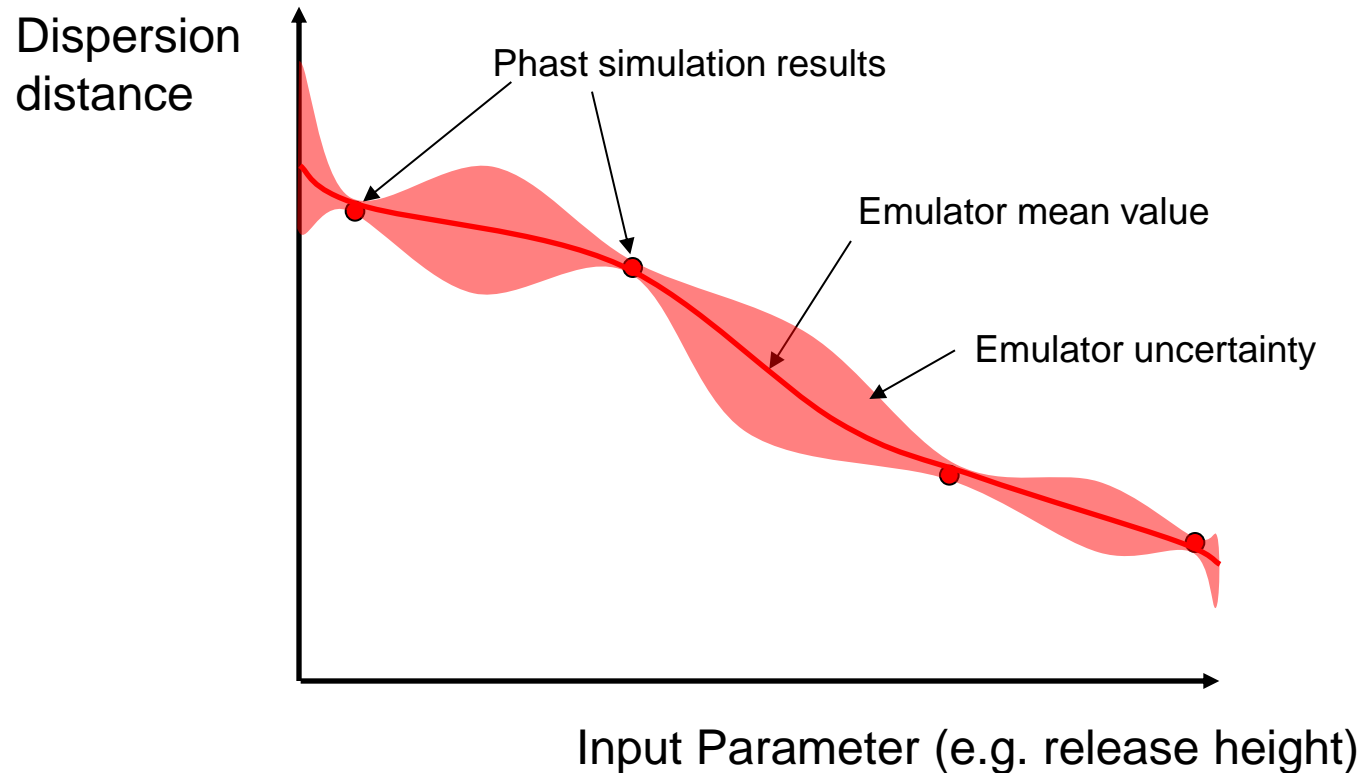
This is one of several [courses](#) offered by Tony O'Hagan and colleagues. Please use the "Contact me" button at the bottom of this page to enquire about when this course may be offered again.

Download instructions

[Download V1.1](#) zip file (1.3MB) MS Windows version.

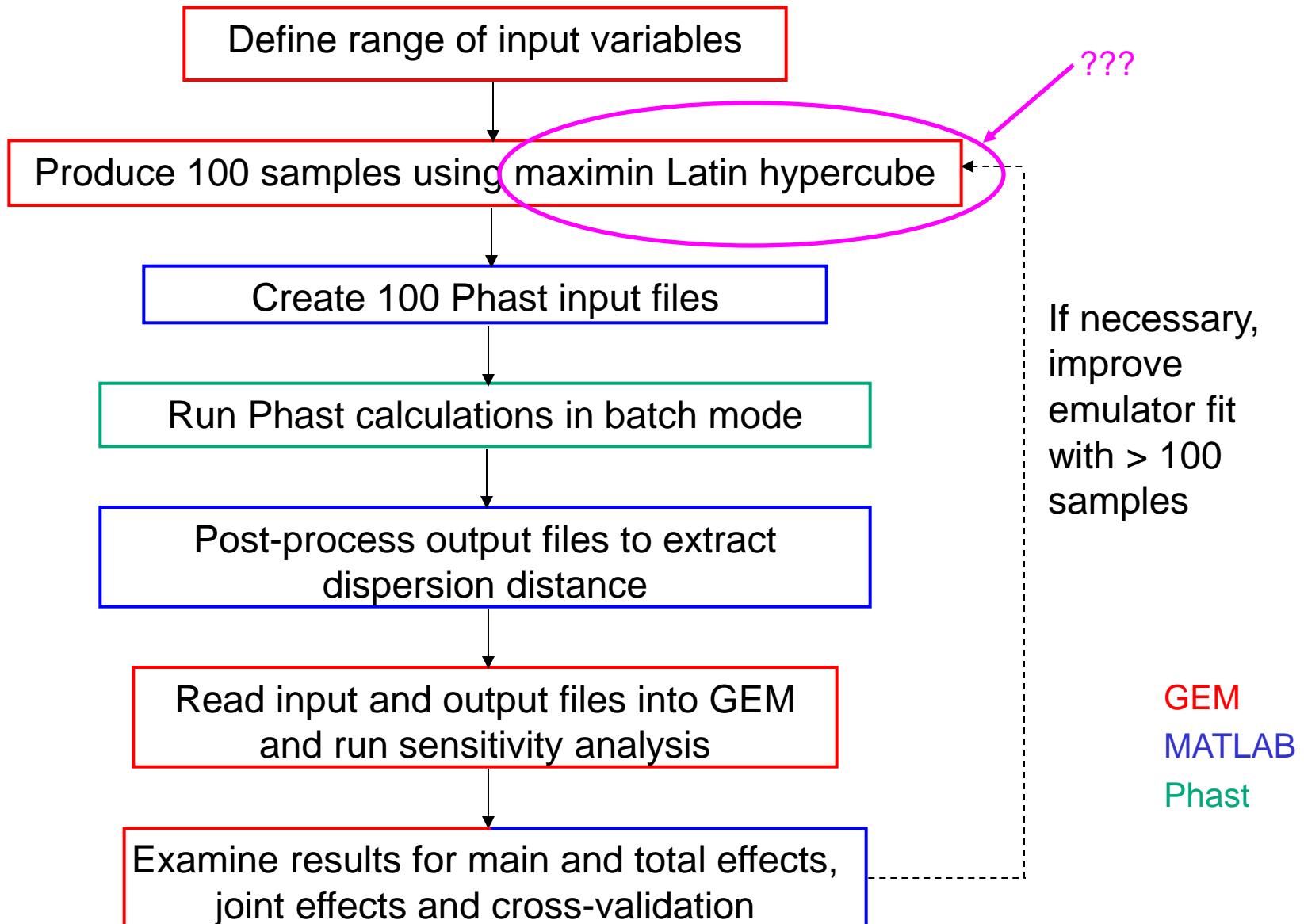
Extract/unzip the zip file to produce a directory GEM-SA containing the following:

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

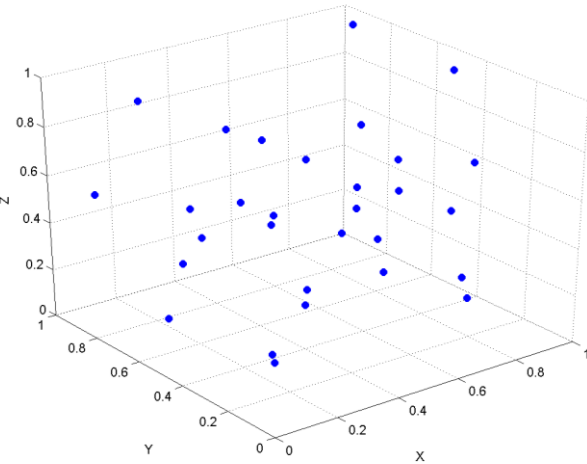
Sensitivity Analysis Process



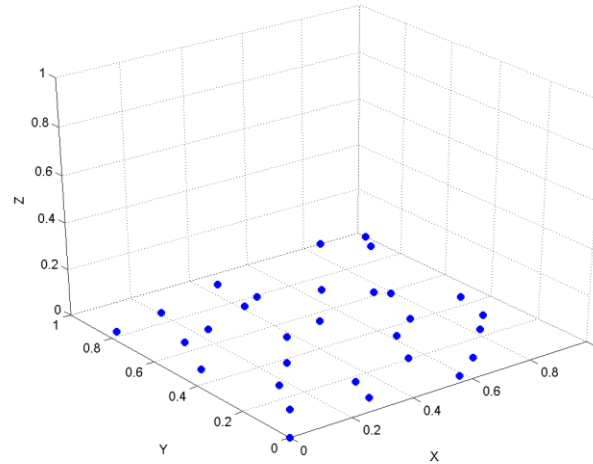
Maximin Latin Hypercube

- Example: 3 input variables, 30 samples

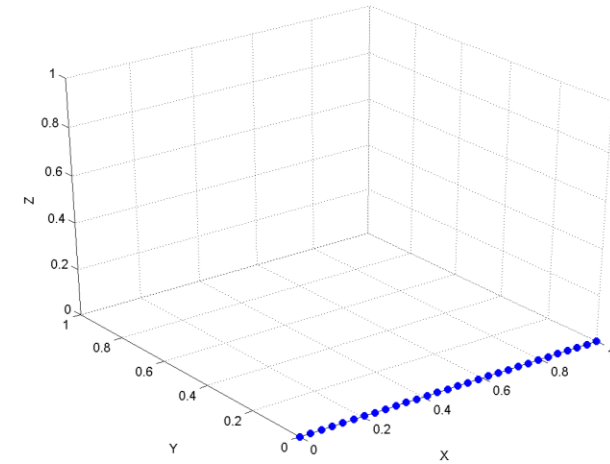
Full 3D sample space



Parameter Z has no effect



Parameters Y and Z have no effect

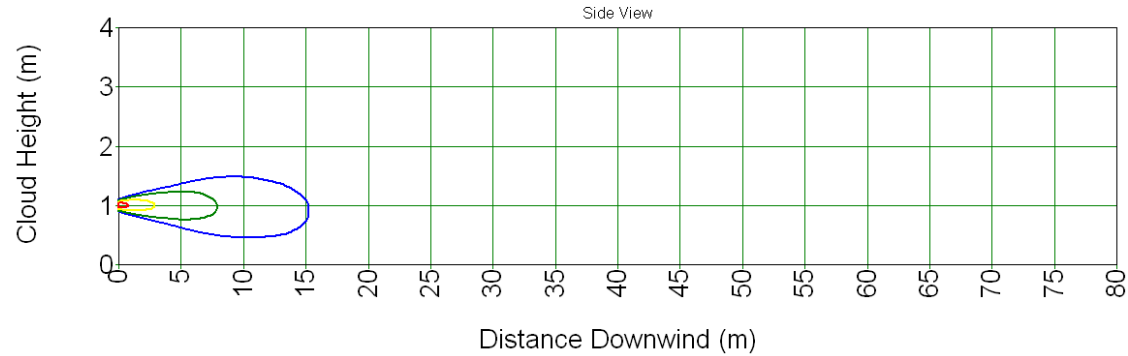


- If Parameters Y and Z had no effect on the results, all 30 samples are equispaced across Parameter X sample space
- Often, just 1 or 2 input parameters dominate model predictions : Latin hypercube maximises coverage from limited number of points

