ATMOSPHERIC DISPERSION AND INDIVIDUAL EXPOSURE OF HAZARDOUS MATERIALS.

VALIDATION AND INTERCOMPARISON STUDIES

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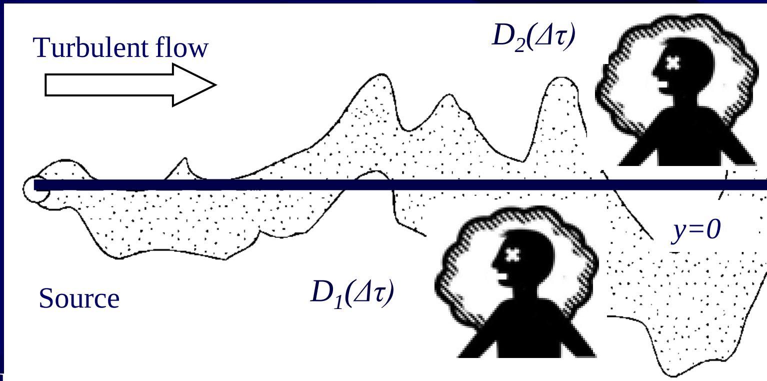
Motivation

- Deliberate or accidental atmospheric release from a near ground point source upwind or in a complex urban environment.

- Prediction of individual exposure at a time interval $\Delta\tau$ downwind the source (Sensor 1, 2).
- Individual exposure = Dosage at a time interval $\Delta\tau$.

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

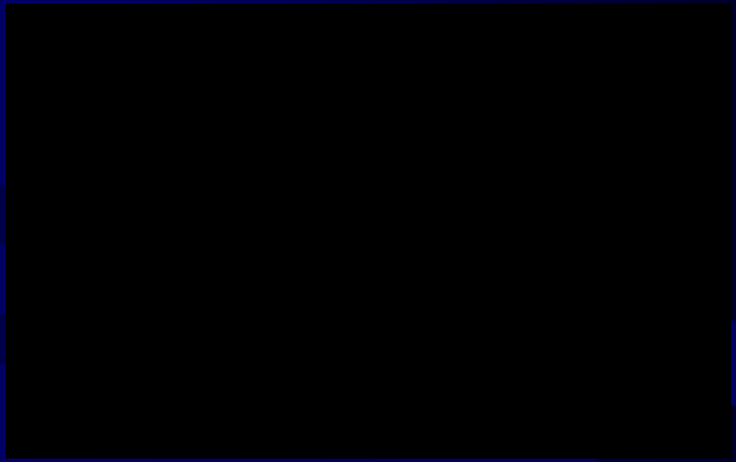


The problem

Stochastic nature of turbulence

$\Downarrow$

Concentration variability



EWTL, University of Hamburg

Conclusion:

The prediction of actual concentration/dosage downwind the source is practically impossible.

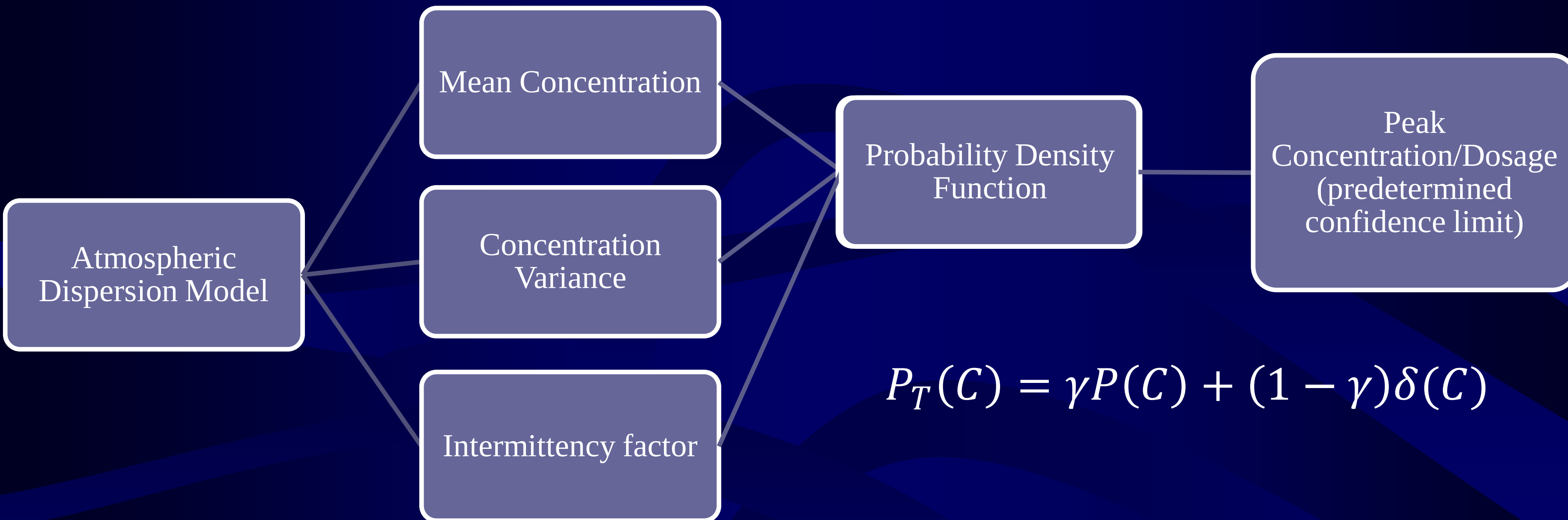
Maximum individual exposure/expected dosage:

