The Importance of Concentration Fluctuations in Hazard Assessment and Source Term Estimation

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Background

- Response to a release of hazardous material depends upon identifying:
  - Where the release occurred.
  - How much material was released.
- Can be addressed by inverse modelling/source term estimation but:
  - Process must be rapid to be operationally useful (<5 minutes).
  - Process is difficult due to the large uncertainties associated with the data.

Aim

- Correlating sensor concentration fluctuations with predictions from a dispersion model is a critical part of the inverse modelling process.
- The aim was to:
  - Determine the impact on the source term estimate of different variance model assumptions.
  - Determine the best representation of variance to use.

MCBDF

- Dstl has prototyped a capability for source term estimation based on dynamic Bayesian graphical modelling:
  - Enables disparate data to be combined in mathematically tractable way with high level of error tolerance.
  - Outputs are source term posterior probability density functions (pdfs).
- Software is known as the Monte-Carlo Bayesian Data Fusion (MCBDF) code.

MCBDF Output

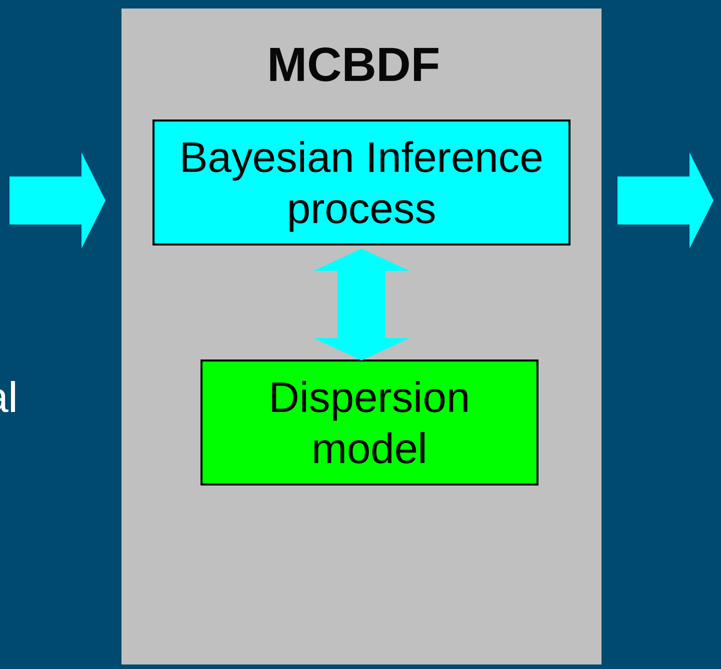
- Source-term estimation for 9 parameters: location (x, y), time (t), release mass (m), agent type (a), wind vector (u, v), roughness length (z_0), Monin-Obukhov length (L):

Input data

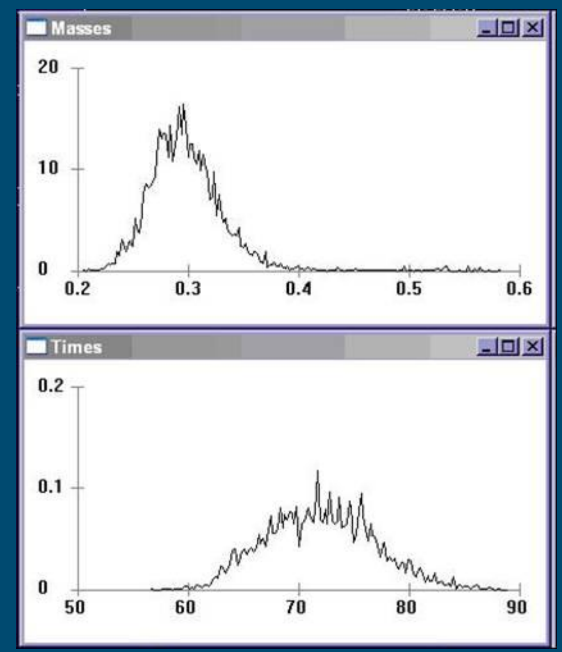
Spatial area

Sensor concentration signals

Meteorological data



Source term pdfs



Concentration variance in MCBDF

- The posterior pdfs are evaluated using Bayes' rule:

$$\underbrace{p(\theta|D)}_{posterior} \propto \underbrace{p(\theta)}_{prior}\underbrace{p(D\,|\,\theta)}_{likelihood}$$