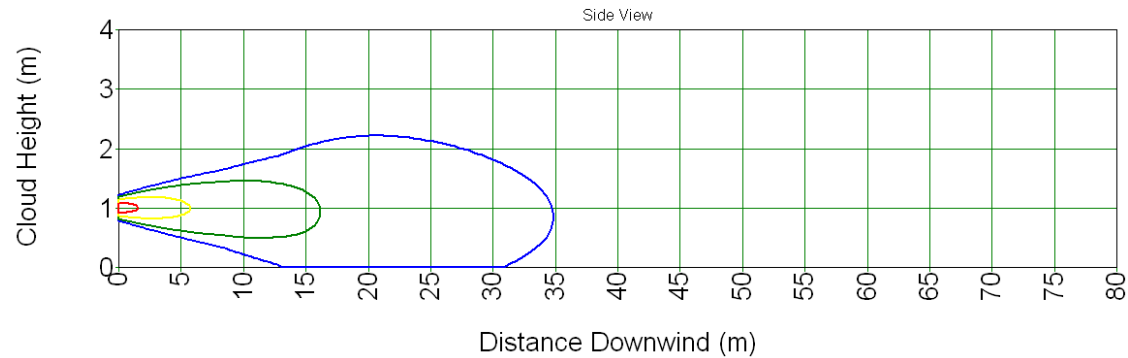
Phast Results

Orifice Diameter

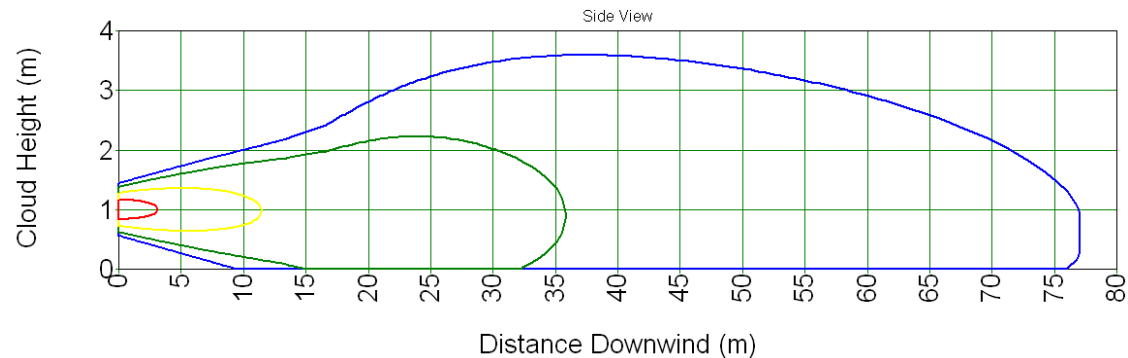
1/2 inch



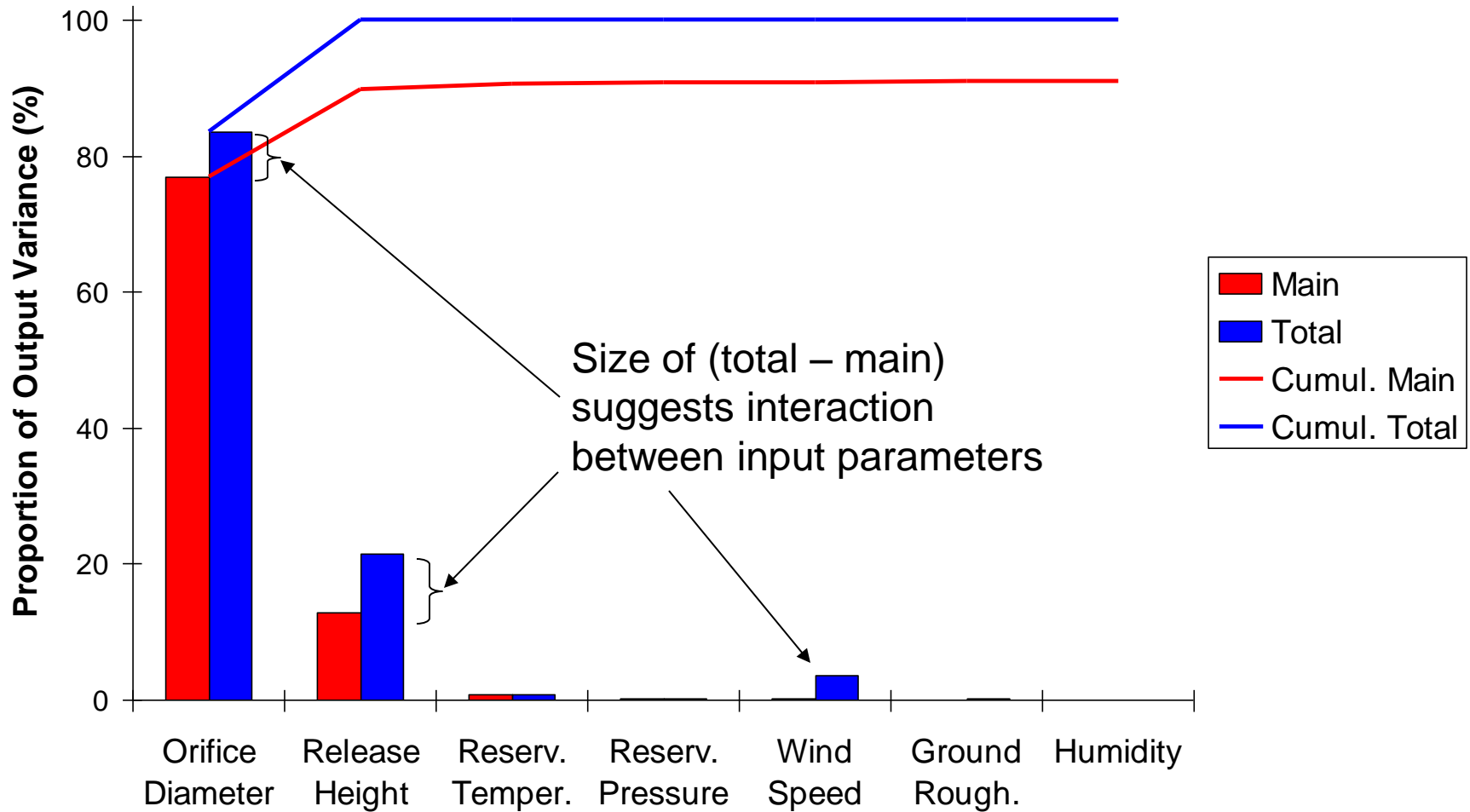
1 inch



2 inch

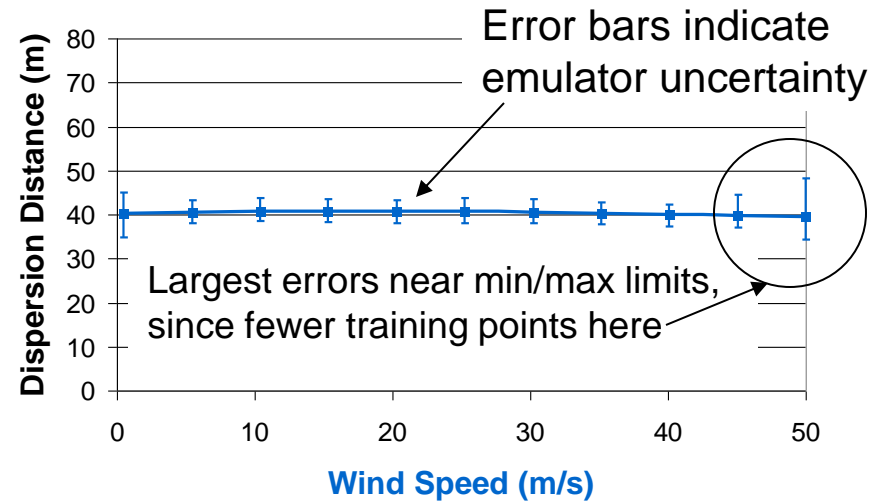
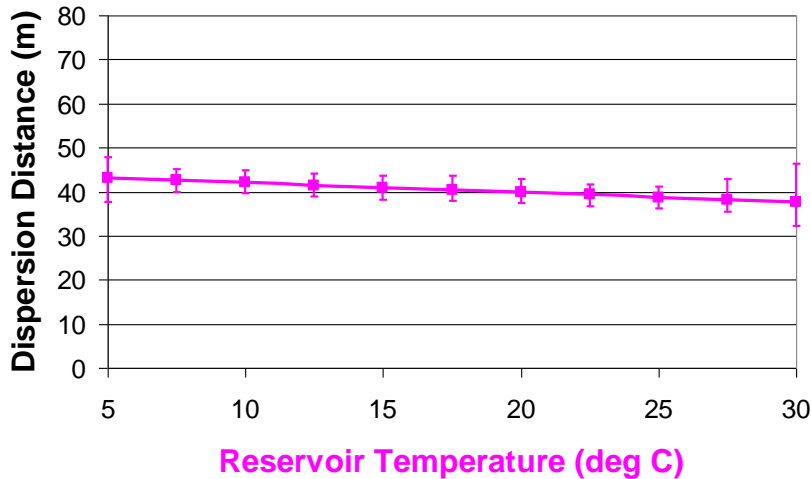
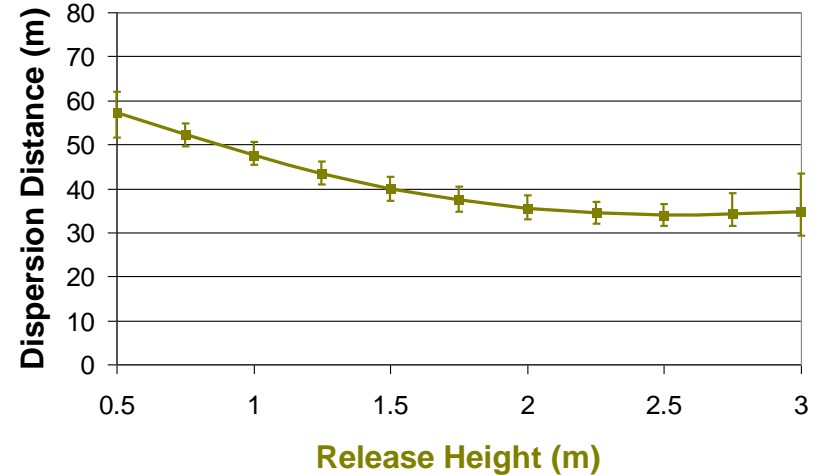
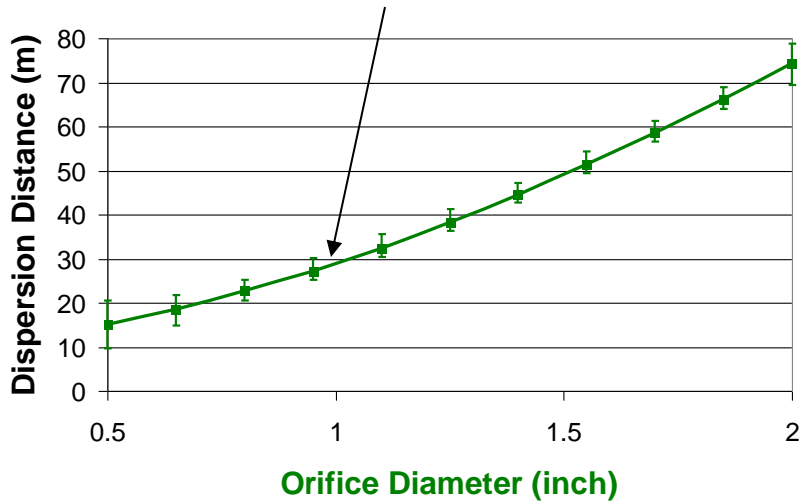