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

$C_{max}(\Delta\tau)$ is the peak time averaged concentration.

Predicting maximum dosage

The Probabilistic Models



$$P_T(C) = \gamma P(C) + (1-\gamma)\delta(C)$$

Research	Gamma	Lognormal	Weibull	Exponential	Chopped normal
Lung et al., (1992)	x	x	x		
Mylne & Mason (1991)				x	x
Yee (1990)		x		x	x
Yee et al., (1993)	x	x	x	x	x
Gailis et al., (2007)	x	x			
Gailis & Hill (2006)	x			x	x

Gamma: $P_\Gamma(C\,|\,a,b) = \frac{1}{b^a \Gamma(a)} C^{a-1} e^{-C/b}$

Lognormal: $P_\Lambda(C) = \frac{1}{C\sqrt{\overline{C'^2}}\sqrt{2\pi}} e^{\frac{-(\ln C-\overline{C})^2}{2\overline{C'^2}}}$

Weibull: $P_W(C) = ba^{-b}C^{b-1} e^{-\left(\frac{C}{a}\right)^b}$

Exponential: $P_E(C) = \frac{1}{\overline{C}} e^{-\frac{C}{\overline{C}}}$

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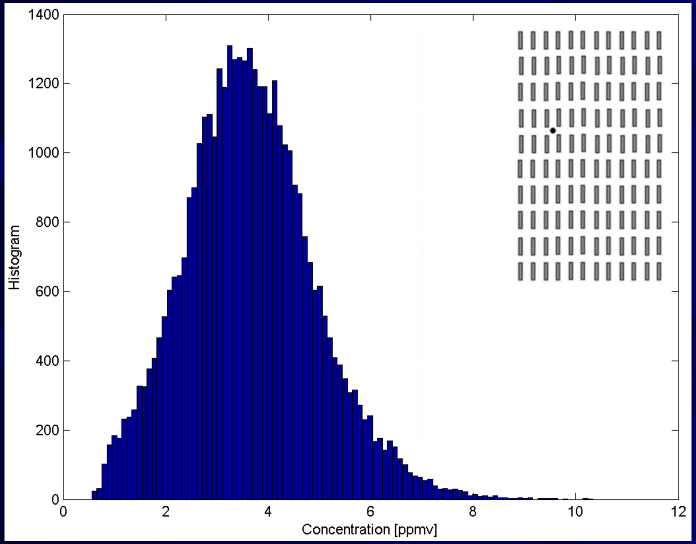
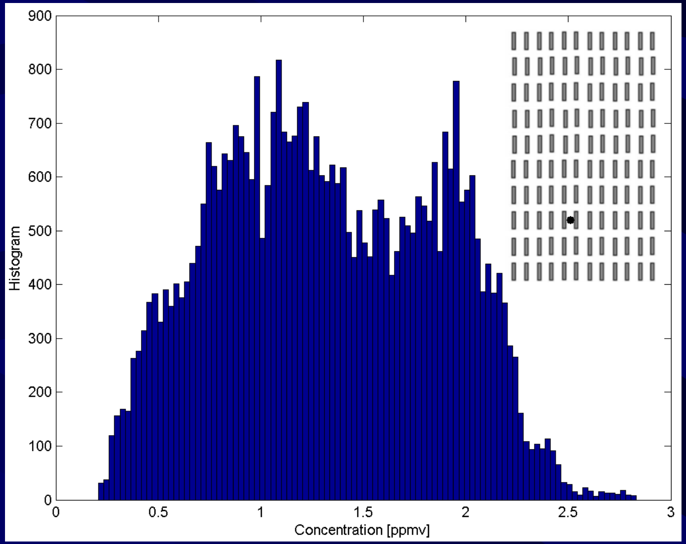
Chopped normal: $P_A(C) = \frac{1}{\sqrt{2\pi\sqrt{\overline{C'^2}}}} e^{\left(-\frac{(C-\overline{C})^2}{2\overline{C'^2}}\right)}$

