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Modelling the Concentration Fluctuation and Individual Exposure in Complex Urban Environments

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Motivation

Understanding and modelling dispersion from point sources over urban areas for practical purposes

Problem one

- The increasing likelihood of accidental or deliberate atmospheric releases of toxic substances in an urban area has focused our attention to the understanding of the dispersion of the gaseous materials in these complex environments and the ability to reliably predict the individual exposure during these events.

- There is often a need to predict the expected dosage in a given exposure time in order to assess if this dosage exceeds or not certain health limits.

Problem one –continued

- Due to the stochastic nature of turbulence, the wind field at the time of the release in the atmospheric boundary layer is practically unknown.

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

- Maximum Dosage over a time interval $\Delta\tau$:

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

.

Problem one – continued

$C_{max}(\Delta T)$ is the maximum (peak) time averaged concentration within this time interval ΔT.

CONCLUSION – I

There is a fundamental need to estimate/predict $C_{max}(\Delta T)$

Problem two

- A modeller likes to test his/her model results against experimental data concerning a point source release in the atmosphere .
- A common approach is to compare the model mean concentrations with the measured mean concentrations at the various sensors positions downstream .
- The model usually predicts true mean ('ensemble average') concentrations. In a stationary state theoretically we are talking for mean concentrations over infinite time.
- The experiment provides mean concentrations that in reality are time averaged concentrations over a 'reasonable' time interval: C (ΔT)
- This time interval cannot be too long since the 'stationarity' of the atmosphere is difficult to be kept long.

Problem two–continued

- Is this comparison 'fair' ?
- Let us assume for the moment 'perfect' stationarity, 'perfect' measurement $C(\Delta T)$ and a 'perfect' prediction $C(\infty)$
- If we repeat the experiment infinite times we will always predict a single $C(\infty)$ and we will measure an infinite number of $C(\Delta T)$ since $\Delta T < \infty$
- The maximum value of $C(\Delta T)$ will be the $C_{max}(\Delta T)$ we mentioned in Problem one.
- In other words the measured mean value represent the true mean value with some uncertainty. The upper bound of the $C(\Delta T)$ is the $C_{max}(\Delta T)$

Problem two – continued

- $C(\Delta T) \approx C_{max}(\Delta T) \approx C(\infty)$ when ΔT is sufficiently large

FACT

In real atmospheric experiments ΔT is never sufficiently large

CONCLUSION – II = CONCLUSION – I

There is a fundamental need to estimate/predict $C_{max}(\Delta T)$

The Purpose of this Study

FACT

There is a fundamental need to estimate/predict C_{max} (ΔT)

QUESTION and POSSIBLE ANSWER

- Can a RANS CFD Model do that ?
- If yes, let us test it in the MUST Field Experiment

The Approach

- Recently Bartzis et al., (2007) have inaugurated an approach relating the parameter $C_{max}(\Delta\tau)/\bar{C}$ to the turbulent fluctuating intensity I and the $\Delta\tau/T_L$ where:

$$I = \frac{\sigma_C^2}{\bar{C}^2}, \qquad \sigma_C^2 = \overline{C'^2} \quad and \quad T_L = \int_0^\infty R(\tau)\, d\tau$$

- TL is the integral time scale and $R(\tau)$ the concentration autocorrelation function.

- It is obvious that the right model needs to provide at least reliable predictions for the mean concentration, the concentration variance and the integral time scale.