Results: Main + Total Effect

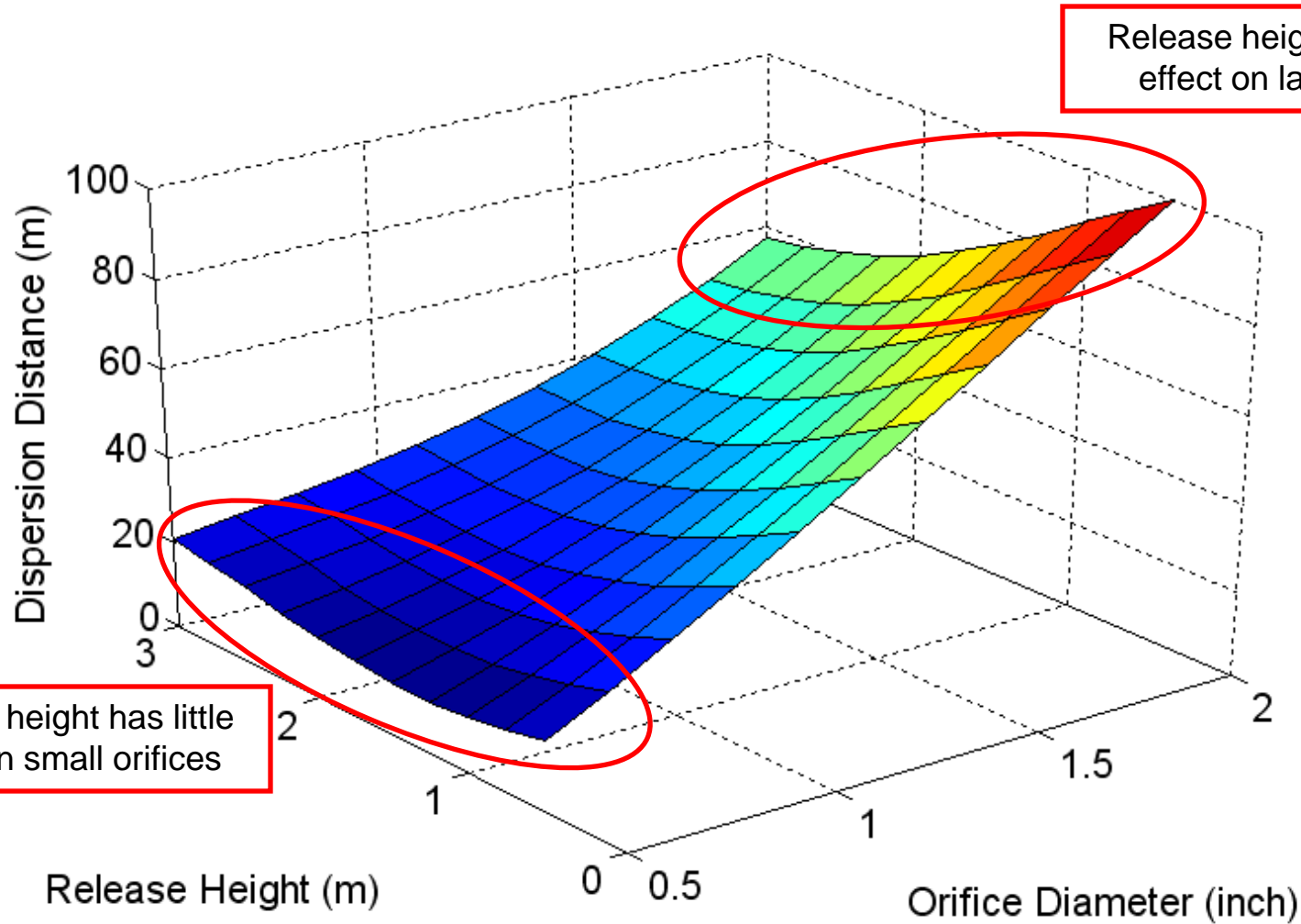


Main Effects

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



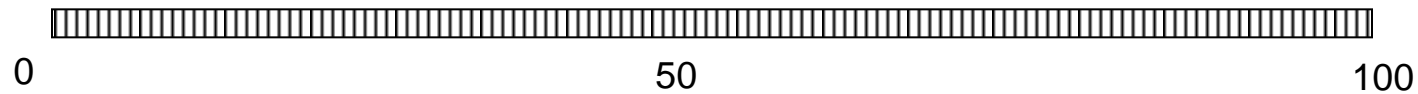
Joint Effects



Emulator Cross-Validation

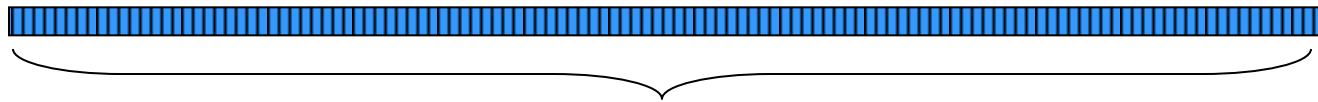
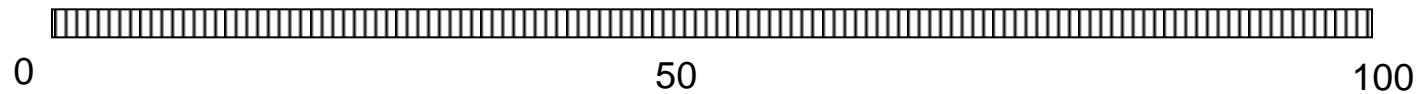


Phast results



Emulator Cross-Validation

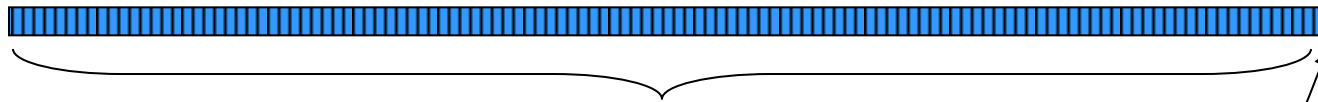
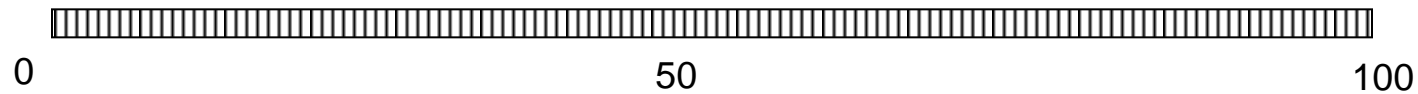
Phast results



Step 1.) Use 99 Phast results to fit emulator

Emulator Cross-Validation

Phast results

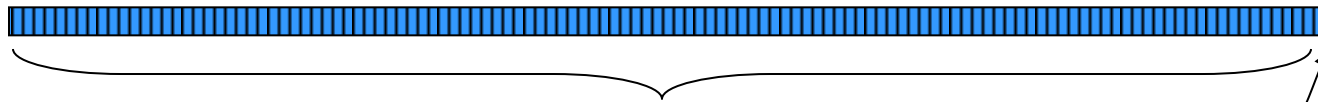
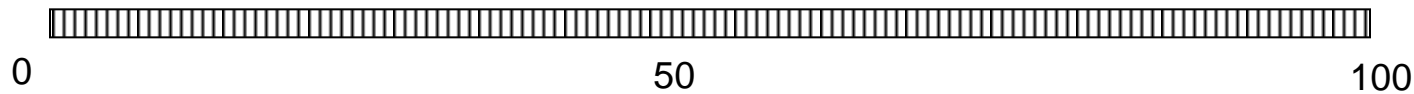


Step 1.) Use 99 Phast results to fit emulator

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

Emulator Cross-Validation

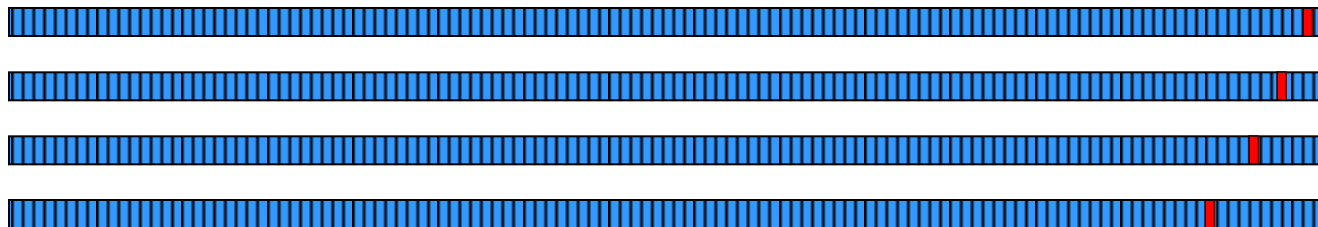
Phast results



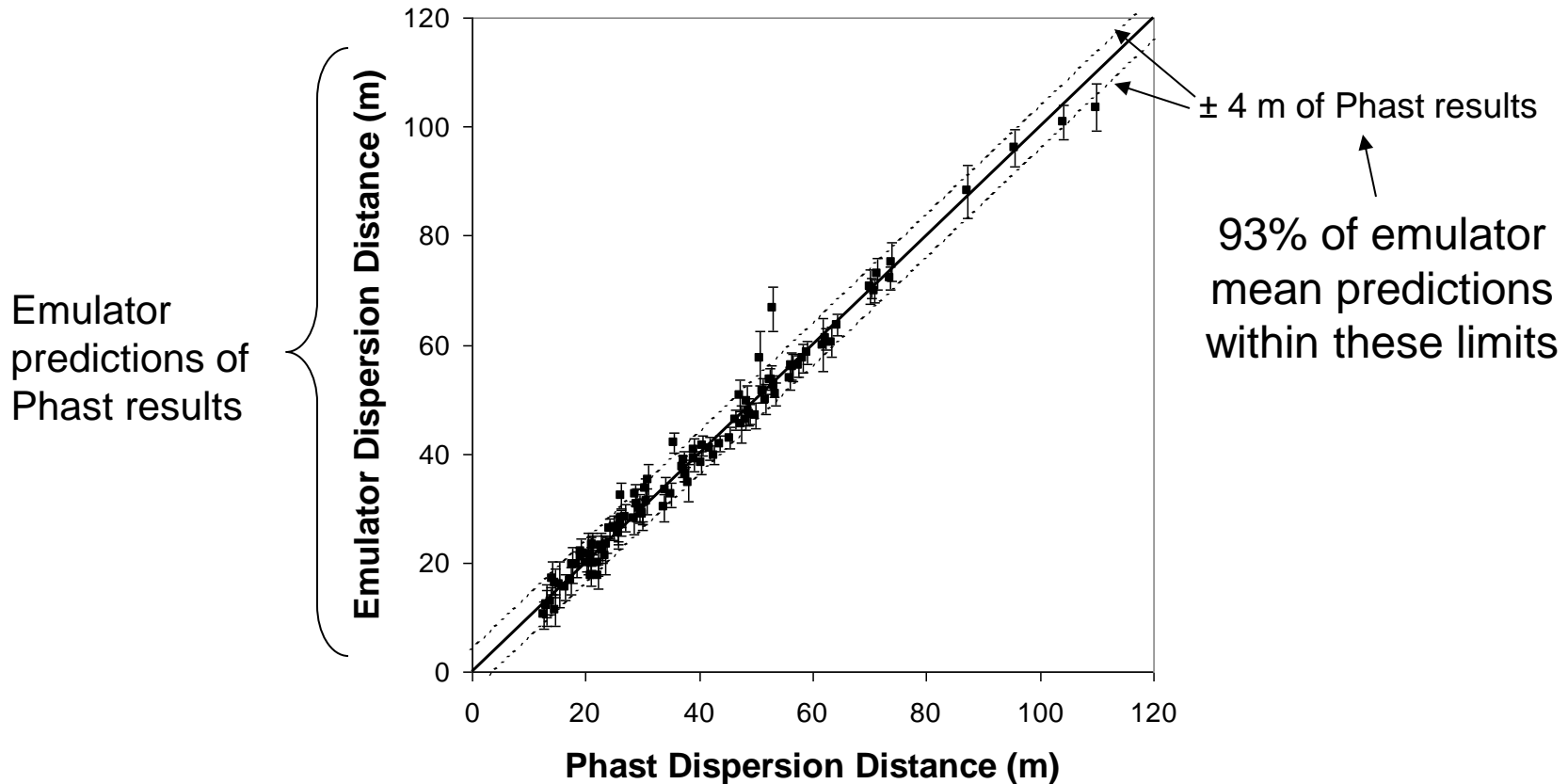
Step 1.) Use 99 Phast results to fit emulator