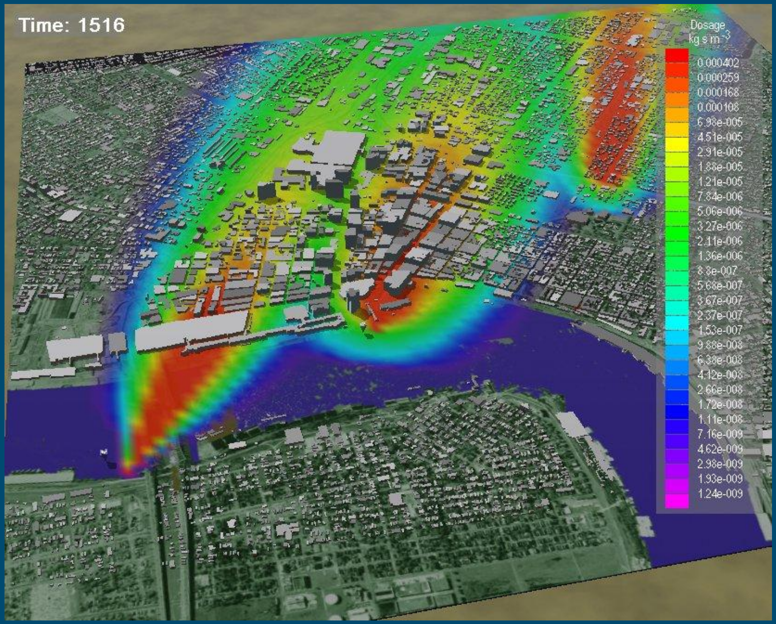
D is the total data set
θ is the source term hypothesis

- Dispersion model concentration mean (μ) and variance (c_{var}) are required to evaluate the likelihood of individual data (d):

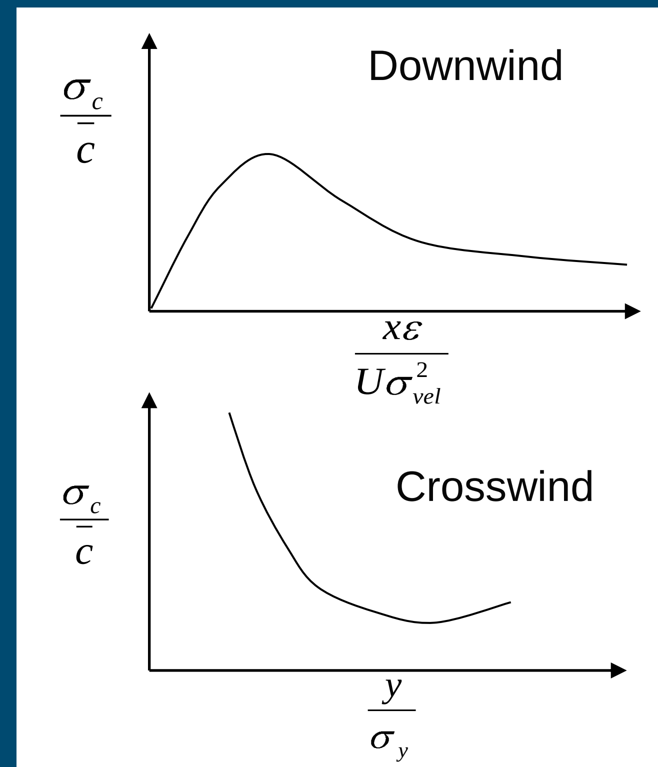
$$\underbrace{p(d\,|\,\mu,c_{\mathrm{var}})}_{likelihood} = \int_0^\infty \underbrace{p(d\,|\,c)}_{\substack{measurement\\ density}}\underbrace{p(c\,|\,\mu,c_{\mathrm{var}})}_{\substack{concentration\\ density}}\mathrm{d}c$$

MCBDF Dispersion Model

- The dispersion model used in MCBDF is the Dstl Urban Dispersion Model (UDM):
  - Gaussian puff model based on the AERMOD equations.
  - Used in non-urban mode.
  - Very rapid execution time on desk-top PC.
  - Enables Bayesian probability reasoning to be applied to a sample set of thousands of hypothesised releases.