The model ADREA

- Mesoscale/local scale
- Stable/unstable ambient conditions
- One equation and two equation turbulence modeling
- Induced turbulence from moving objects (e.g. vehicles)
- One (dense/buoyant) pollutant
- 3-D RANS finite volume, transient
  - one/two phase release and dispersion
  - instantaneous/continuous releases
  - jets of arbitrary orientation (e.g. pipe exhaust, pipe/tank rupture etc)
- N passive substances reactive or not
  - CBM - IV gas chemistry (up to 36 species)
  - radioactivity
  - moist atmosphere (dispersion on gas and water phase in the atmosphere)

ADREA : The presently utilized Transport Equations

- **Reynolds averaged Momentum Equations (u,v,w)**
- **Continuity Equation**
- **Two Equation Turbulence (k - ζ) model**

  (Bartzis,2005) (ζ : wavenumber scale)

- **Pollutant Mass Conservation (concentration) Equation**
- **Pollutant Concentration Variance Equation**

ADREA: The Concentration Variance Equation & Modeling

- Transport equation for the concentration variance:

$$\frac{\partial\left(\rho\,\overline{C'^2}\right)}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho\,\overline{u}_i\overline{C'^2}\right)=-2\rho\,\overline{u_i'C'}\frac{\partial\overline{C}}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\rho\,D\frac{\partial\overline{C'^2}}{\partial x_i}-\rho\,\overline{u_i'C'^2}\right)-2\rho\,D\overline{\frac{\partial C'}{\partial x_i}\frac{\partial C'}{\partial x_i}}$$

- The modeling approach for the production term and the turbulent diffusion term is the standard gradient-transfer approximation.

- For the dissipation term the common approximation has as follow:

$$D\overline{\frac{\partial C'}{\partial x_i}\frac{\partial C'}{\partial x_i}}=\frac{\overline{C'^2}}{T_{dc}}$$

T_{dc} = Turbulent dissipation time scale

ADREA: Concentration Variance Equation Modeling

- The most common modeling approach for T_{dc}:

$$T_{dc} \propto \frac{k}{\varepsilon}$$

k = Turbulent kinetic energy

ε = Turbulent energy dissipation

- In the present study the concentration variance predictions have been obtained by utilizing two approaches for dissipation time scale:

$$T_{dc} = c_{dc} k^{-\frac{1}{2}} \zeta^{-1} \qquad T_{dc} = T_{dc0} = constant$$

ADREA: The Peak Time-Averaged Concentration Modeling

- Bartzis et al (2007):

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

I = Turbulent fluctuating intensity

T_L = Integral time scale

$$I = \frac{\sigma_C^2}{\overline{C}^2}, \qquad \sigma_C^2 = \overline{C'^2} \quad and \quad T_L = \int_0^{\infty} R(\tau)\, d\tau$$

R(T) = Autocorrelation function

- In the present study: $T_L \approx T_{dc0}$

The MUST Field Experiment

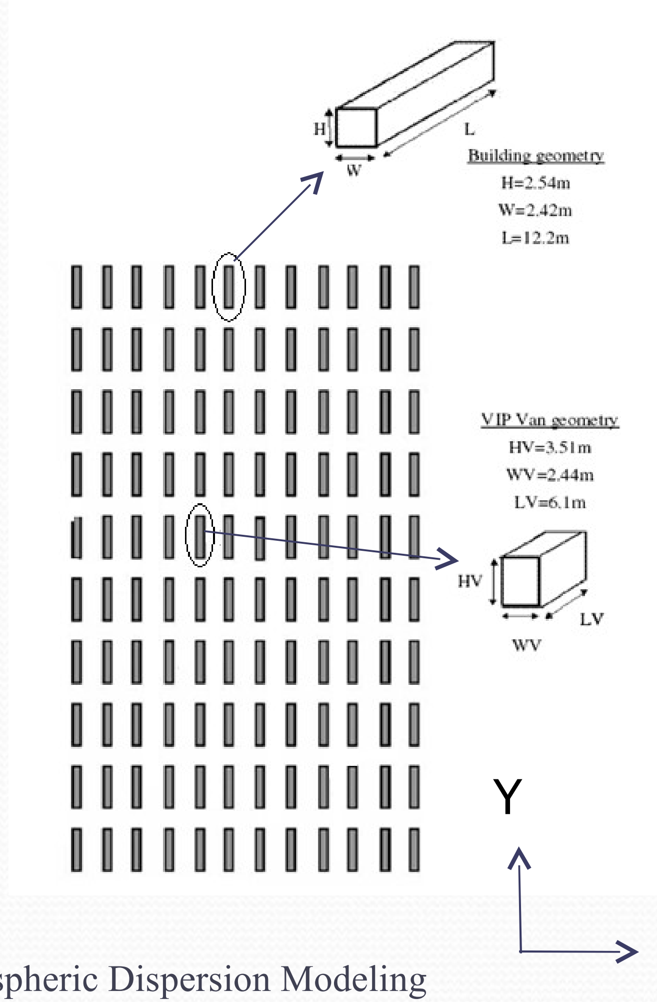
Mock Urban Setting Test (MUST):