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

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



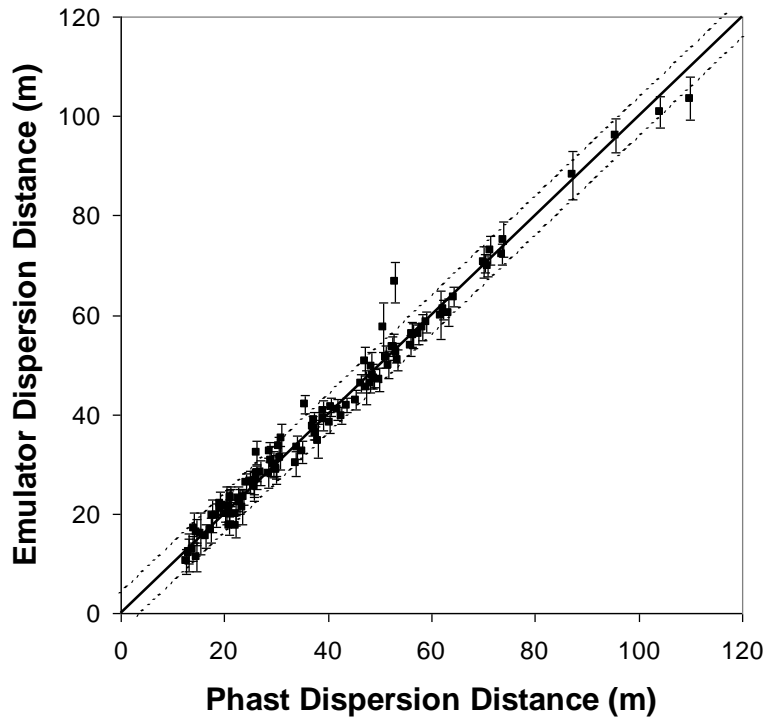
Emulator Cross-Validation



- 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

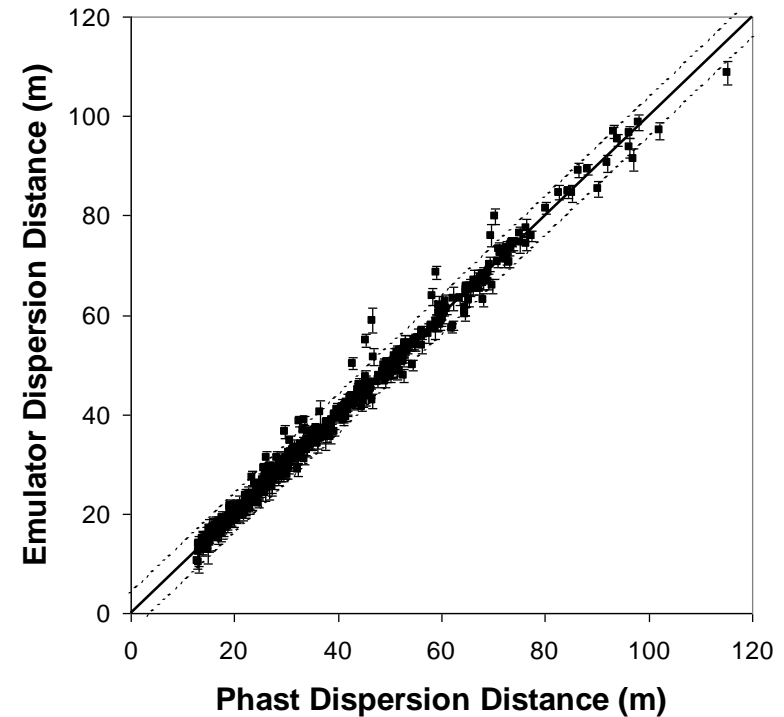
Emulator Cross-Validation

100 Phast training data points



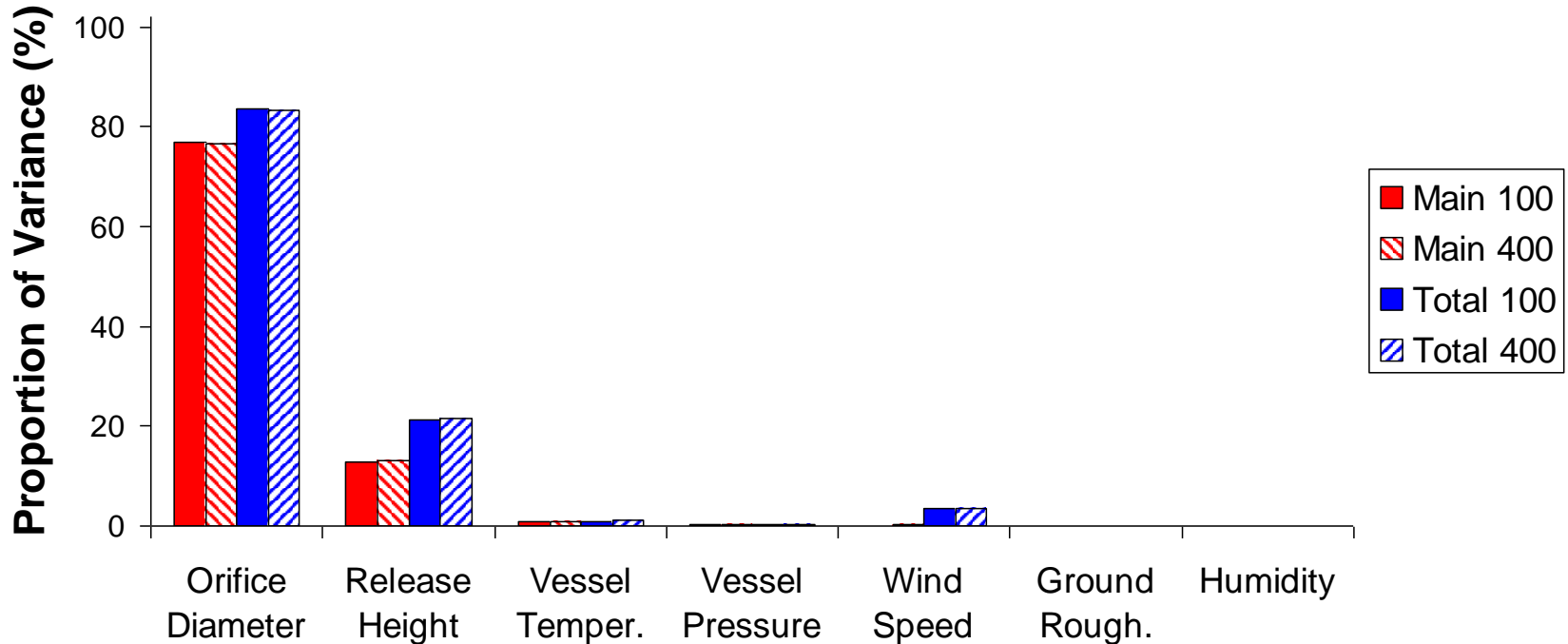
93% within $\pm 4m$

400 Phast training data points



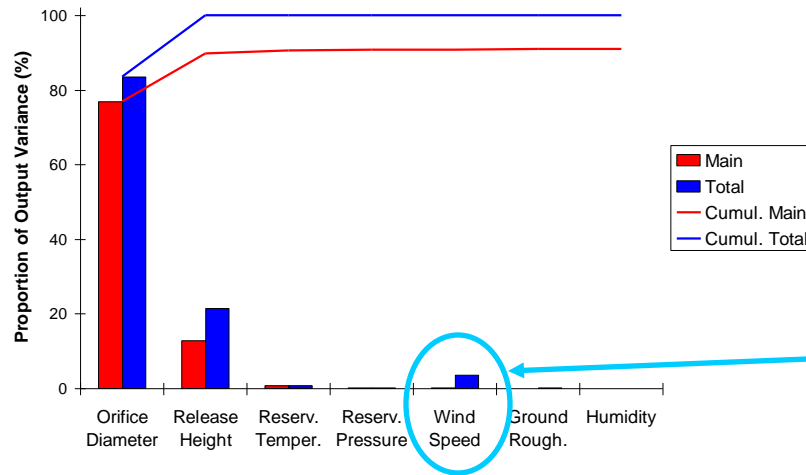
95% within $\pm 4m$

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

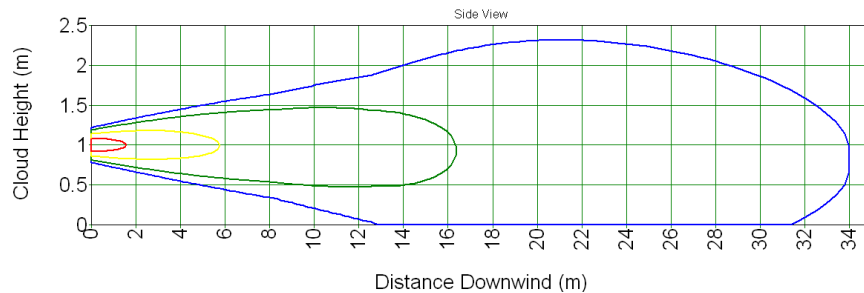
Do results make sense?



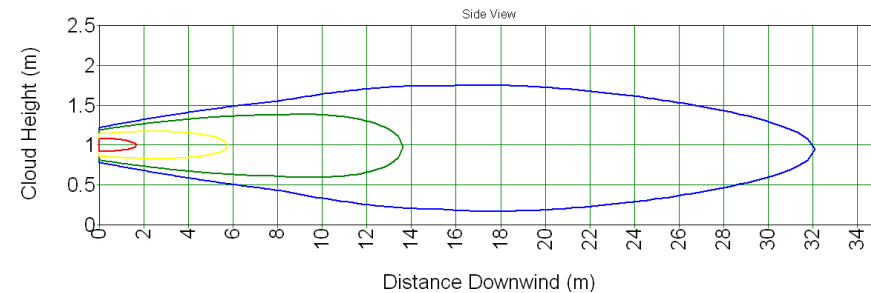
Dispersion distance hardly affected by atmospheric conditions

Even wind speed 0.5 – 50 m/s ?!

