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MAXIMUM INDIVIDUAL EXPOSURE ESTIMATION

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Motivation

- The need to reliably predict **individual dosage** during the event of a deliberate or accidental atmospheric release from a near ground point source in a complex urban environment.

- In many cases the releases are short and/or the concentrations are high and there is a need to estimate the **individual exposure in relatively short times.**

The problem

- A hazardous air pollutant is released from a point source.
- The release could be **instantaneous** or **finite** and it is characterized by its **peak release rate** and its **duration.**
- We need to predict at a certain receptor point downstream **the dosage** in a specific time **interval $\Delta\tau$**.

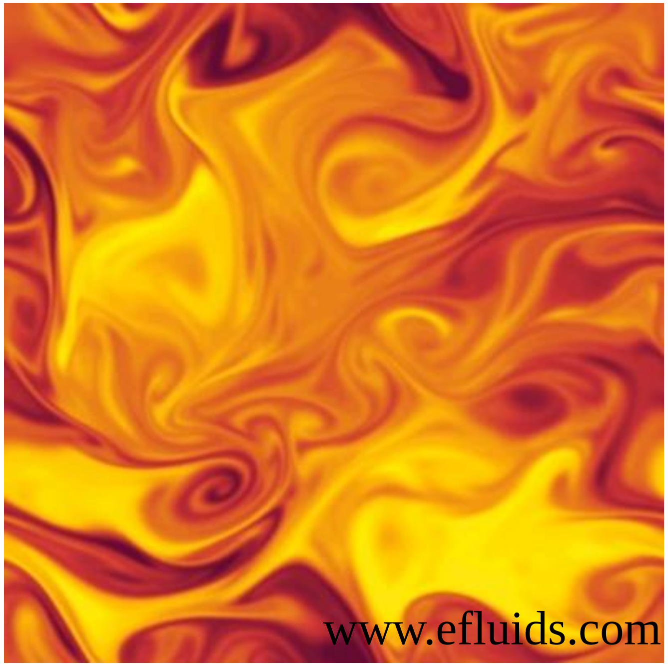
$$D(\Delta\tau) = \int_{0}^{\Delta\tau} C(t)\,dt$$

where C(t) is the instantaneous concentration

Fact

- Due to the stochastic nature of turbulence, the instantaneous wind field at the time of the release is practically unknown.

- For this reason the prediction of **actual exposure is impossible**.



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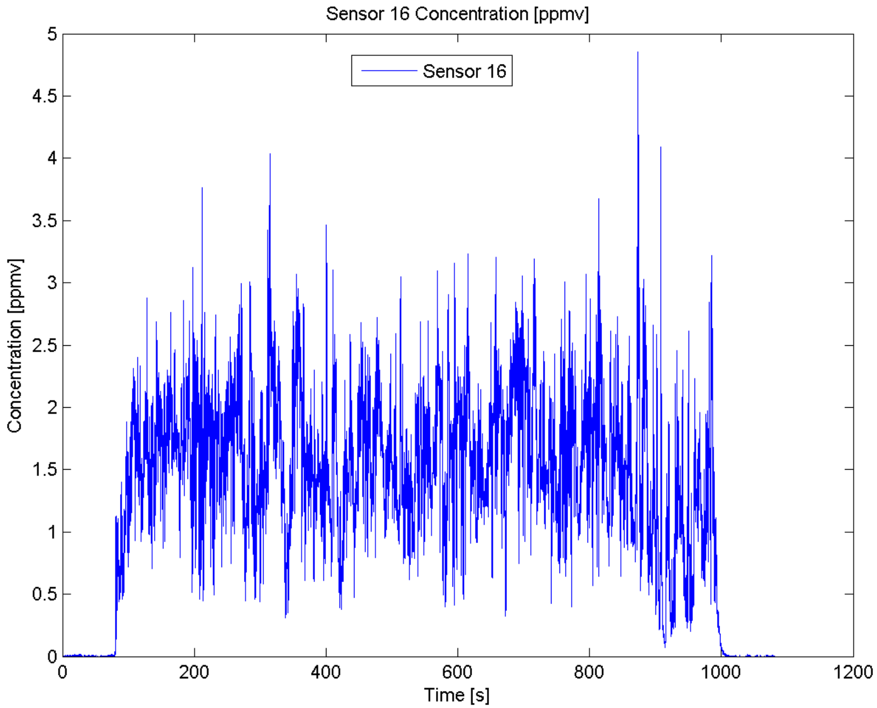
The approach

- Therefore, is more realistic to talk not for actual dosage but for **maximum dosage with a given exposure time**.

$$D_{\max}(\Delta\tau) = \left[\int_0^{\Delta\tau} C(t)dt \right]_{\max}$$

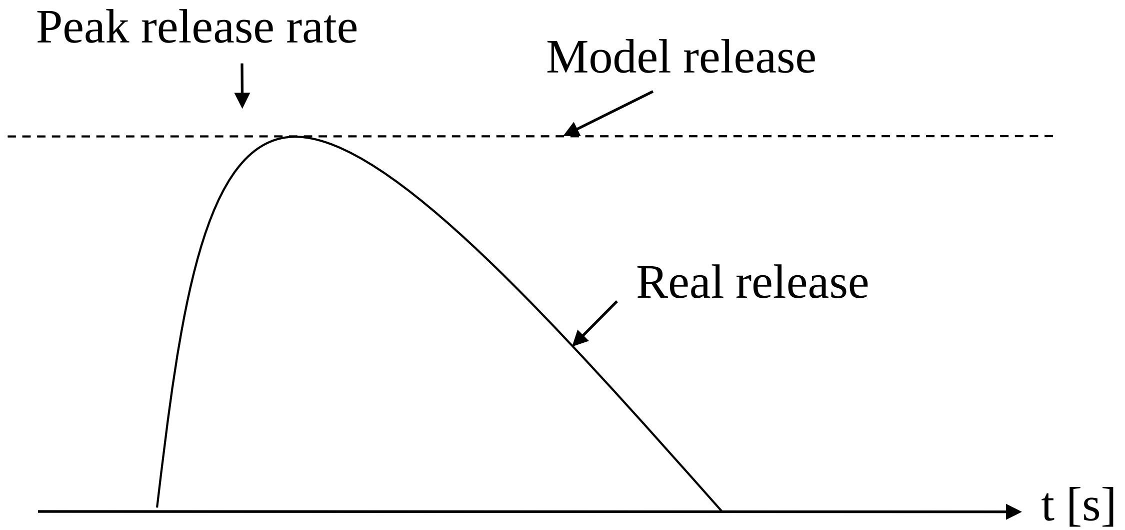
A basic realistic assumption

The turbulence field within the time range from the start time of the release to the ending time of the plume passage from the receptor is stationary.