Limits of probabilistic method

- There is not a common well known distribution that can be used to describe the concentration in all the locations.





2. Results sensitive to the confidence interval 95%, 99%, 99.8%, 99.98%.
   For 100% $C_{max} \longrightarrow \infty$

Predicting maximum dosage

The Deterministic Models (Bartzis et al., 2008)

$$\frac{D_{\mathbf{max}}(\Delta\tau)}{\overline{C}} = f\left(I, \frac{\Delta\tau}{T_C}\right) \Longrightarrow \boxed{D_{\mathbf{max}}(\Delta\tau) = \overline{C}\left[1 + \beta\, I\left(\frac{\Delta\tau}{T_C}\right)^{-n}\right]\Delta\tau}$$

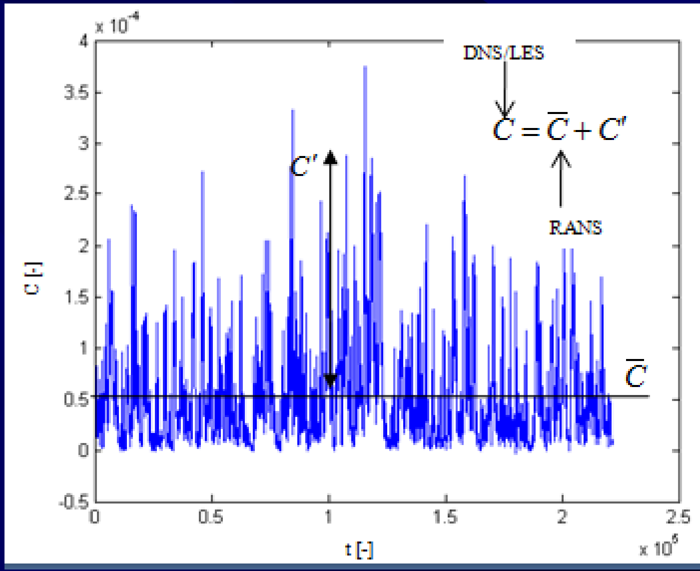
- Turbulence autocorrelation time scale $T_C = \int_0^\infty R_C(\tau)d\tau$
- Autocorrelation function $R_C(\tau) = \dfrac{\overline{C'(t)C'(t+\tau)}}{\overline{C'^2}}$
- Mean value: $\overline{C}$ Fluctuation: C' Variance: $\overline{C'^2}$
- Fluctuation intensity: $I = \overline{C'^2} / \overline{C}^2$
- β and n are parameters that are estimated experimentally FLADIS: β = 1.5, n = 0.3

  MUST: β = 1.64, n = 0. 3

The prediction requirements

- The mean concentration $\overline{C}$
- The concentration variance $\overline{C'^2}$
- The turbulent time scales T_C

- The simplest and practical approach for complex terrains
  - CFD RANS models
  - Two-equation turbulent closure