Near Ground point source release over simulated urban environment.

The MUST field experiment

General Description

- MUST consists of 120 standard size shipping containers that are setup in a nearly regular array of 10 by 12 obstacles covering an area of around 200 by 200 m.

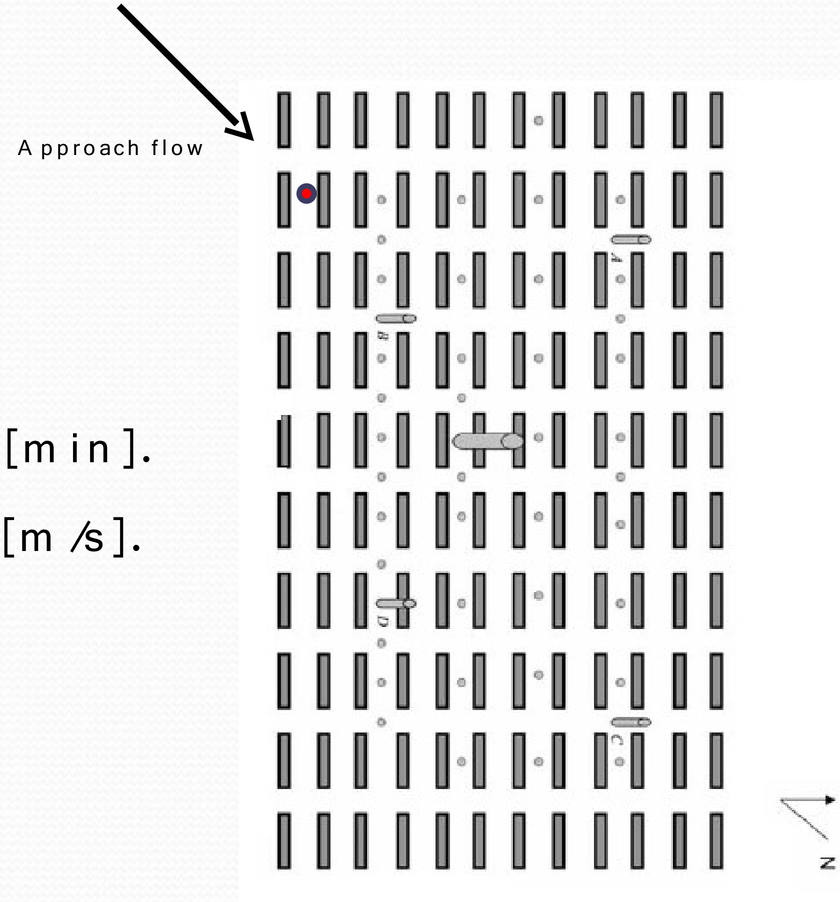


- The terrain of the field site is characterized as ‘flat open terrain’, an ideal horizontally homogeneous roughness.