Problem Simplification - I

- Since the key target is the prediction of $D_{max}(\Delta\tau)$, the whole modelling approach can be reduced to a simplified problem:
  - The source is replaced by a continuous source of constant release rate equal to the peak release rate.



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Problem Simplification - II

- The abovementioned stationarity assumption on turbulence is extended for an infinite time.

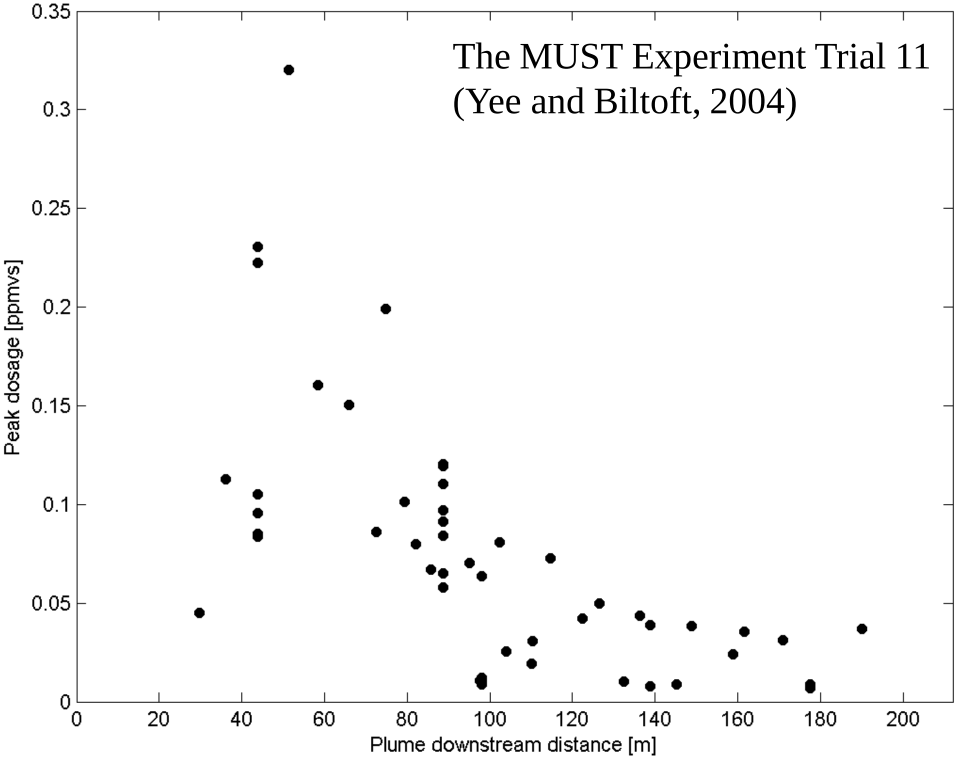
- The extreme value of $D_{max}(\Delta\tau)$ of the simplified problem is expected to be at least equal to the one of the real problem as defined above. This can be explained from the fact that in the simplified problem the $D_{max}(\Delta\tau)$ value is expected to be greater or equal of the one in the real problem.

An important note

- $D_{max}(\Delta\tau)$ has a finite value. (It cannot be higher than the dosage at the release point).

- $D_{max}(\Delta\tau)$ is expected to dilute downstream.

The fact that $D_{max}(\Delta\tau)$ is a finite quantity makes the deterministic models more attractive in principle, than the probabilistic ones.



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Probabilistic Models

In this methodology someone tries to obtain first the knowledge of the mean concentration ($\overline{C}$), the concentration standard deviation (σ_C) and the intermittency factor (γ).

The maximum expected concentrations with a given confidence level, are derived from the corresponding concentration cumulative distribution function (cdf) which is considered to be a function of $\overline{C}$, σ_C and γ, by assuming a particular shape of the concentration probability density function:

Authors	Distributions
Lung et al, 2002	Gamma
	Weibull
	Log-normal
Mylne, K.R. and P.J. Mason, 1991	Exponential
	Chopped-normal
Sykes et al., 2000	Chopped-normal

Then the concentrations are multiplied with $\Delta\tau$.

A Deterministic Model -I

Recently Bartzis, et al., (2007), have inaugurated an approach relating the individual maximum dosage during a time interval $\Delta\tau$ to parameters such as concentration variance and the turbulence integral time scale:

$$D_{\max}(\Delta\tau) = \left[1 + \beta \cdot \mathrm{I} \cdot \left(\frac{\Delta\tau}{T_L}\right)^{-n}\right] \cdot \overline{C} \cdot \Delta\tau$$

where T_L is the turbulence integral time scale derived from the autocorrelation function $R(\tau)$:

$$T_L = \int_0^{\infty} R(\tau)\, d\tau$$

The fluctuation intensity I is defined as:

$$\mathrm{I} = \frac{\sigma_C^2}{\overline{C}^2}$$

where σ_C^2 is the concentration variance and $\overline{C}$ is the mean concentration.

A Deterministic Model-II

β and n are constants derived from experimental evidence. The indicative values given, have as follows: $\beta = 1.5, \; n = 0.3$

The $D_{max}(\Delta\tau)$ model until now has been calibrated by a limited number of field data from neutral flows.

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Testing the approach with the MUST data