Transport equation for concentration variance

(using the concept of eddy viscosity/diffusivity)

$$\underbrace{\frac{\partial \rho \overline{C'^2}}{\partial t}}_{\text{Change in time}} + \underbrace{\frac{\partial \rho \overline{u_i}\,\overline{C'^2}}{\partial x_i}}_{\text{Advection by the mean velocity field}} = \underbrace{-2\rho K_C \left(\frac{\partial \overline{C}}{\partial x_i}\right)^2}_{\text{Generation of fluctuations due to gradients in the mean concentration}} + \underbrace{\frac{\partial}{\partial x_i}\left[\rho\left(K_C + D\right)\frac{\partial \overline{C'^2}}{\partial x_i}\right]}_{\text{Diffusive transport produced by turbulent velocity fluctuations; Diffusive transport produced by molecular diffusion}} \underbrace{-2\rho D \frac{\overline{\partial C'}}{\partial x_i}\frac{\overline{\partial C'}}{\partial x_i}}_{\text{Dissipation by molecular diffusion of the fine scale concentration fluctuations}}$$

Turbulent concentration fluxes: $-\overline{u_i' C'^2} = K_{C'}\frac{\partial \overline{C'^2}}{\partial x_i} = K_C \frac{\partial \overline{C'^2}}{\partial x_i} = \frac{K_m}{\sigma_h}\frac{\partial \overline{C'^2}}{\partial x_i}$

The dissipation rate of concentration variance

The usual approach → algebraic modelling (Csanady, 1967):

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

T_{dc} = dissipation time scale of concentration variance

The dissipation rate of concentration variance:

A new approach (Efthimiou & Bartzis, 2011)

$$\frac{T_{dc}}{T_{dc\infty}} = \frac{T_C}{T_{C\infty}}$$

Assumptions:

1. The time scales T_{dc} and T_C are analogous variables.

2. The time scales T_{dc} and T_C depends on the pollutant travel time.

3. The time scales $T_{dc\infty}$ and $T_{C\infty}$ correspond to full mixing conditions and depends on the flow turbulent characteristics.

The new approach has been tested until now with the k-ζ model (Bartzis, 2005).

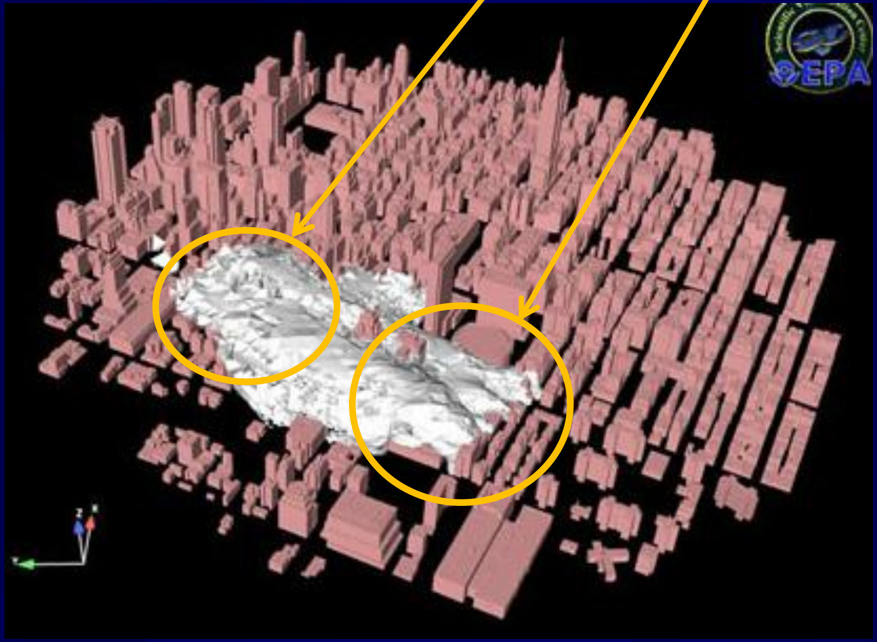
In the present study: Incorporation of the widely used k-ε model (Launder, B. E. and D. B. Spalding, 1974) to the new methodology.

The autocorrelation time scale T_C

Experimental evidence: T_C is highly correlated with the pollutant travel time especially near the source.

$$\boxed{T_C = \mathbf{min}(c_u T_{travel},\ T_{C\infty})}$$

$c_u = 0.11$



Pollutant travel time
Radioactive tracer method

Remarks:

1. In Eulerian CFD models the estimation of the pollutant travel time is not direct.

2. The use of the physical law *x/U* is questionable in complex urban environments.

Radioactive tracer method

➢Two tracers are released simultaneously from the same source with the same experimental conditions.