0.5 m/s wind



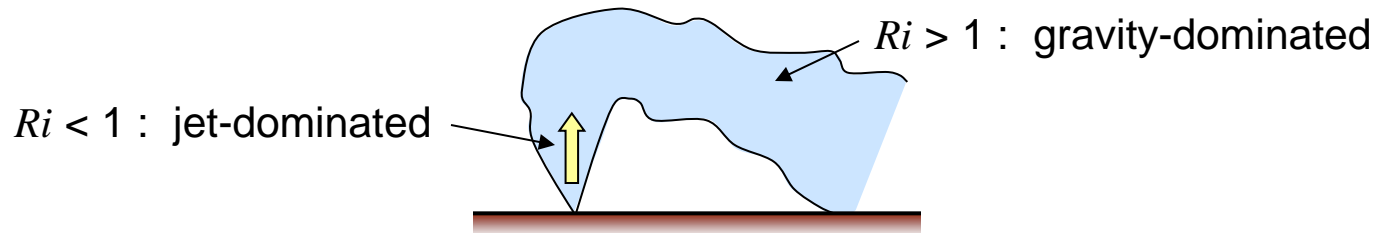
50 m/s wind



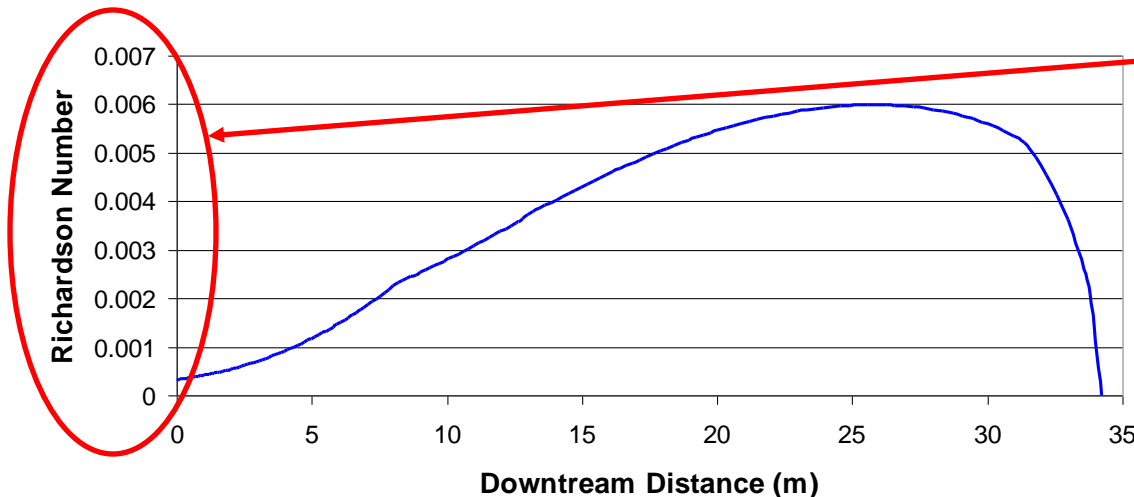
Plume Behaviour

- Plume behaviour characterised by Richardson Number

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



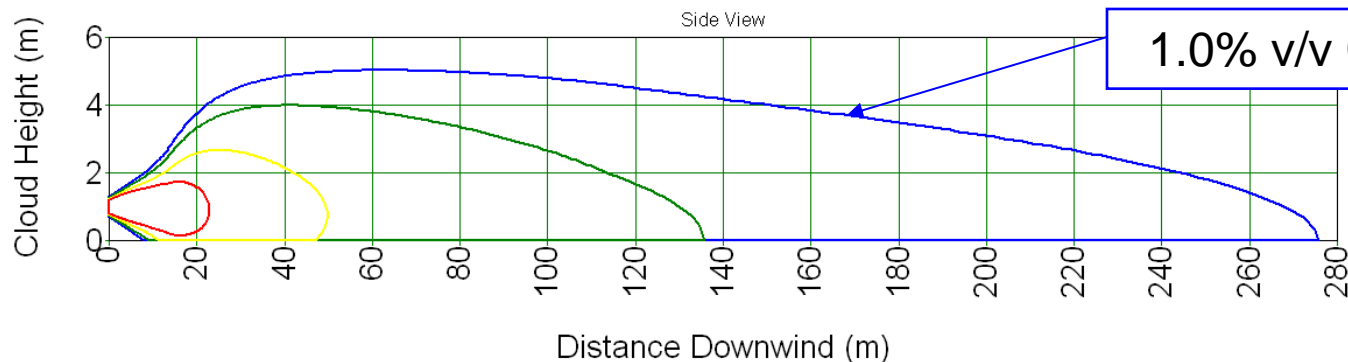
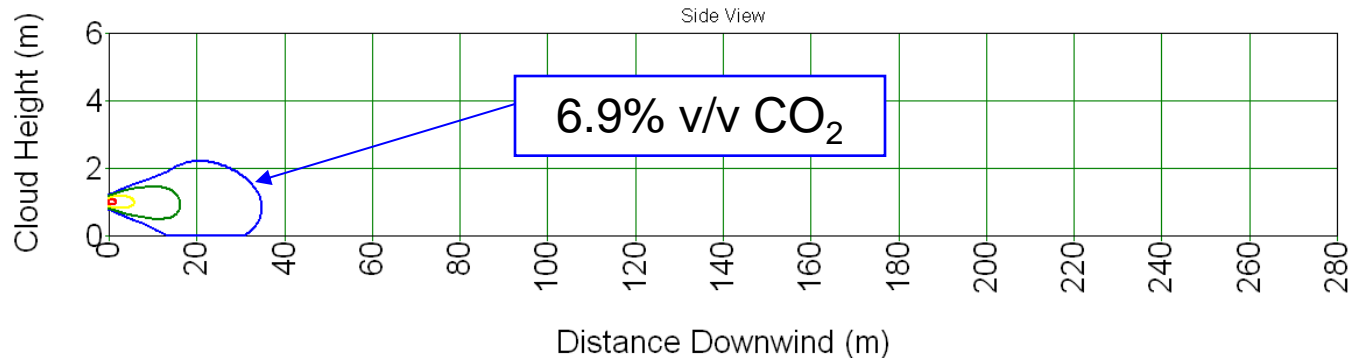
Phast results for 1-inch orifice with 0.5 m/s wind:



Plume behaviour is governed by jet momentum

Wind Speed Effects

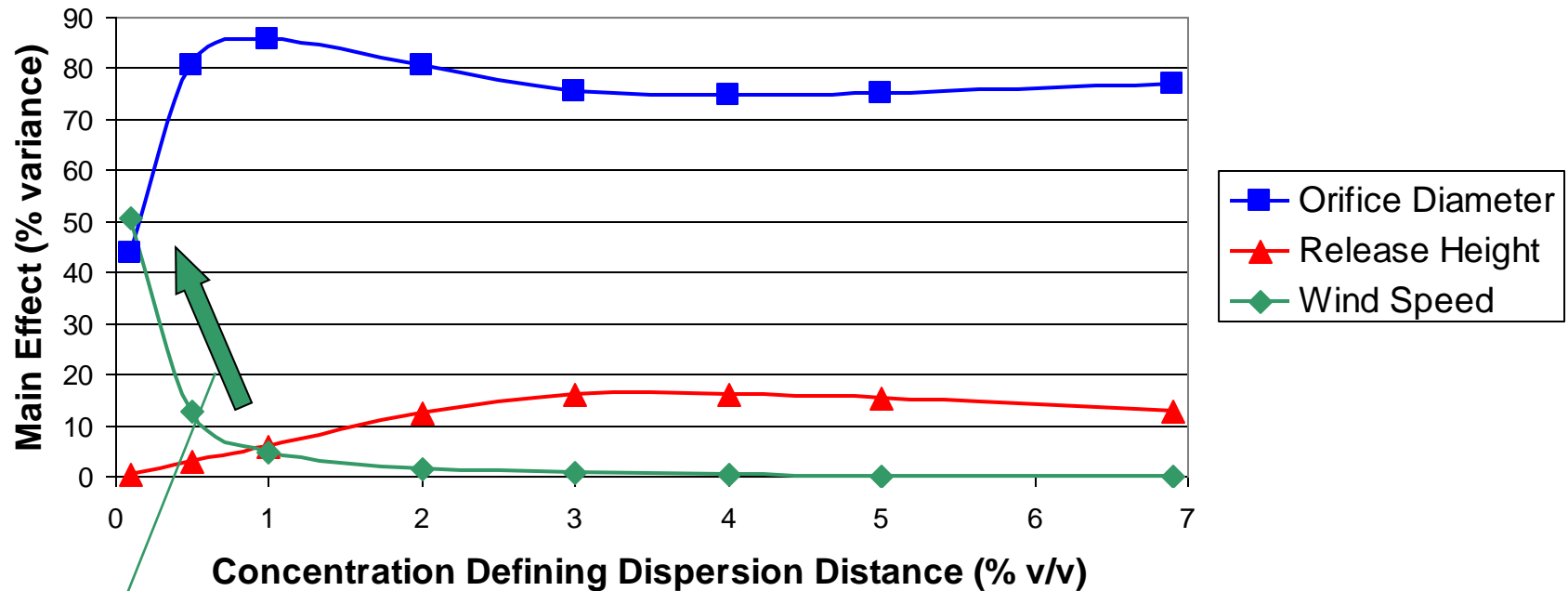
Defining the edge of cloud using a lower concentration:



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

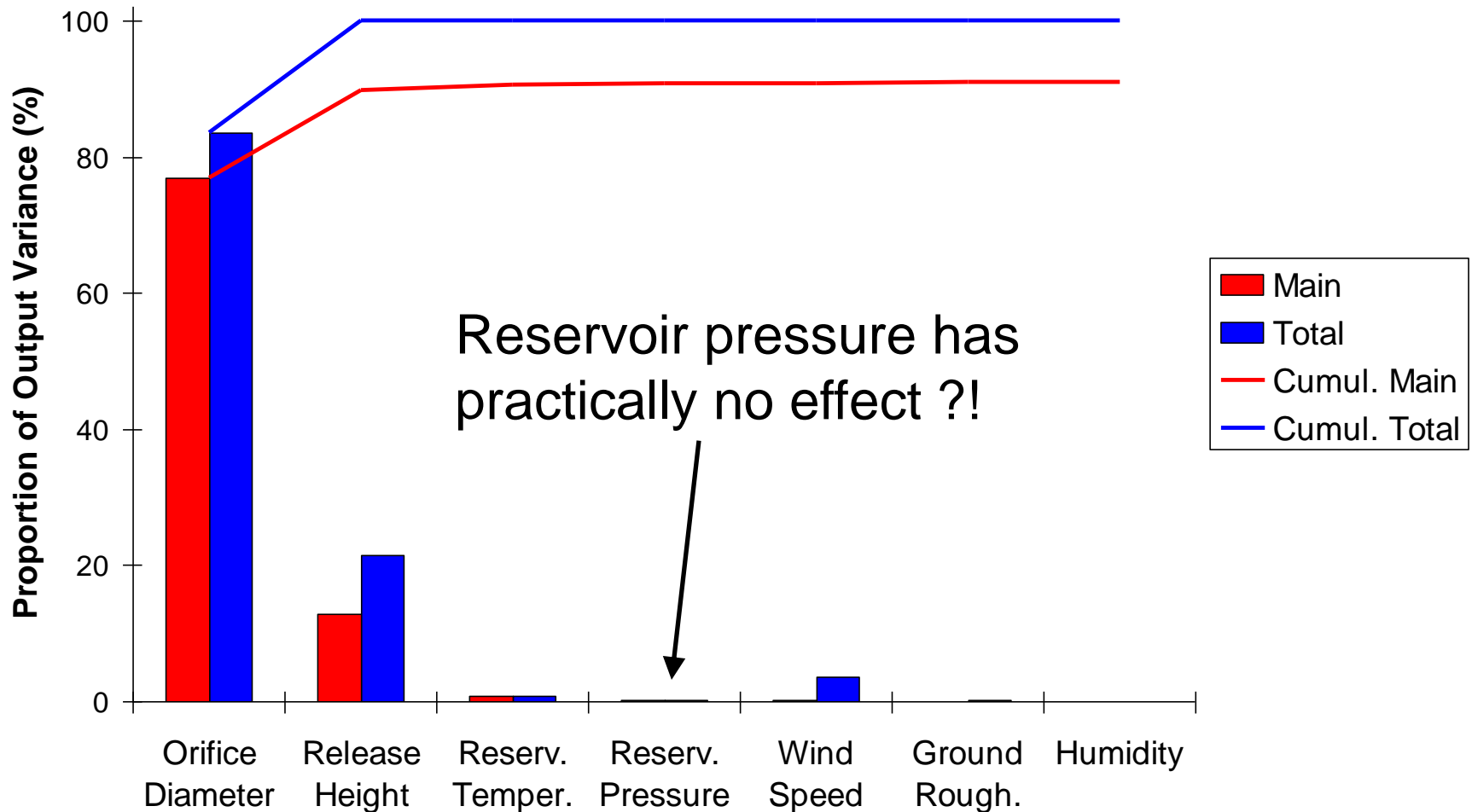
Wind Speed Effects

- Repeated sensitivity analysis with different model output



At concentrations below 1% CO₂, the wind speed has a significant effect

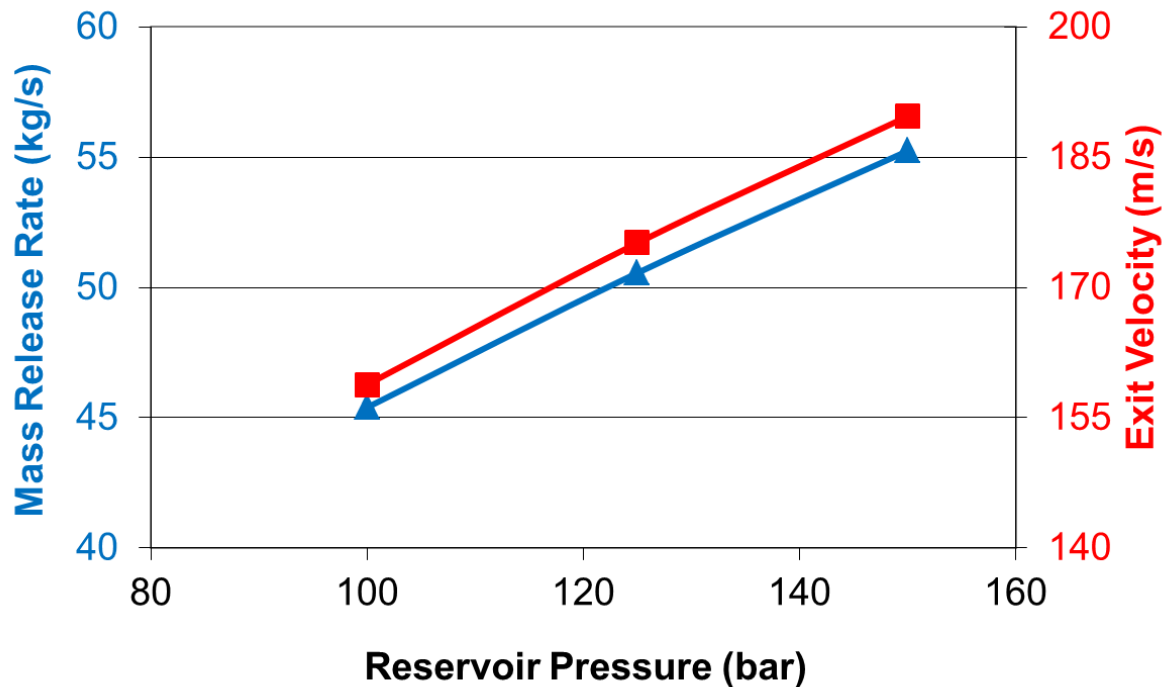
Effect of Reservoir Pressure



Effect of Reservoir Pressure

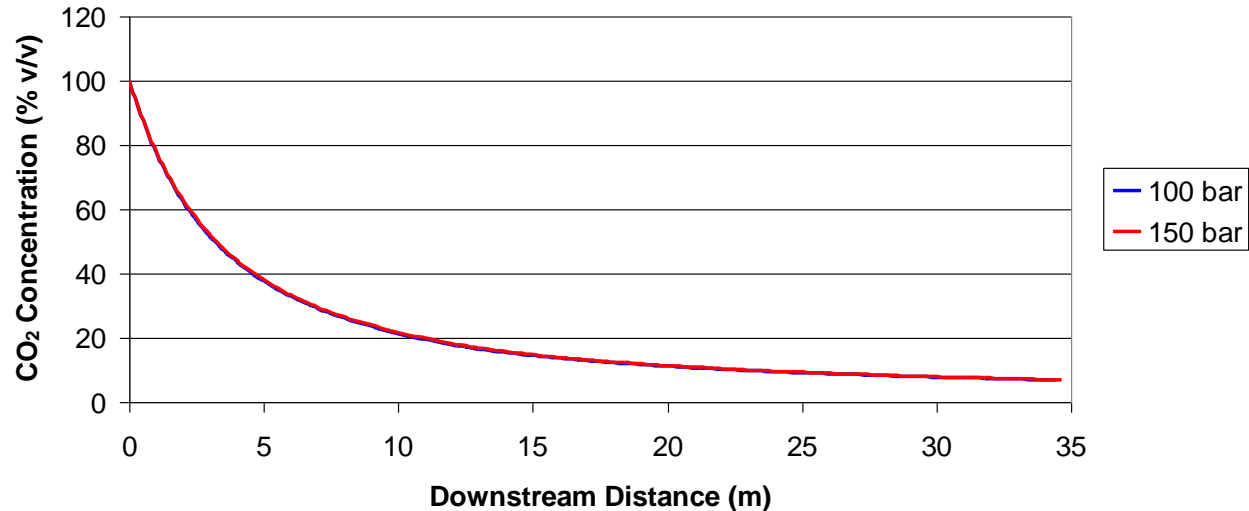
Increasing “Reservoir Pressure” has competing effects:

- 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 CO₂ 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

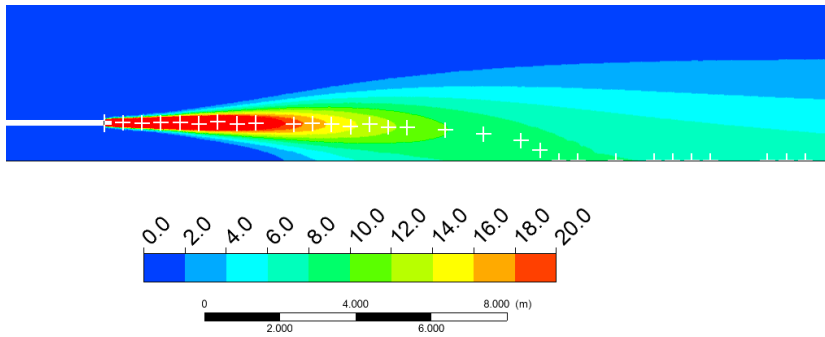
Weaknesses of Emulators

- 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

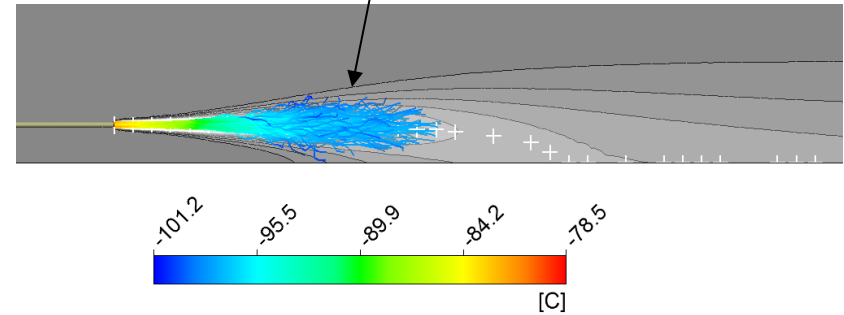
ANSYS-CFX

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

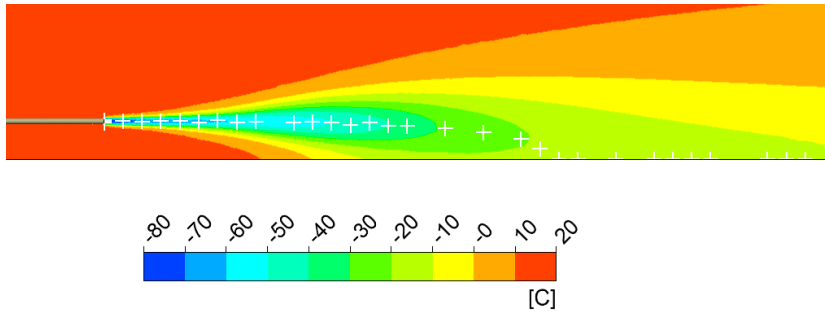
CO₂ Gas Concentration (% vol/vol)



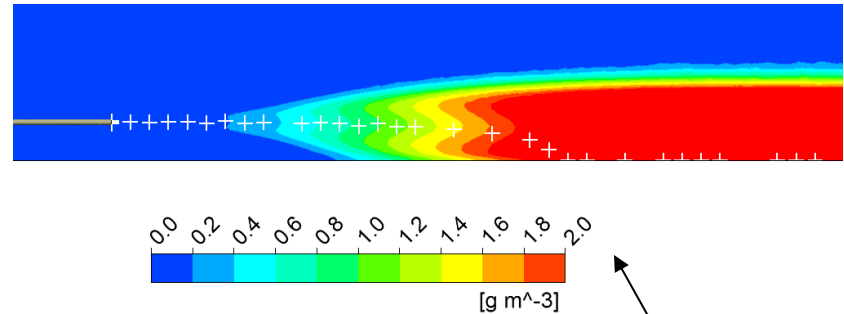
CO₂ Particle Temperature (deg C)



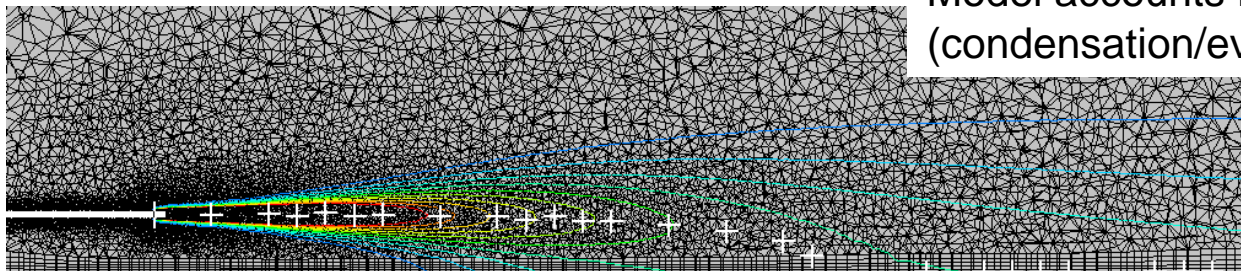
Gas Temperature (deg C)