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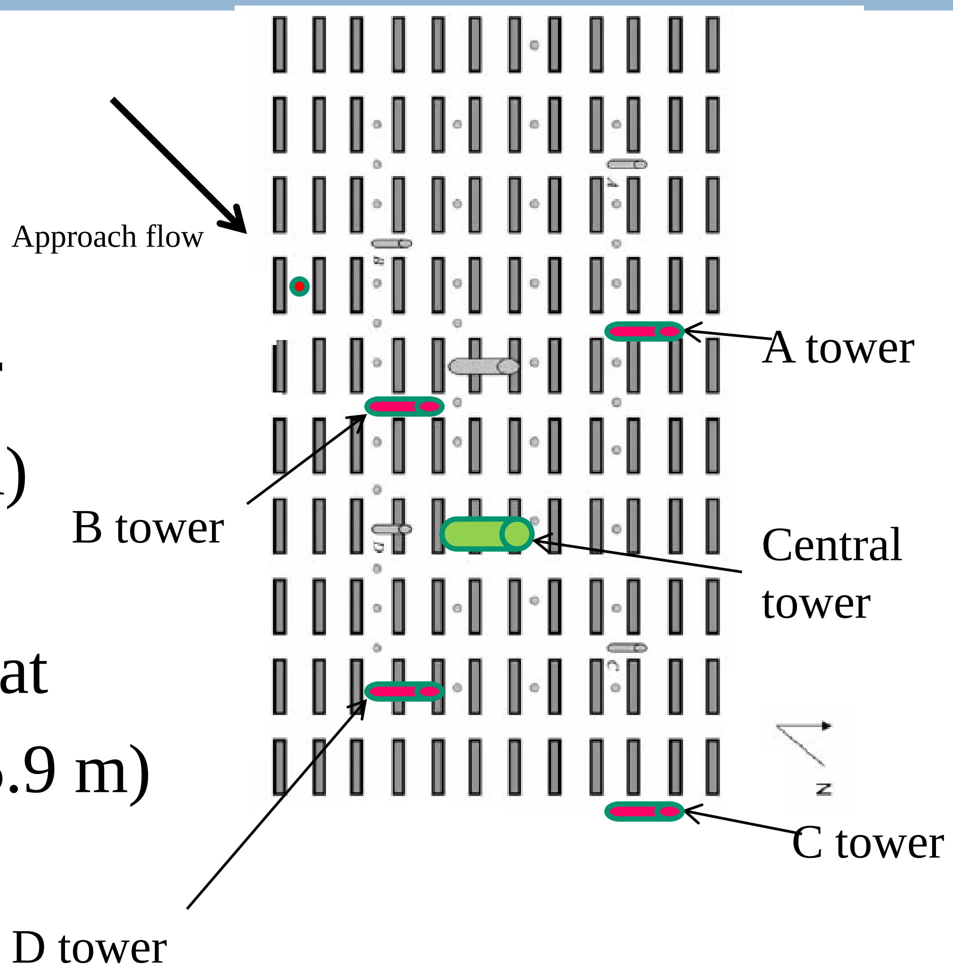
The MUST field experiment

MUST = Mock Urban Setting Test:

Near Ground point source release over simulated urban environment.

The MUST field experiment selected case. The sensors positions

- 40 locations on 4 horizontal sampling lines (at z = 1.6 m)
- 8 sensors on 32-m central tower (at z = 1, 2, 4, 6, 8, 10, 12, 16 m)
- 6 sensors on each of 6-m tower at A, B, C, D (at z = 1, 2, 3, 4, 5, 5.9 m)



(Yee and Biltoft, 2004)

Description of the MUST data

- The MUST data (Yee and Biltoft, 2004) includes:
  - 81 trials of all stability classes and various atmospheric conditions.
  - 5,832 sensor measurements with time resolution of 0.01 – 0.02s.
  - $1.36 \cdot 10^8$ data

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Data analysis

- The purpose of the data analysis was to select the time series that were appropriate for the present analysis.

- For each trial specific time periods (e.g. 200s, 900s, 450s) were selected for the calculation of statistical measures (mean, variance, maximum and integral time scale). These periods were originally chosen by Yee, E. and C. Biltoft, (2004) and were primarily based on the stationarity (i.e., speed and direction) of the wind over the period.

- From the 5,832 sensor concentration data only the 4,004 non zero concentration sensor data have been found.

Validation strategy

- The coefficients β and n show some variation when trying to fit the experimental data (Bartzis, et al., 2007). This could be attributed not only to the model imperfectness but also to the fact that perfect stationarity does not exist especially for long times and the measured signals are often 'contaminated' by non local large scale disturbances.

- In order to make the whole validation procedure simple and workable it has been decided to keep the exponent n constant (=0.3) and leave the proportionality factor β to be varied from signal to signal. In this case the imperfectness of the model as well the possible errors on measurements are going to be reflected to β value and its variability/uncertainty.

- Applying this strategy to every signal, it has been also clear that for practical reasons it was not realistic to perform a quality assurance of the signals with respect to errors or/and stationarity.

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Detection of outliers for β - values

Known statistical methods to identify outliers have been applied.

- The Box Plot method (MATLAB, 2008) which gave 194 outliers and 3,810 remaining data with a maximum value 3.2.

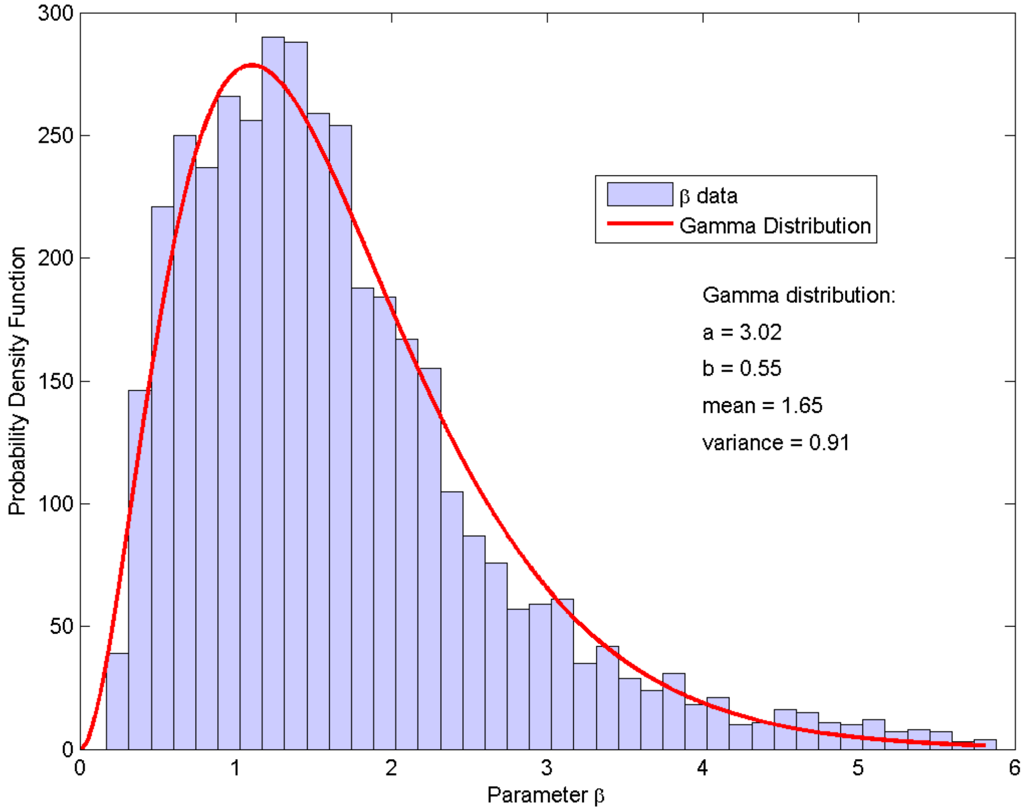
- The Grubbs Test (Grubbs, F., 1969) which gave 45 outliers and 3,959 remaining data with a maximum value 5.88.