➢One tracer is considered passive (C_0) while the other is considered radioactive (C) with a decay constant λ (s^{-1}).

<u>Pollutant travel time:</u>

$$T_{travel} = -\frac{1}{\lambda} \ln \frac{C}{C_0}$$

The time scale $T_{C\infty}$ (full mixing)

k-ζ model (Efthimiou et al., 2011)

$$T_{C\infty} = c_h k^{-1/2} \zeta^{-1} \qquad c_h = 1.0$$

Standard *k-ε* model (Andronopoulos et al., 2002, Milliez and Carissimo, 2008)

$$T_{C\infty} = k\varepsilon^{-1}$$

The time scale $T_{dc\infty}$ (full mixing)

$$T_{dc\infty} = c_{dc} T_{C\infty}$$

k-ζ model:

Efthimiou et al., 2011: $c_{dc} = 3.05$

Standard *k*-ε model:

Andronopoulos et al., 2002: $c_{dc} = 0.8$

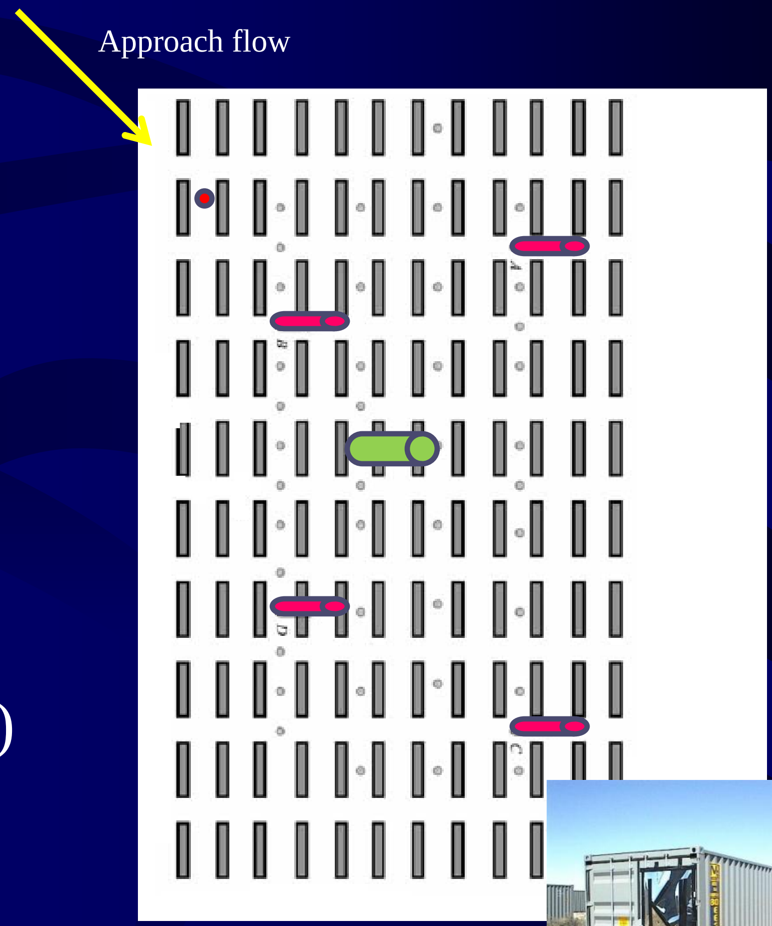
Milliez and Carissimo, 2008: $c_{dc} = 1.0$

The MUST experiment (Yee & Biltoft, 2004)

- 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)