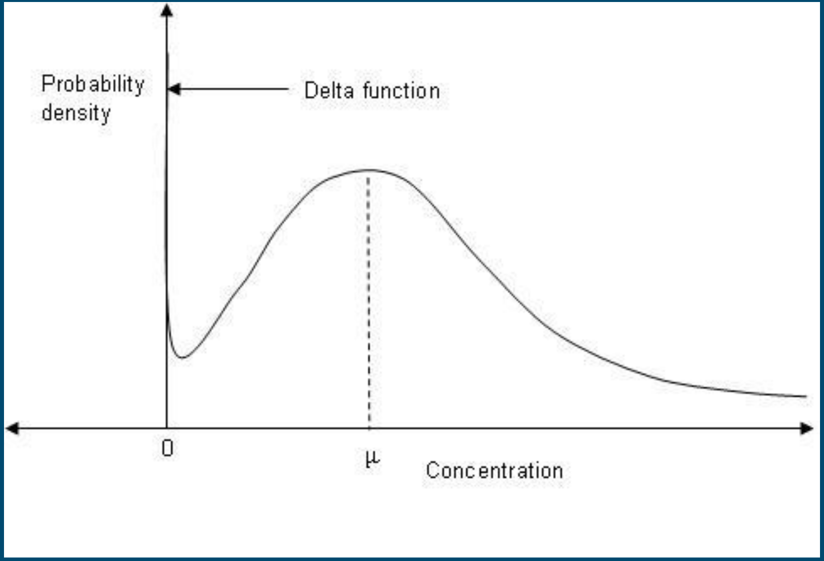
Concentration Variance



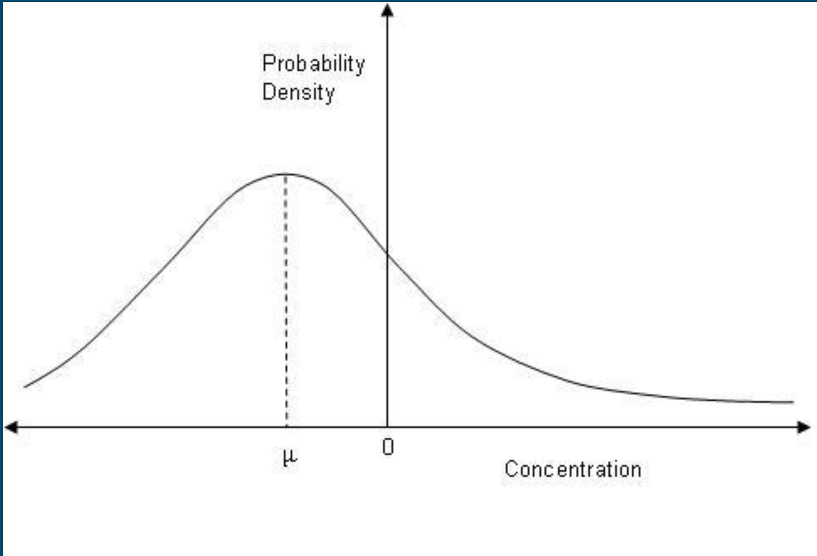
- Concentration variance at a point is dependent upon:
  - The local turbulence scales.
  - The time since release.
  - Position relative to the puff centre.
  - The puff interaction history.