- For conservative reasons the second method has been adapted. Thus, the 45 above mentioned outliers were removed from the population of β.

- The 3,959 β - values have been used in the following analysis.

Probability Density Function of β

- The experimental probability density function of the parameter β.



It is reminded, that the Gamma probability density function (pdf) is given by the relation:

$$f(x|a,b) = \frac{1}{b^a \Gamma(a)} \cdot x^{a-1} \cdot e^{-\frac{x}{b}}$$

where a is the shape parameter and b is the scale parameter.

Probability Density Function of β

Parameters	MLEs	95% confidence intervals	
		Lower bound	Upper bound
a	3.02	2.89	3.14
b	0.55	0.52	0.57
Mean	**1.65**	1.51	1.8
Variance	0.91	0.79	1.03

- These results strengthen further the validity of $D_{max}(\Delta\tau)$ model. It should be noted that the mean value 1.65 is well comparable with the indicative value 1.5 given by Bartzis, et al., (2007).

Extreme value of β

- Since the parameter β is expected to have a finite value it is not enough to express its variance only by a pdf in which its extreme value goes theoretically to infinity. There is a need to try to estimate its upper bound.

- One method of extracting this value is to use Extreme Value Theory (Gumbel, E.J., 1958) one method of which is to take the exceedances over a predetermined parameter threshold β = u (Reiss, R.D. and M. Thomas, 2007).

- Following by Balkema, A.A. and L. de Haan, (1974) and Pickands, (1975), the pdf of these exceedances can be approximated by the Generalized Pareto Distribution (GPD) (Reiss, R.D. and M. Thomas, 2007).

Estimation of the GPD parameters

- The Generalized Pareto Distribution approach can conclude to a finite extreme value:

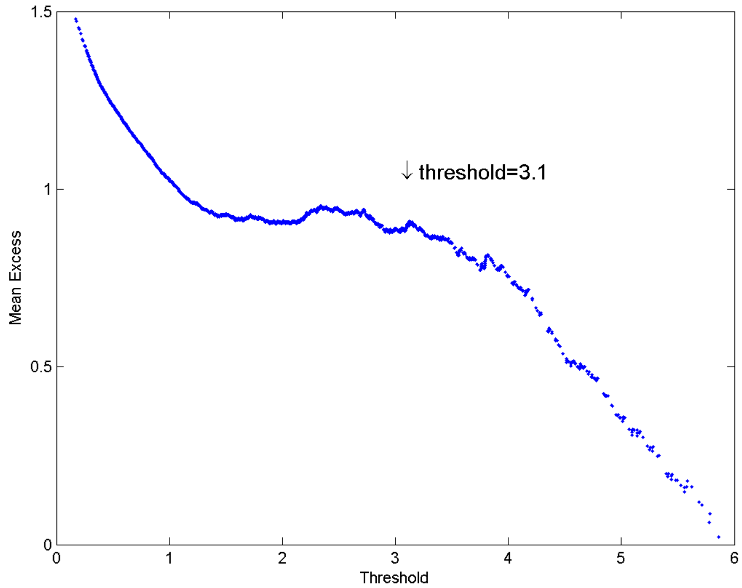
$$\beta_{max} = u - \frac{\sigma}{\xi}$$

where ξ is the GPD shape parameter and σ its scale parameter.

- The threshold value u can be obtained by applying the mean excess plot method (Munro, R.J. et al., 2001). The mean excess is the sum of the excesses over the threshold u divided by the number of data points which exceed the threshold u (Gencay, R., 2001).

Estimation of the GPD parameters

- The mean excess parameter as a function of the selected threshold should be approximately linear as the theory of GPD imposes (Reiss, and Thomas, 2007).



- In the tail of the distribution (threshold > 3.1) we expect the extreme values of β_{max} to be constant.

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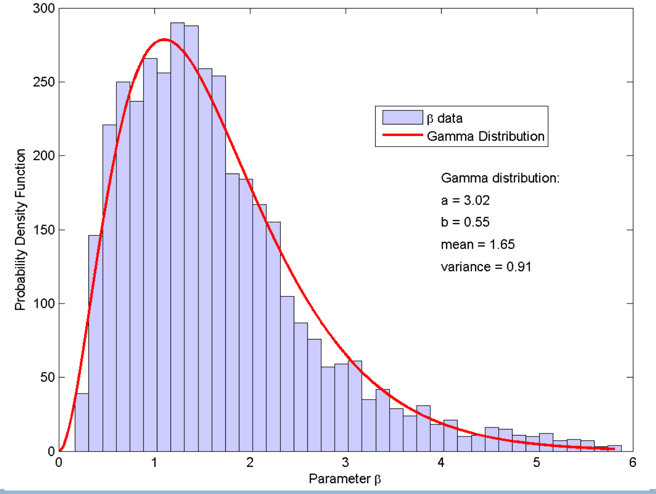
Estimation of the GPD parameters

- The ξ and σ parameters are derived by the Maximum Likelihood Estimation (MATLAB, 2008) applied to the data above threshold and their corresponding values are $\xi = -0.35$ and $\sigma = 1.2$.