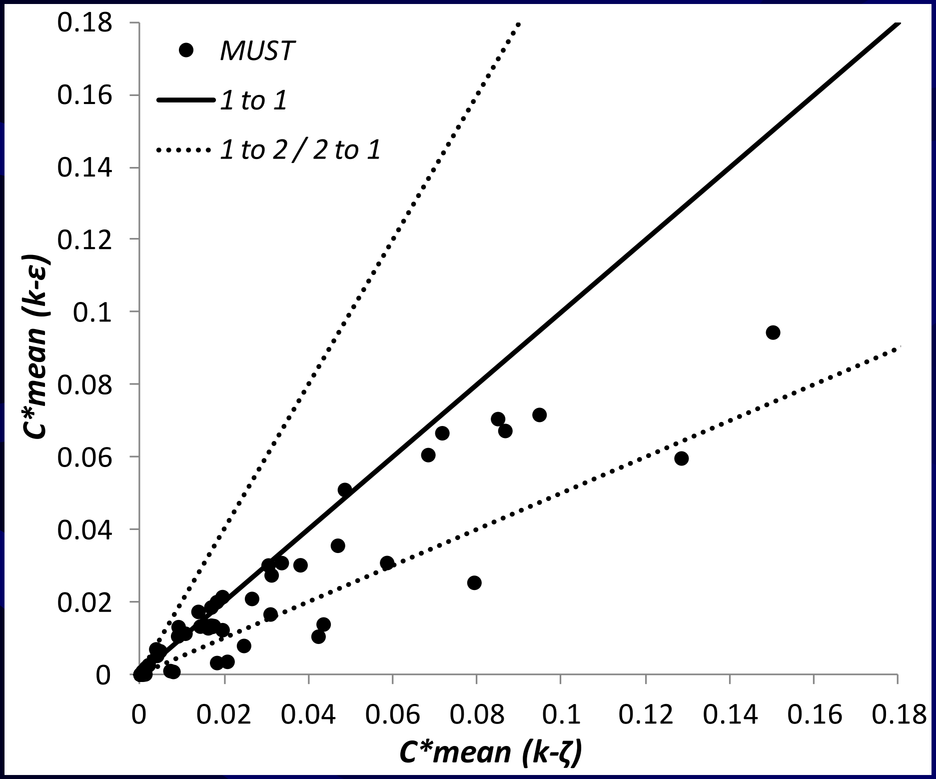
The selected validation trials

Experimental parameters	MUST	
	Trial 11	Trial 12
Date	25/9/2001	25/9/2001
Hour of emission	18:29:00	18:49:00
Tracer	Propylene (C_3H_6)	
Emission duration	15 min	
Emission rate	0.00457 kg s^{-1}	
Source area	0.00196 m^2	
Source height	1.8 m	0.15 m
Reference velocity	7.93 m s^{-1}	7.26 m s^{-1}
Wind direction	-40.54^o	-41.23^o
Mean atmospheric temperature	304.94 K	304.32 K
Roughness height	0.127 m	0.086 m
Manipulation time period	200 s	
Friction velocity	0.92 m s^{-1}	0.76 m s^{-1}
Monin-Obukhov length	-28000 m	2500 m
Exponential exponent	0.25	0.23

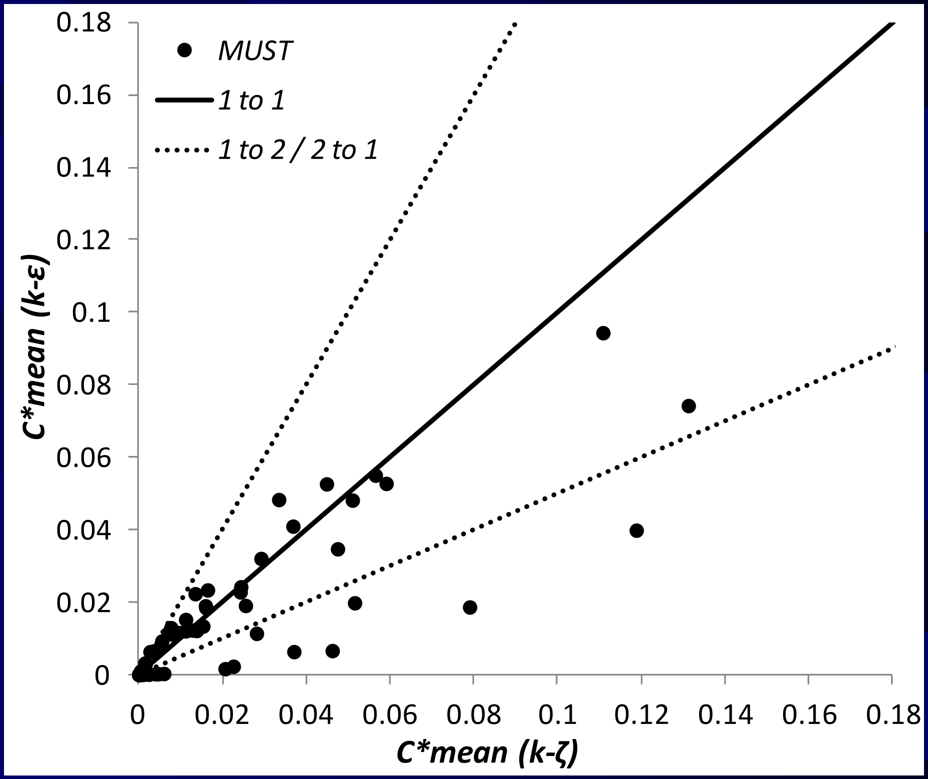
The simulations are performed with the CFD code ADREA (Bartzis et al., 1991).