The MUST field experiment

The selected case key characteristics

- The 25 September 2001 experiment.
- Near neutral conditions.
- Release rate: 0.00375 [$m^3 s^{-1}$].
- Release duration 15 min .
- Selected period for assessment : 5 – 8.3 [min].
- Average wind speed at 4-m : V_h = 7.93 [m/s].
- Wind direction at 4-m : A_{dir} = -40.54°.
- Ambient temperature: $T_{mean} \approx$ 31 [°C]
- Relative humidity: $H_{mean} \approx$ 13 [%]

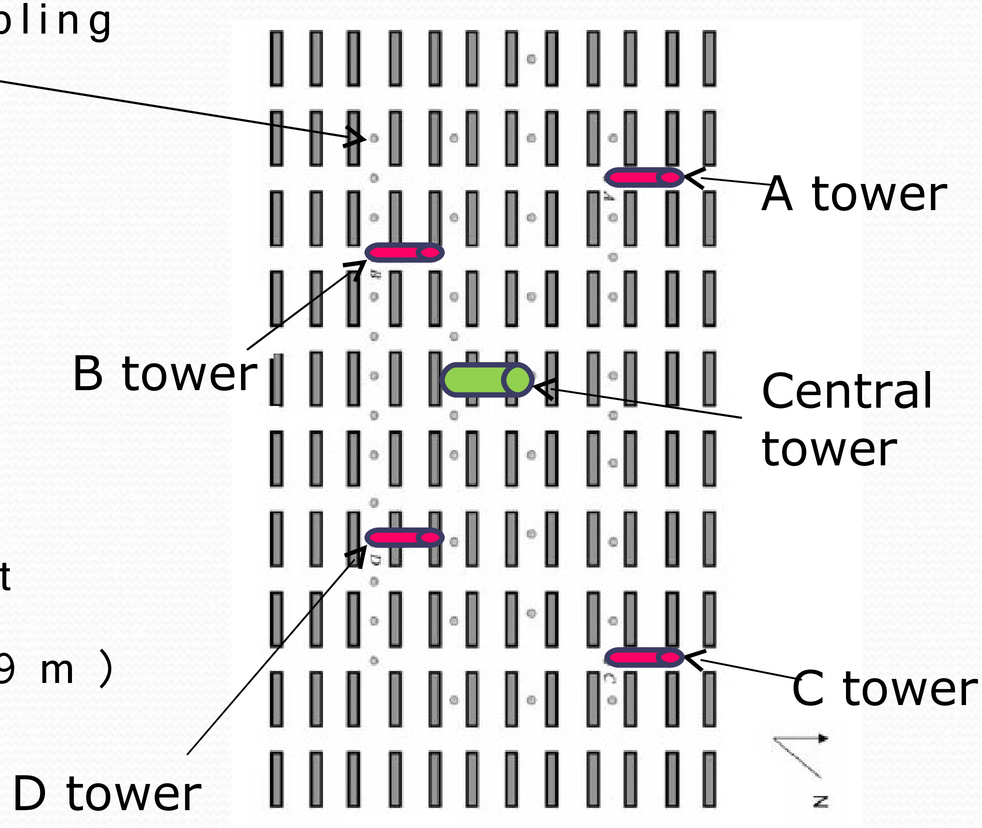


(Yee and Biltoft, 2003)

The MUST field experiment selected case

The sensors Position

- 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)