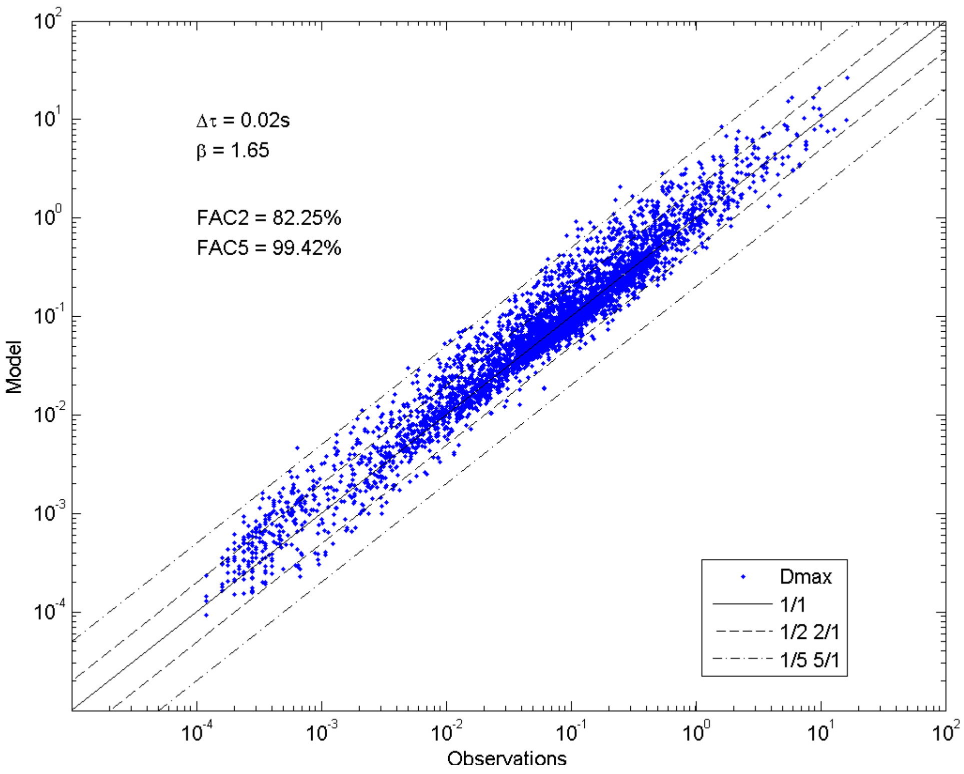
- Thus the GPD gives $\beta_{max} = 6.5$. This value appears to be approximately four (4) times higher than the mean β value of 1.65 obtained above.

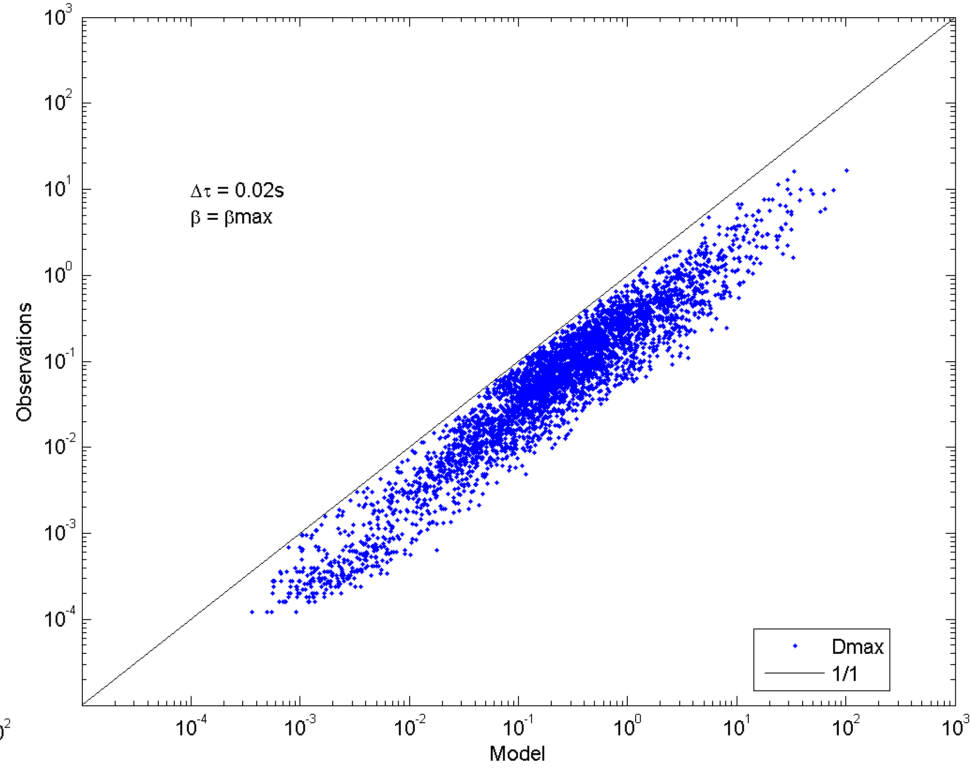
- If we adopt the gamma pdf as defined above to describe β variability/uncertainty, this value corresponds to a confidence limit 99.94%.



$D_{max}(\Delta\tau)$ model results

- All D_{max} data are compared with the model equation $D_{max}(\Delta\tau)$ with $\beta = 1.65$, $\beta = \beta_{max}$ and $n = 0.3$.





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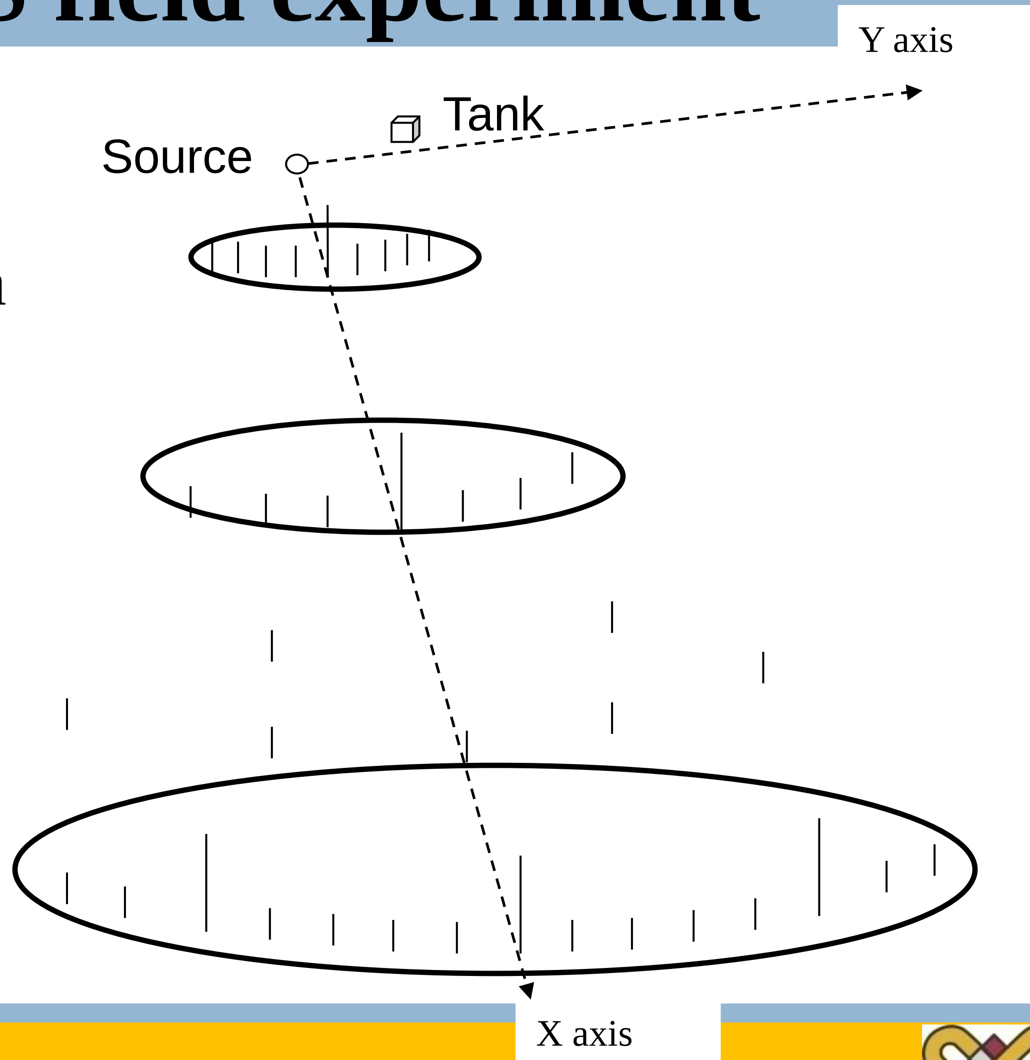
The FLADIS field experiment