Mean concentration results (I)

Trial 11



Trial 12



Mean concentration results (II)

Factor of two of observations

$$FAC2 = \frac{N}{n} = \frac{1}{n}\sum_{i=1}^{n} N_i \qquad N_i \begin{cases} 1, & 0.5 \le \dfrac{C_{pi}}{C_{oi}} \le 2.0 \\ 0, & \dfrac{C_{pi}}{C_{oi}} < 0.5 \text{ ή } \dfrac{C_{pi}}{C_{oi}} > 2.0 \end{cases}$$

Fractional Bias (underestimation/overestimation)

$$FB = \frac{\left(\overline{C_o} - \overline{C_p}\right)}{0.5\left(\overline{C_o} + \overline{C_p}\right)}$$

Normalized mean square error (dispersion)

$$NMSE = \frac{\overline{\left(C_o - C_p\right)^2}}{\overline{C_o}\,\overline{C_p}}$$

Quality acceptance criteria (Schatzmann et al., 2010)

$|FB| < 0.3$

$NMSE < 4$

$FAC2 > 0.5$

	Validation metrics		
	FAC2	FB	NMSE
Near ground measurements			
Trial 11 (k-ζ / k-ε)	0.60 / 0.43	-0.08 / 0.52	0.35 / 0.77
Trial 12 (k-ζ / k-ε)	0.89 / 0.52	-0.22 / 0.39	0.33 / 0.53
Total measurements			
Trial 11 (k-ζ / k-ε)	0.48 / 0.44	-0.24 / 0.11	0.69 / 0.73
Trial 12 (k-ζ / k-ε)	0.70 / 0.46	-0.19 / 0.12	0.42 / 0.53

Concentration standard deviation results (I)

$$T_{dc\infty} = c_{dc} T_{C\infty}$$

Selection of the parameter c_{dc}:

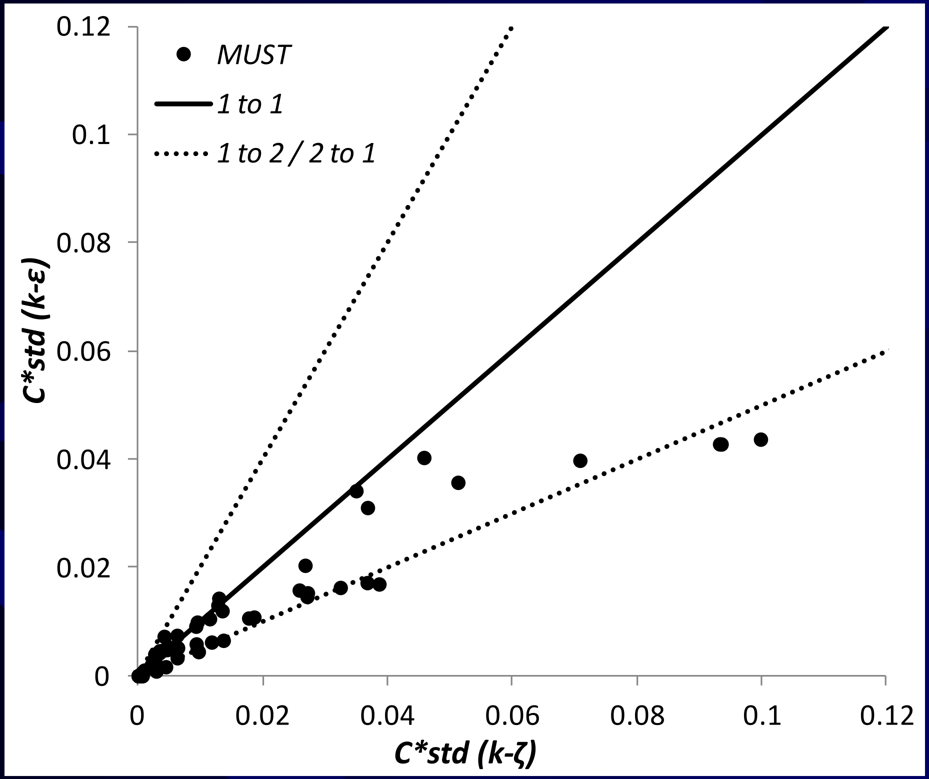
Sensitivity study on the influence of this parameter to the results has been performed for both Trials using the k-ε model.