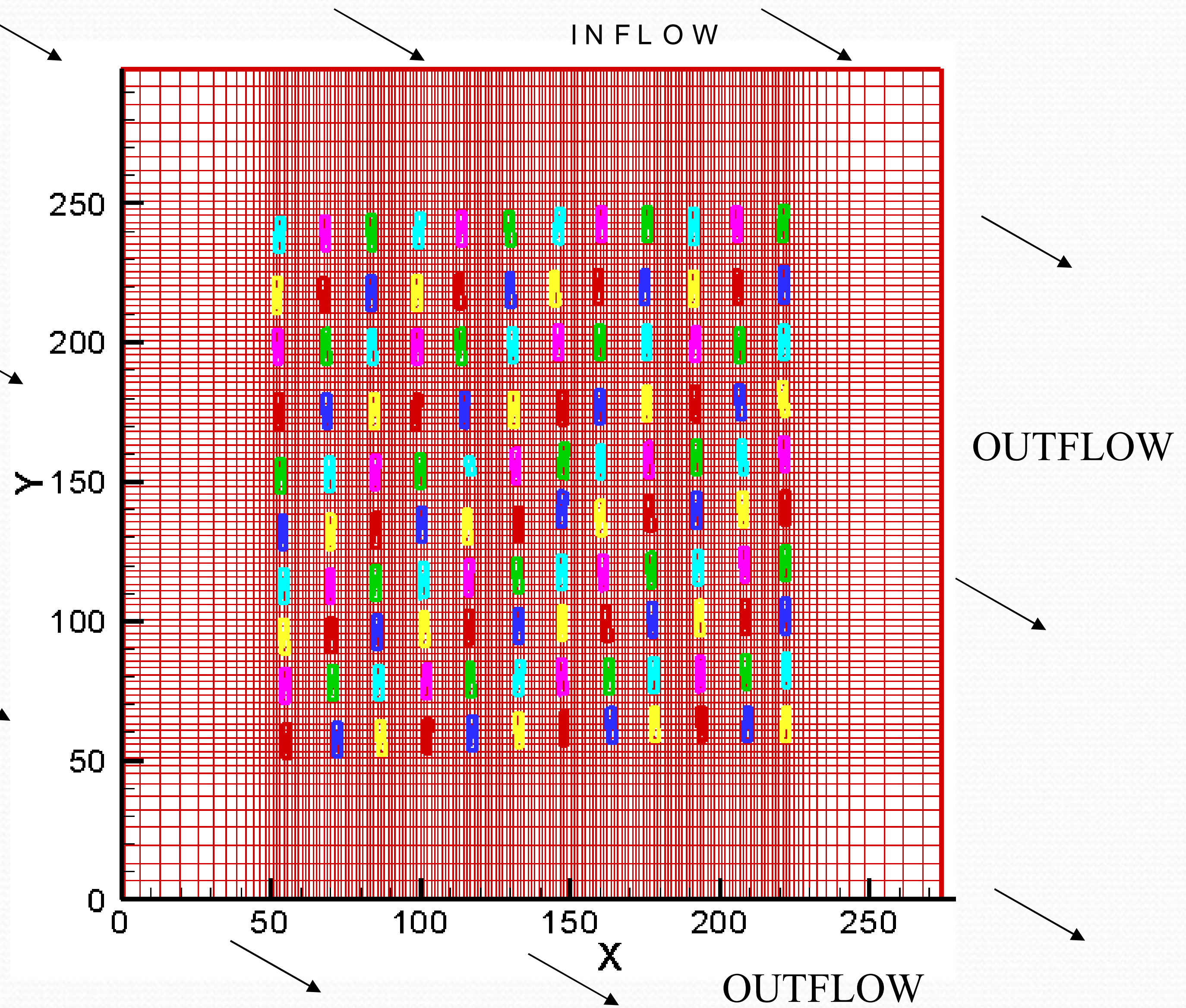


(Yee and Biltoft, 2003)

ADREA :The Domain/Grid

- 3D domain 170 x 99 x 32
- Non-uniform logarithmic grid
  - X = 274.1 m Δx_{min} = 1.1983 m, Δx_{max} = 6.48 m
  - Y = 298.9 m Δy_{min} = 2.4982 m, Δy_{max} = 6.59 m
  - Z = 19.43 m Δz_{min} = 0.3175 m, Δz_{max} = 1.0 m

Grid description



Total number of Cells: 538,560

Results – I

- Statistical metrics for comparison of the concentration fluctuations with the two models of the dissipation decay time T_{dc}

Variable	Metrics	Model for Decay Time (T_{dc})	
		$T_{dc} = T_{dc0}$	$T_{dc} = c_{dc} k^{-\frac{1}{2}} \zeta^{-1}$
σ_C^*	FB	-0.407	-0.533
	NMSE	2.43	3.09
	R	0.718	0.635
	FAC2	0.447	0.404
	HR	0.64	0.47