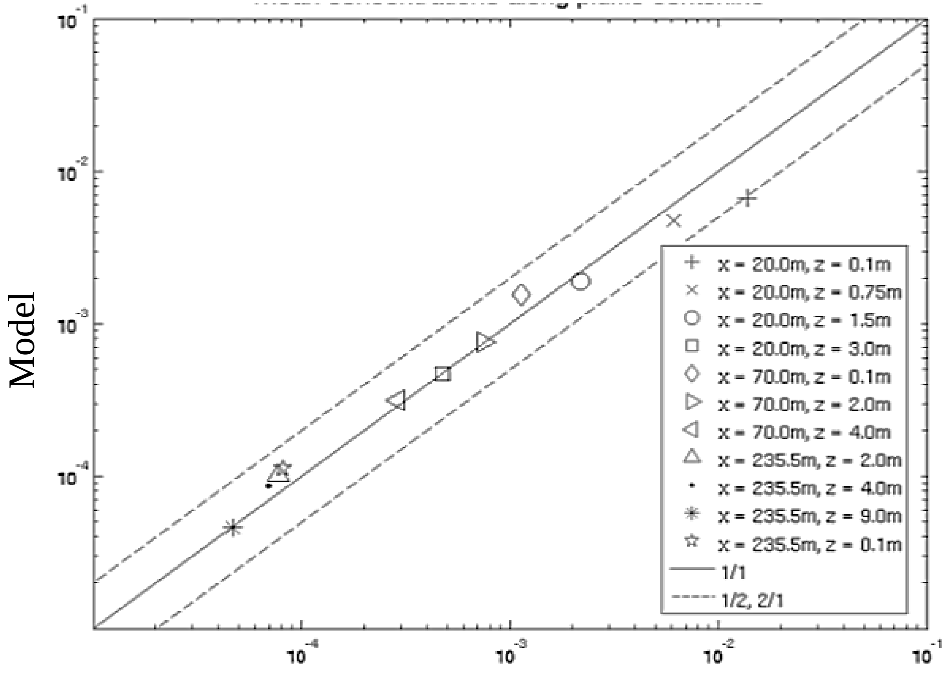
In the FLADIS experiment (Nielsen, 1994) the ammonia was released horizontally as a flashing jet.

The sensors were mainly arranged in three arcs:
 20, 70 , 235m
:

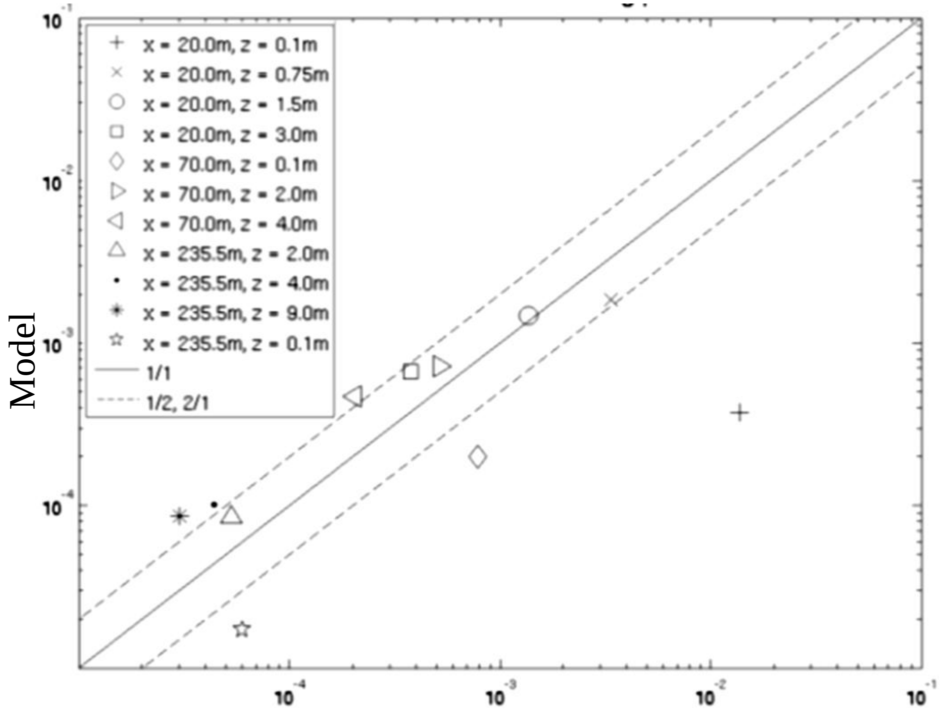


CFD-RANS PREDICTIONS (ADREA)
The FLADIS T16 results: Concentrations

Max Arc Mean Concentration



Max Arc Standard Deviation



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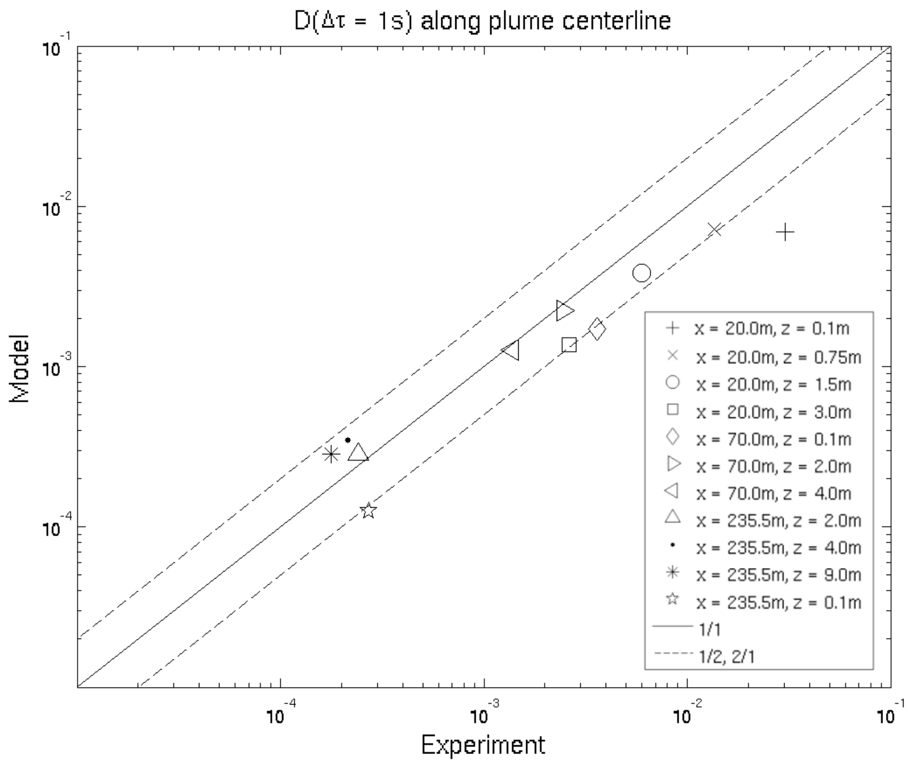
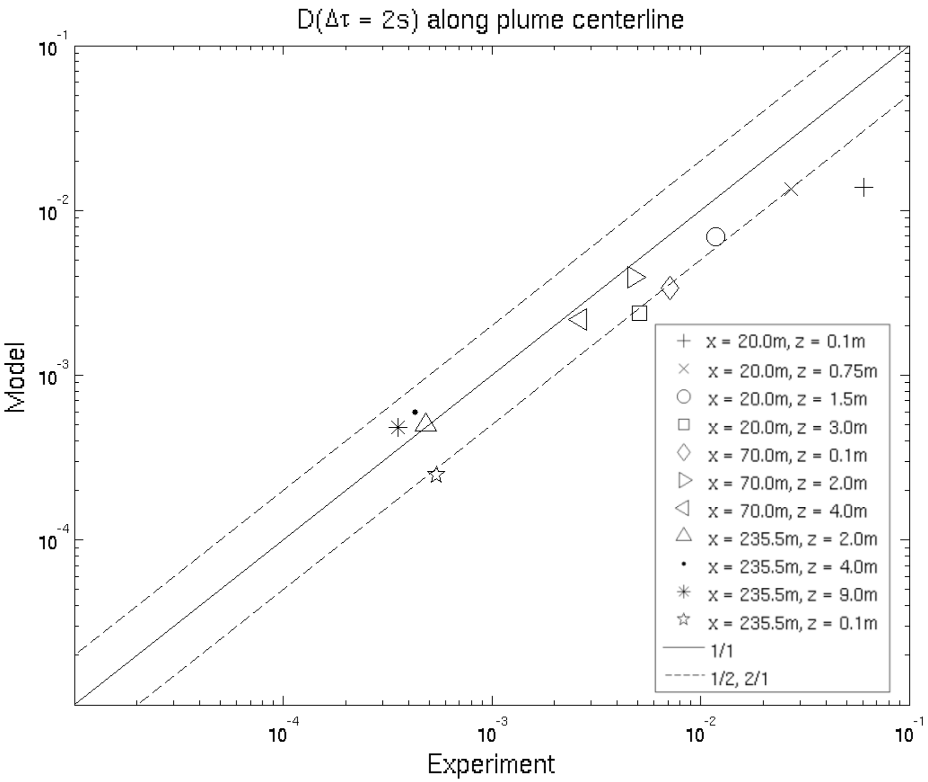
CFD-RANS PREDICTIONS (ADREA)
The FLADIS T16 results: Dosages

Max Arc Dosage for Δτ = 1s and Δτ = 2s





The Conclusions

- The present work is addressed on the validation of Bartzis, et al., (2007) empirical model for $D_{max}(\Delta\tau)$ to predict reliably the individual maximum exposure in case of deliberate or accidental atmospheric releases of hazardous substances for various atmospheric stability classes.

- For the first time a vast amount of data has been utilized for this purpose. The extensive dataset of the MUST experiment was analyzed which included 81 trials of various stability classes and contained in total 5,832 concentration sensor data with time resolution of 0.01 – 0.02 s.

- The present analysis of the data strongly supports the validity of $D_{max}(\Delta\tau)$ equation to predict maximum individual exposure in short time intervals. For this purpose a steady state CFD – RANS model could provide the necessary input parameters (i.e. $\overline{C}$, σ_C^2, and T_L). It is recommended that the nominal value for β to be changed to 1.65.

The Conclusions

- For the first time the β variation and uncertainty has been systematically studied. It shows very clearly a gamma function variation with the parameters a = 3.02 and b = 0.55. (Uncertainties for a and b are also given).

- An extreme value $\beta_{max} = 4 \times 1.65$ is also estimated based on Extreme Value Theory which corresponds to probability 99.94% of the Gamma pdf.

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Acknowledgements

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Thanks to U S Defence Threat Reduction Agency (DTRA) for providing the MUST data to the COST732 community.