Clipped Gaussian distribution

- Past analysis has suggested that the variability can be best represented by a clipped Gaussian distribution:



Clipped Gaussian



Under-lying Gaussian

$\bar{c}$

UDM Variance Calculation

- Concentration variance due to a number of over-lapping puffs is:

$$c_{\mathrm{var}} = \frac{\bar{r}^2 \bar{c}^2}{\bar{G}}$$

Where: $\bar{c}$ is the average puff concentration, $\bar{r}$ is the average fluctuation intensity, $\bar{G}$ is the average Gaussian factor

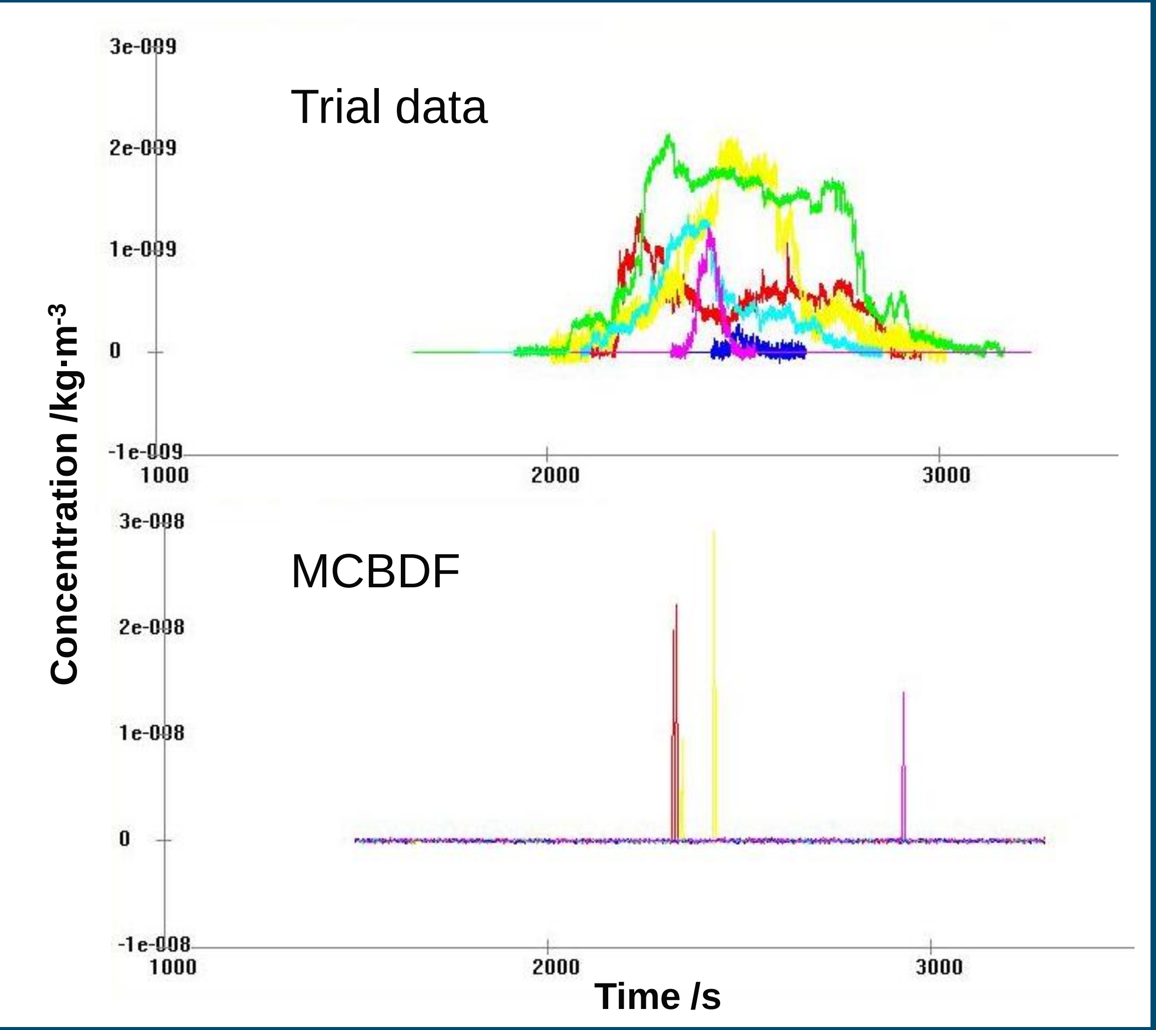
- Fluctuation intensity is:

$$r = \sqrt{\frac{\sigma_{ex}\sigma_{ey}\sigma_{ez}(1+K^2)}{\sigma_{ix}\sigma_{iy}\sigma_{iz}} - 1}$$

Where: subscript '*e*' refers to ensemble average puffs, and subscript '*i*' to instantaneous puffs. *K* is the internal fluctuation constant (= 0.3).