FB = Fractional Bias

NMSE = Normalised Mean Square Error

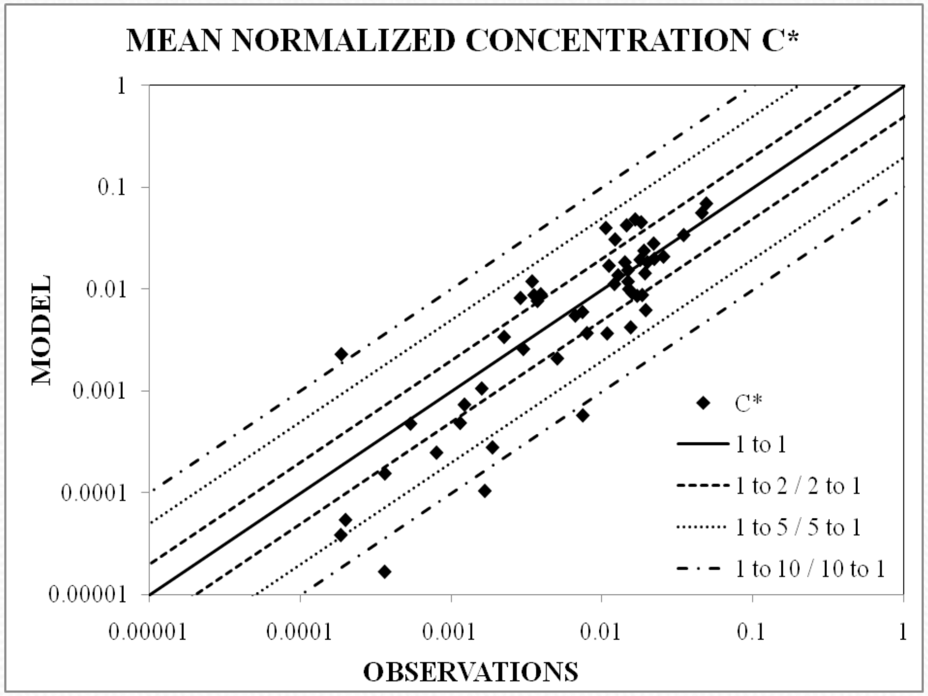
R = Correlation Coefficient

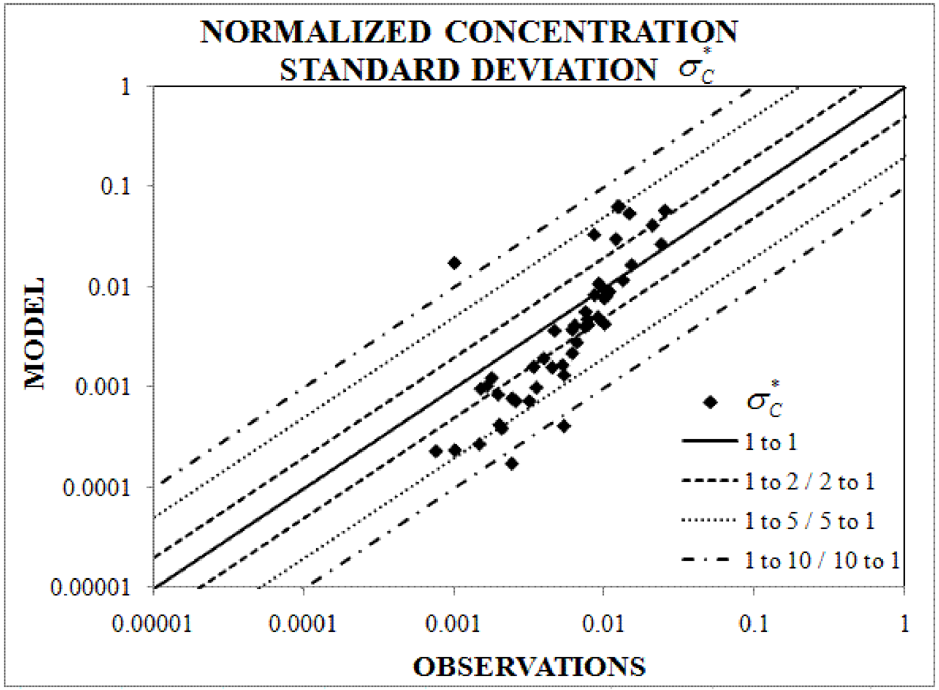