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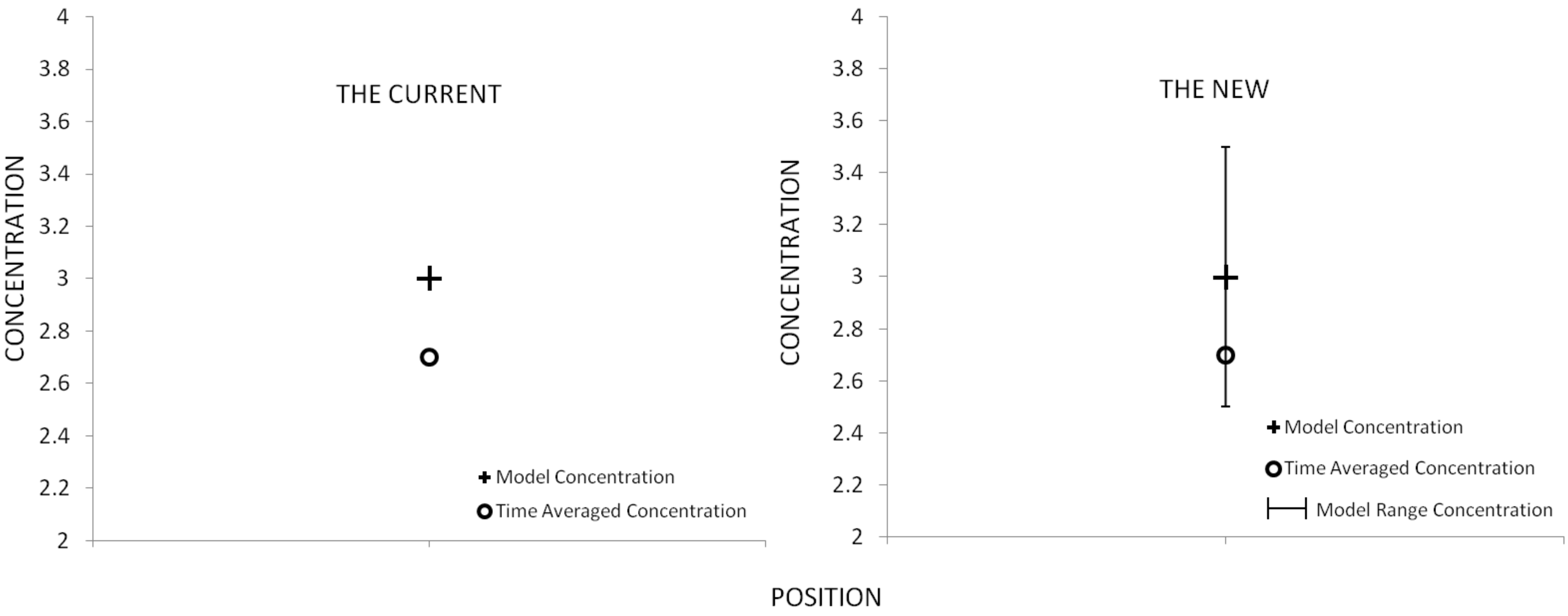
A 'BY PRODUCT' OF THE PRESENT METHODOLOGY

A new concept in concentration model comparison with experiments

COMPARISON OF MODEL CONCENTRATION vs TIME AVERAGED CONCENTRATION



A Proposed Approach

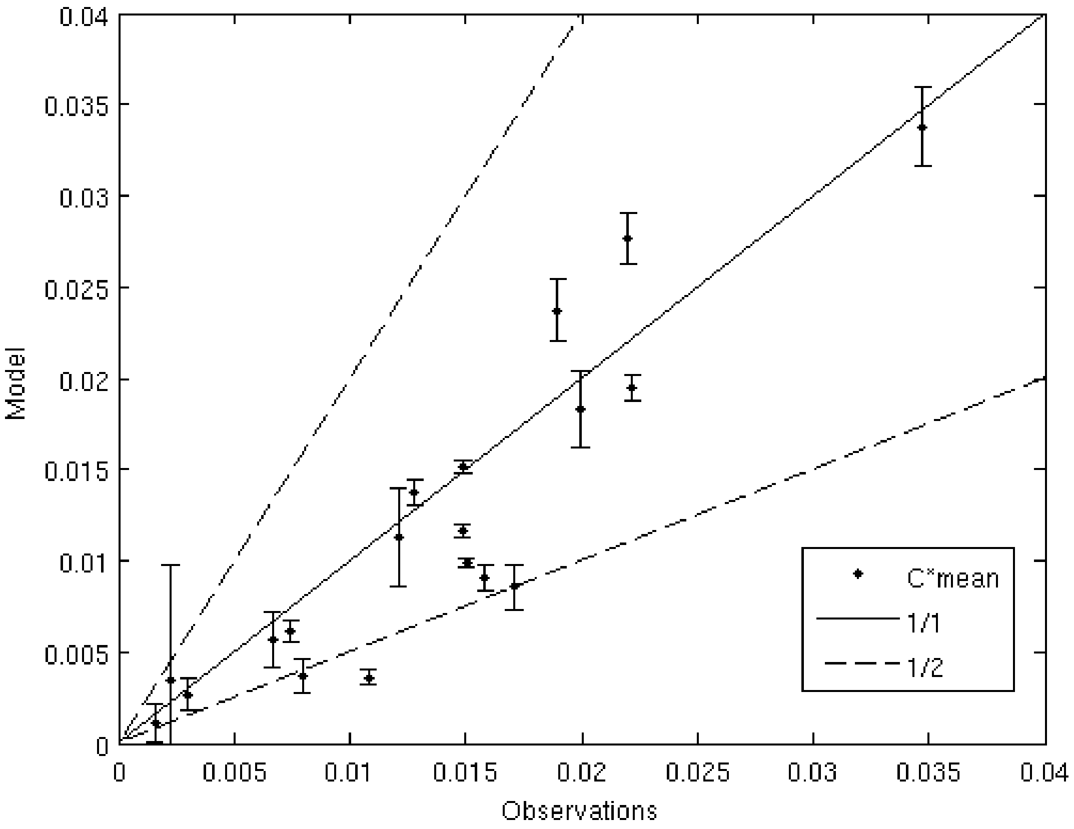
Assume : $C_{max}(\Delta\tau) - C(\infty) \approx C(\infty) - C_{min}(\Delta\tau)$ for $C_{min}(\Delta\tau) > 0$

$C(\infty)$: The model mean concentration

Bartzis et al (2007) :

$$\frac{C_{max}\quad \Delta\tau}{\overline{C}} = 1 + b \cdot I \cdot \left(\frac{\Delta\tau}{T_L}\right)^{-n} \qquad b = 1.5 \quad n = 0.3$$

MUST Field Data :
Time Averaged (200s) Concentration vs Predicted Concentration (200s)



Thank you for your attention

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