Water Droplet Concentration (g/m³)



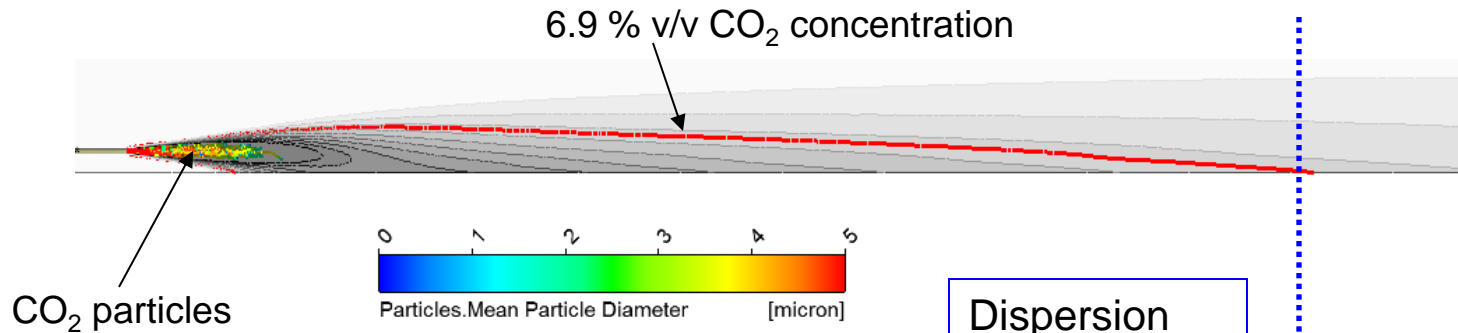
Model accounts for humidity effects (condensation/evaporation)



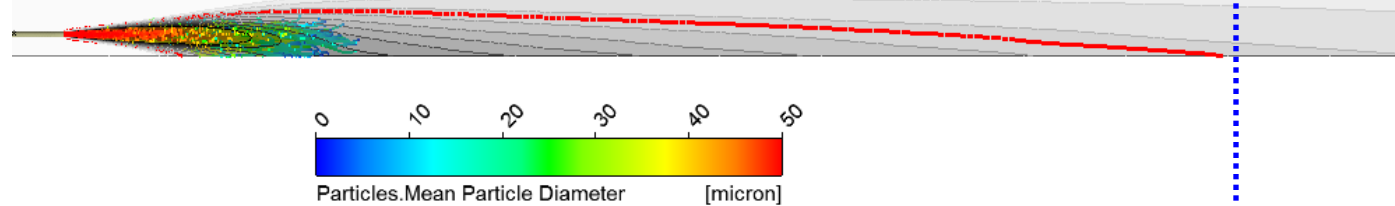
CFD Results

Particle Size

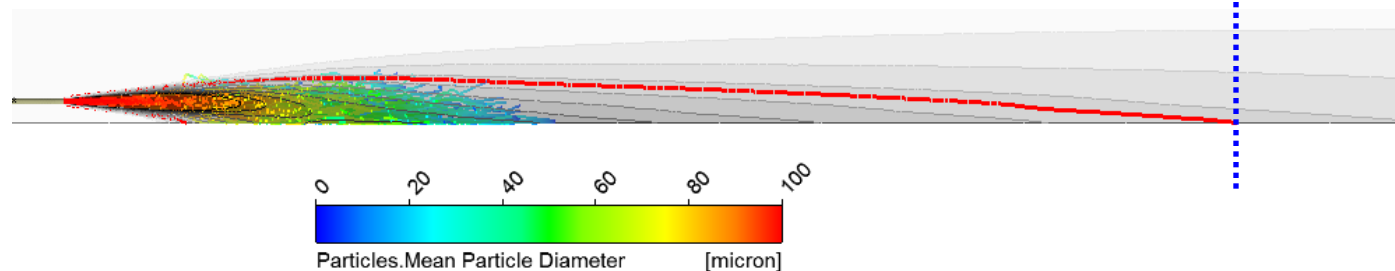
5 μm



50 μm

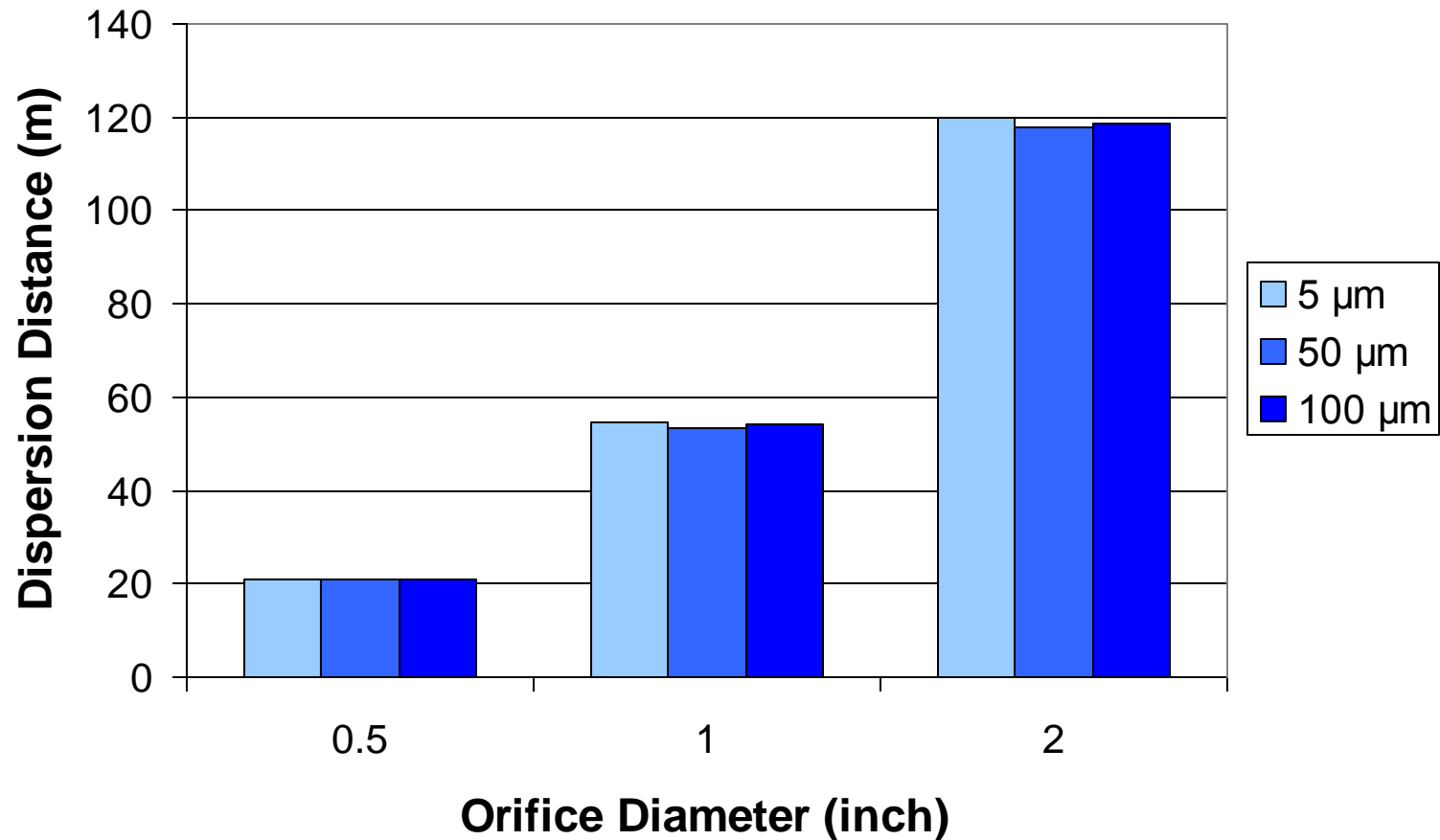


100 μm



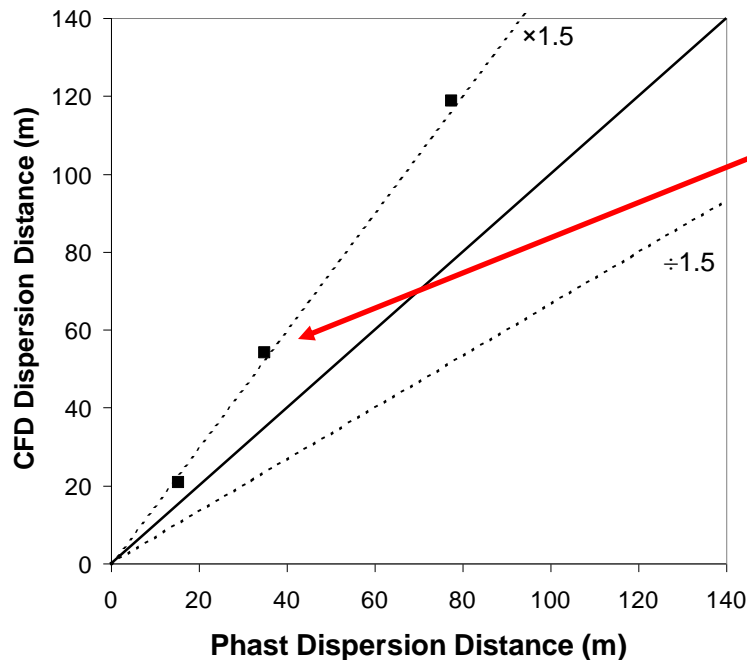
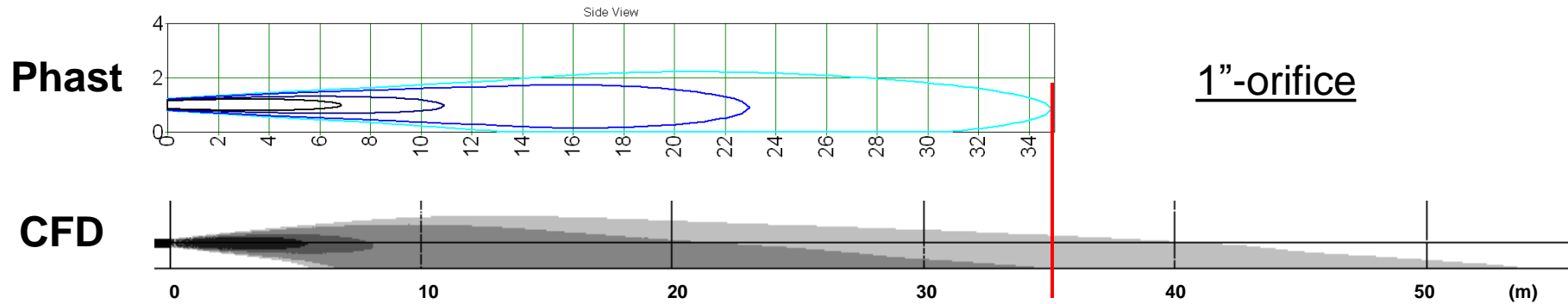
CFD Results

- 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

- 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!