FAC2 = Fraction within a Factor of Two

HR = Hit Rate

Results – II

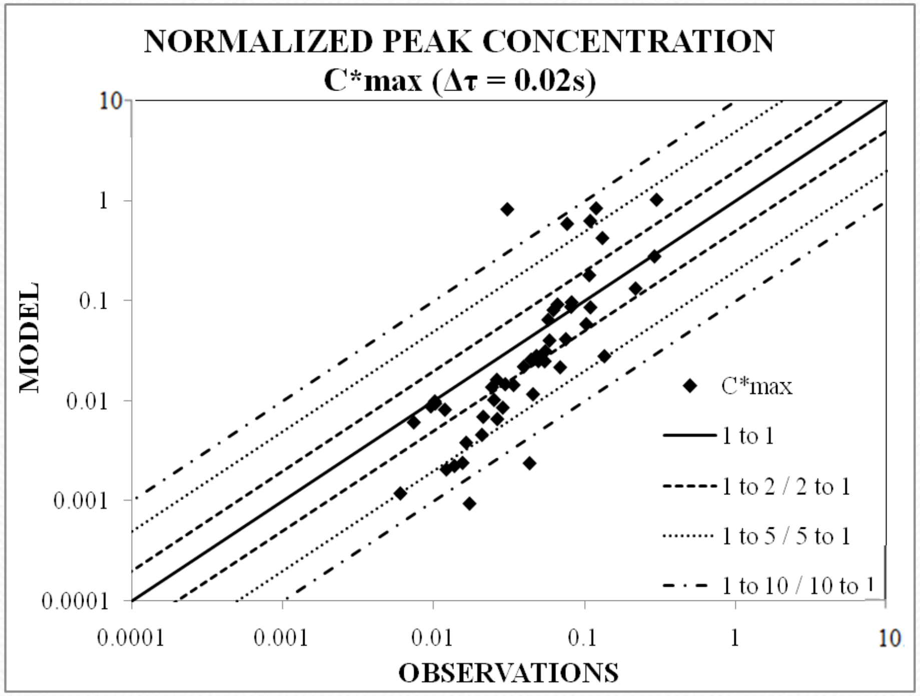
- Mean normalized concentration and normalized standard deviation for $T_{dc} = T_{dc0}$.