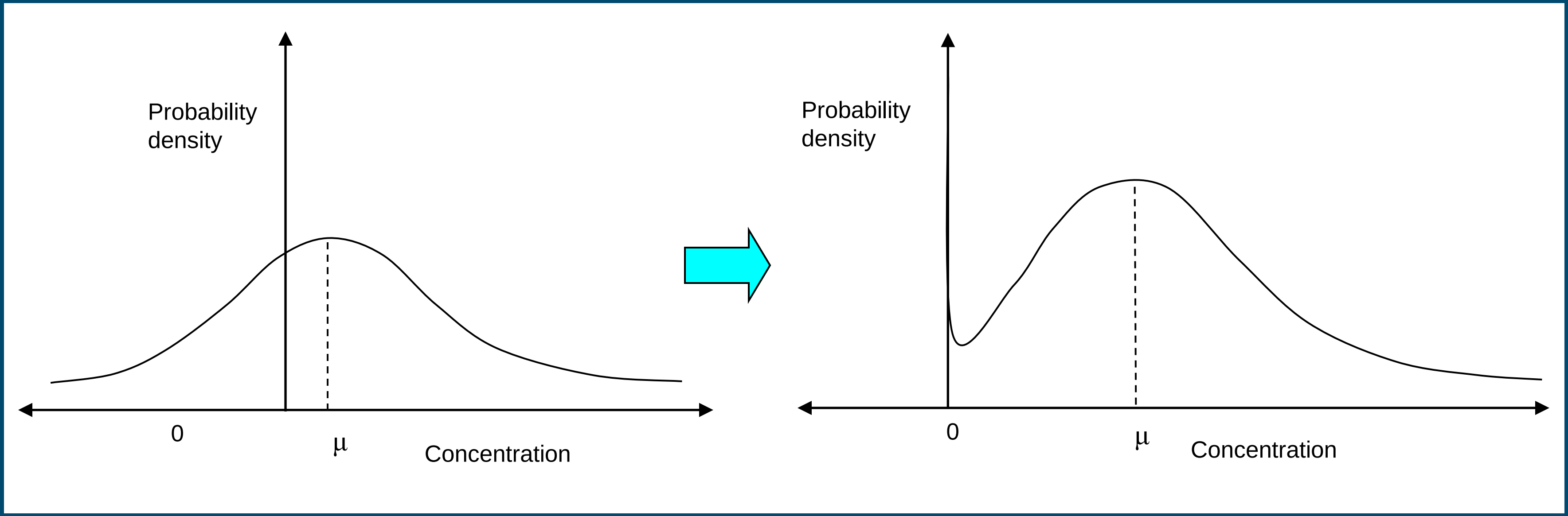
Testing of MCBDF against DP26

- Dipole Pride 26 (DP26) arranged to test the SCIPUFF variance model.
- UDM mean and variance values assumed to refer to clipped-Gaussian distribution.
- Inference concentration time-series had little in common with trial data.



An Alternative Assumption

- Assume that the mean and variance from UDM refer to an unclipped Gaussian distribution, and derive a clipped distribution:

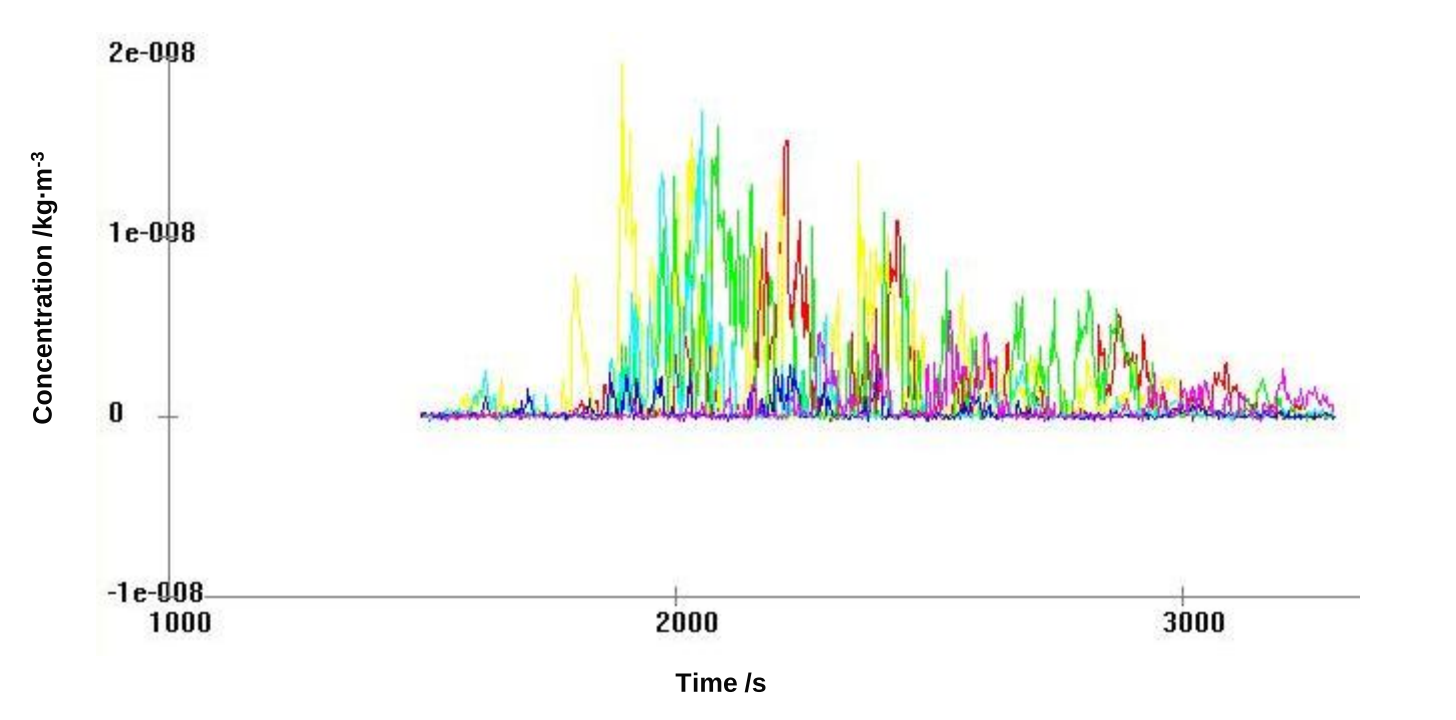


unclipped Gaussian

clipped Gaussian

Testing of MCBDF against DP26

- Unclipped Gaussian assumption provided much more realistic concentration time-series.