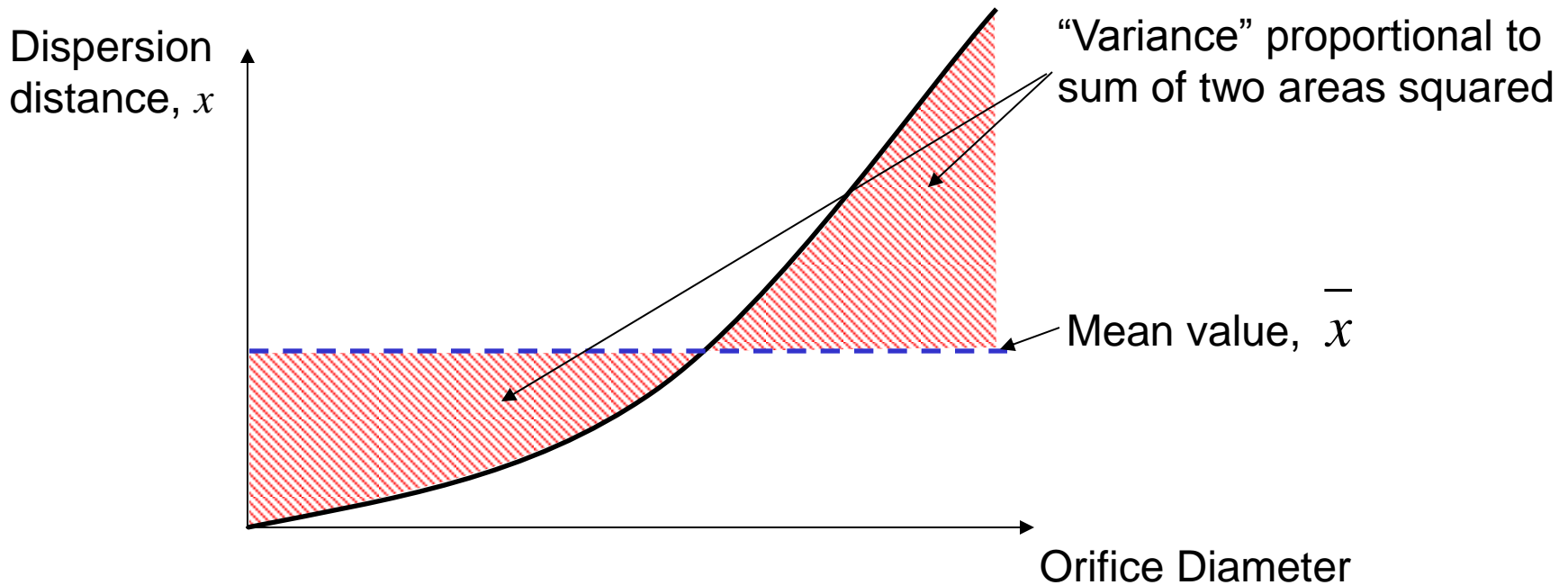
P.S. See me if you would like a demonstration of GEM

Variance-Based Sensitivity Analysis

- What is “variance”?

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

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

- **Main Effect of Parameter A:**

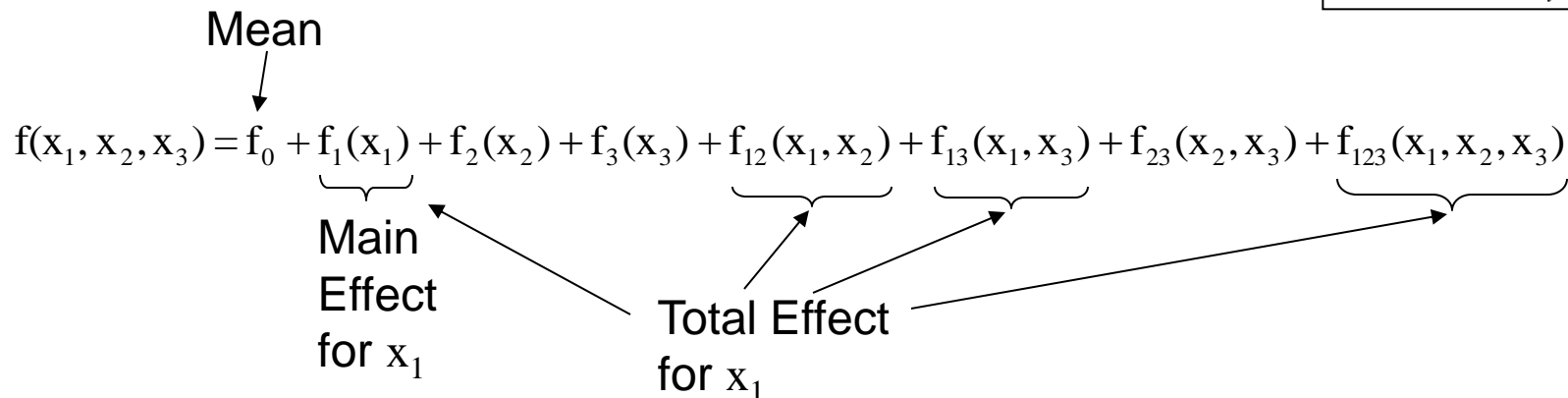
- The amount of variance that would be removed from the total output variance if we learnt of the true value of A

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

- **Total Effect of Parameter A:**

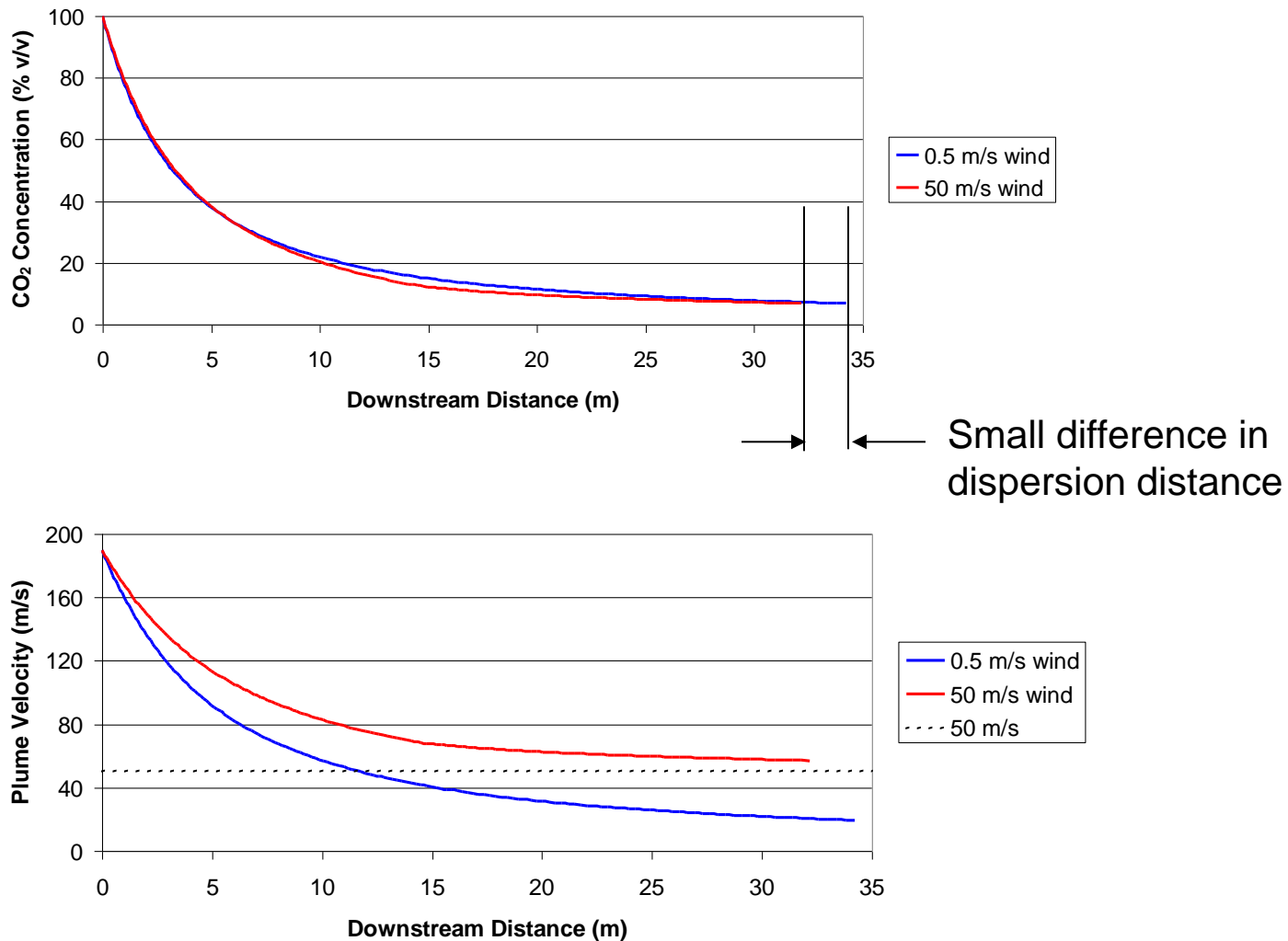
- The amount of variance that would remain unexplained if the values of all other parameters except A were known, and the variance was produced only by varying A

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



Effect of Wind Speed

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



What are we interested in?

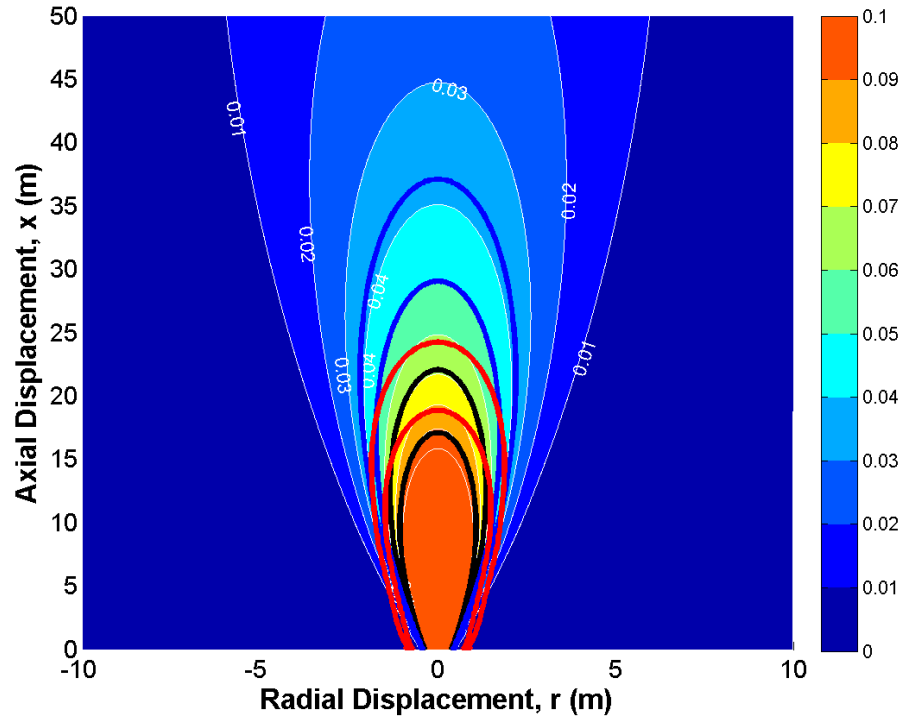
- Cloud extent based on HSE contours of Toxic Load:
 - Specific Level of Toxicity (SLOT)
 - Significant likelihood of Death (SLOD)

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

	SLOT	SLOD
DTL (ppm ⁿ .min)	1.5 x 10 ⁴⁰	1.5 x 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 CO₂

Concentration Fluctuations



- CO₂ jet : diameter 0.5m and exit velocity 50 m/s.
- Coloured contours show the CO₂ 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