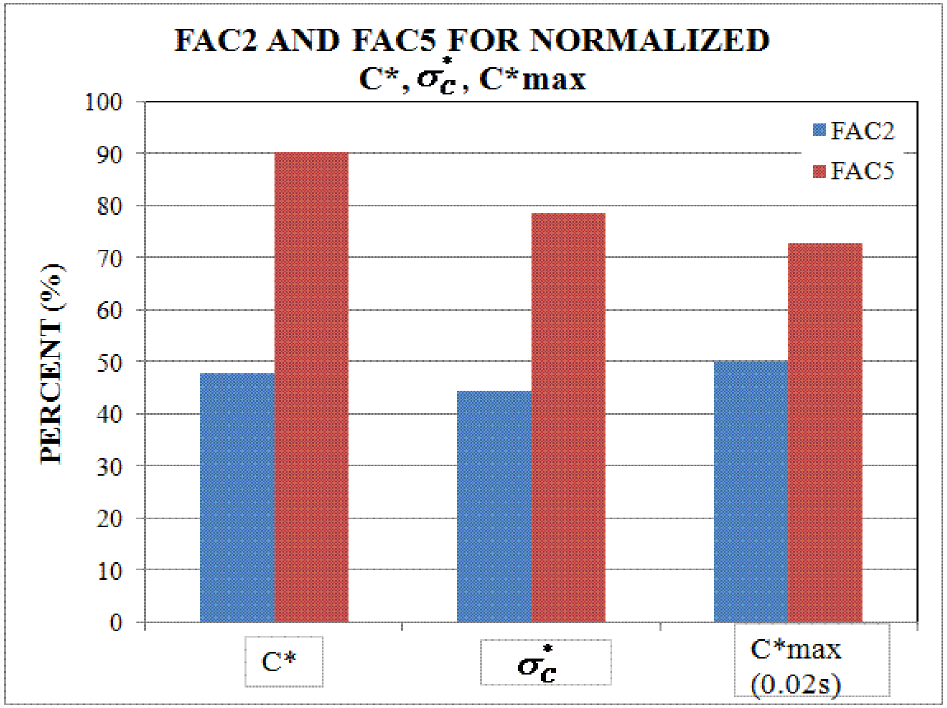




Results – III

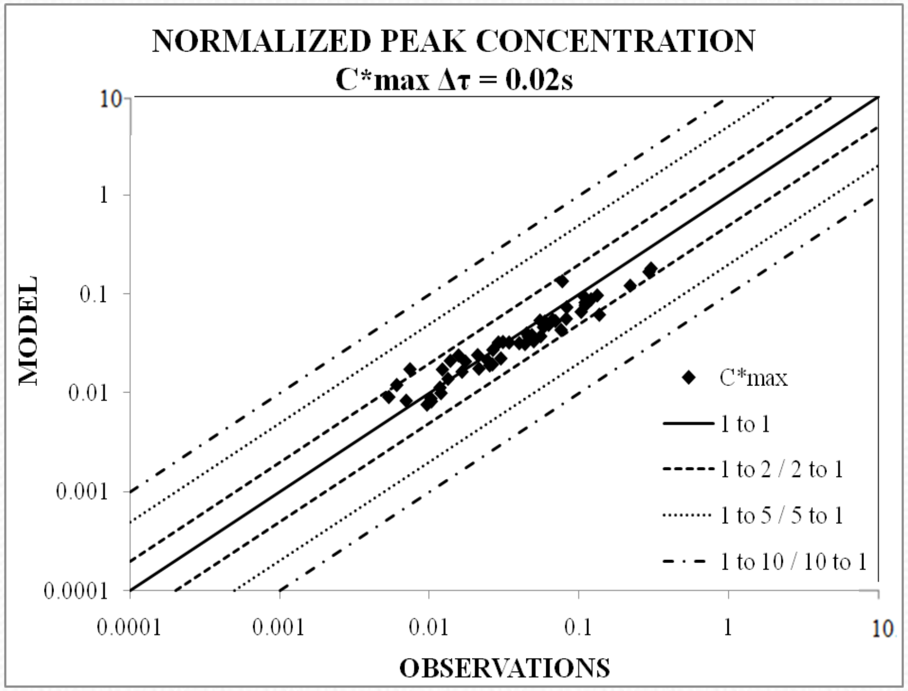
- Peak time averaged concentrations for $\Delta\tau$ = 0.02 [s] (time resolution for most of the measurements) and FAC2 and FAC5 metrics.





Results – IV

- Peak concentrations using for concentration means and variances the experimental ones.



- Figure supports further the validity of Bartzis et all (2007) model to predict peak concentrations within a factor of two.

Conclusions

- In this work a CFD RANS modelling approach incorporated to ADREA code has been presented capable of predicting mean concentrations, concentration variances and peak concentrations necessary to estimate pollutant hazard and individual exposure at any time interval.

- Concerning plume turbulent time scale modelling, the average value approach gave better results compared with the widely used approach of local scale modelling.

- The comparisons with the MUST field dispersion experiment are quite encouraging, although there is still a room for improvements especially in the plume turbulent time scaling.

- The present results support the validity of Bartzis et al. (2007) empirical model to predict peak time concentrations.

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Thank you for your attention