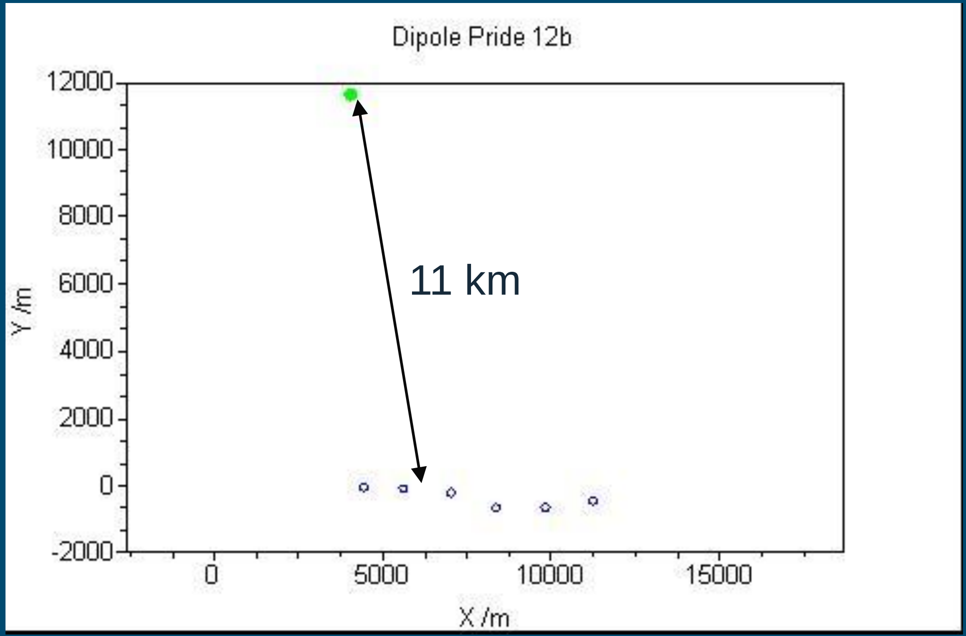
Testing of MCBDF against FFT07

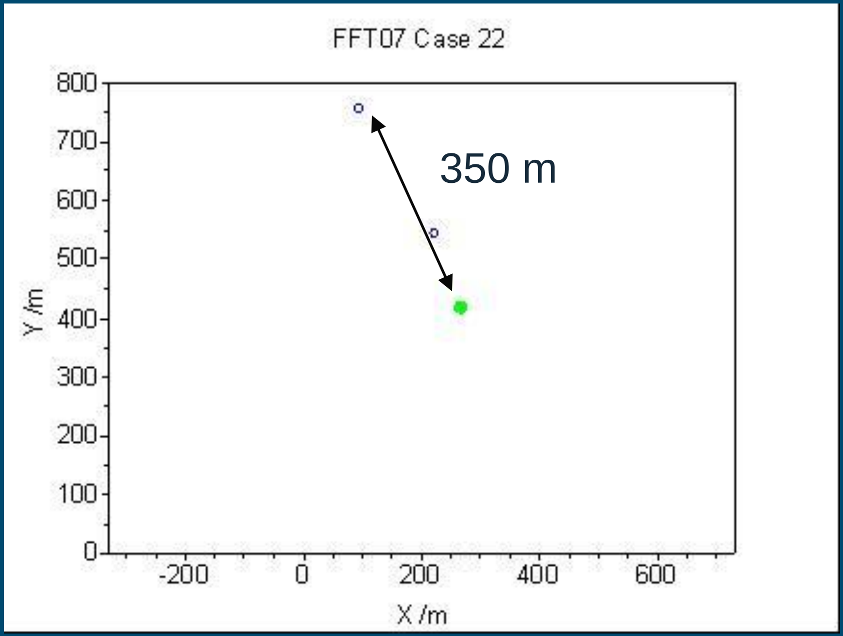
- Trial arranged to provide test data for inverse modelling.
- MCBDF applied in 'blind test' exercise.
- Most likely hypothesis output.
- Unclipped Gaussian assumption applied.
- Release location and time generally good.
- Release mass systematically under-estimated.

Case	Actual release mass (kg)	MCBDF release mass (kg)
16	0.698	0.185
22	1.159	0.294
61	1.159	0.292
70	0.698	0.231

Comparison of DP26 and FFT07 cases

- Both provided challenging cases; but had different temporal and spatial scales:





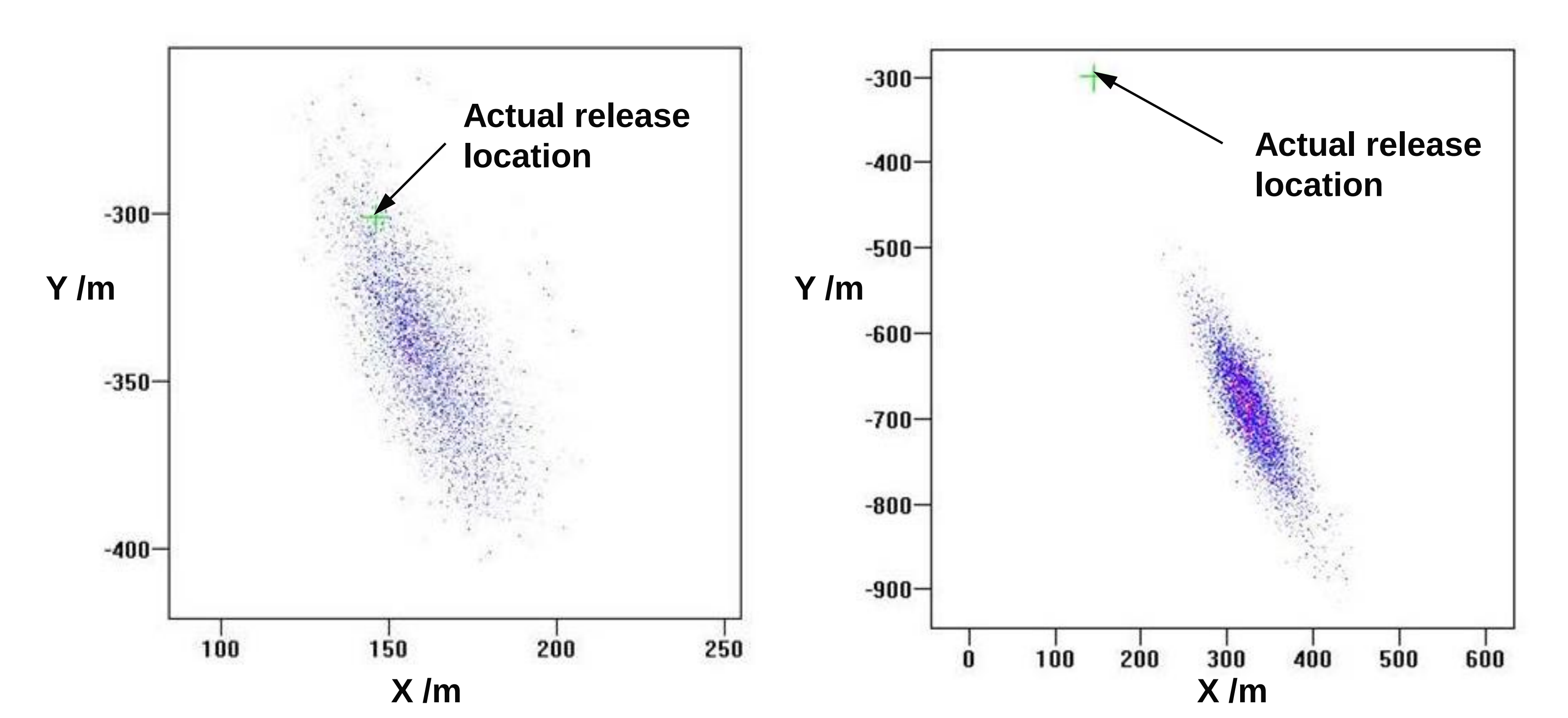
Release locations green circles; sensor locations blue circles

Comparison of clipped/unclipped results

- DP26 and FFT07 cases analysed with clipped and unclipped assumptions.
- Unclipped assumption:
  - True source location always within pdf.
  - Release mass 20-40% of true value.
  - Release time consistently later than actual time.
- Clipped assumption:
  - True source location not within output pdf.
  - Earlier release times and larger release masses.

Comparison of results

- Location pdfs and actual release location:



- Clipped Gaussian assumption did not provide useful output.

Why is unclipped assumption best?

- Provided more concentration density values for comparison with sensor time-series data.
- Provided less precise hypotheses with low individual significance.
- Having more data at each step helped MCBDF construct sensible pdfs, as it does not take account of past history.
- Assumption did not provide a better model of the concentration variance.

Under-estimation of release-mass

- Unclipped assumption gave consistent under-estimation of release mass.
- This could stem from:
  - The assumption results in an effective loss of mass.
  - The variance values were too large.
- Further analysis based on applying simple factors to the concentration variance did not show a consistent benefit.
- Resolution requires a more sophisticated concentration variance model that captures more of the physics, and relates variance to local turbulence.

Conclusions

- If MCBDF is used, assuming that current UDM mean and variance values refer to an unclipped Gaussian distribution a partial solution is achieved: release location and time.
- A complete solution requires a more accurate concentration variance model.
- Complete inverse modelling solutions require variance calculations appropriate to the environment.

Questions?