First simulation: $c_{dc} = 0.8 \rightarrow$ underprediction (e.g. for Trial 11 and for all sensors: FAC2 = 5.7%, NMSE = 2.49, FB = 1.03).

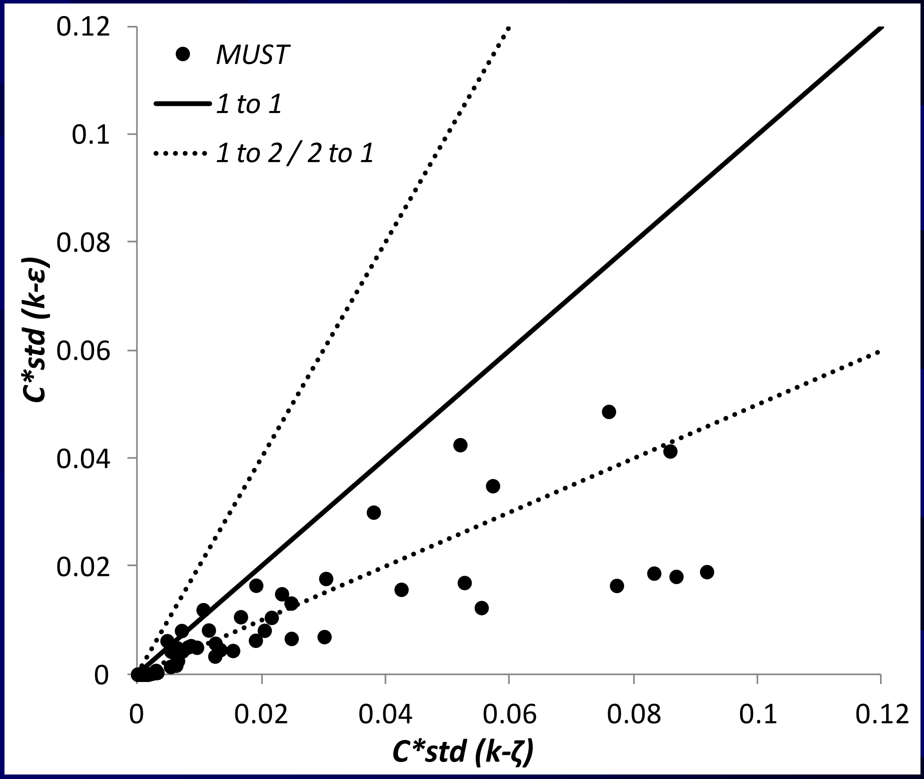
Best performance: $c_{dc} = 1.7$.

Concentration standard deviation results (II)

Trial 11



Trial 12



Concentration standard deviation results (III)

Factor of two of observations

$$FAC2 = \frac{N}{n} = \frac{1}{n}\sum_{i=1}^{n} N_i \qquad N_i \begin{cases} 1, & 0.5 \leq \dfrac{C_{pi}}{C_{oi}} \leq 2.0 \\ 0, & \dfrac{C_{pi}}{C_{oi}} < 0.5 \text{ ή } \dfrac{C_{pi}}{C_{oi}} > 2.0 \end{cases}$$

Fractional Bias (underestimation/overestimation)

$$FB = \frac{\left(\overline{C_o} - \overline{C_p}\right)}{0.5\left(\overline{C_o} + \overline{C_p}\right)}$$

Normalized mean square error (dispersion)

$$NMSE = \frac{\overline{\left(C_o - C_p\right)^2}}{\overline{C_o}\,\overline{C_p}}$$

Quality acceptance criteria (Schatzmann et al., 2010)

$|FB| < 0.3$

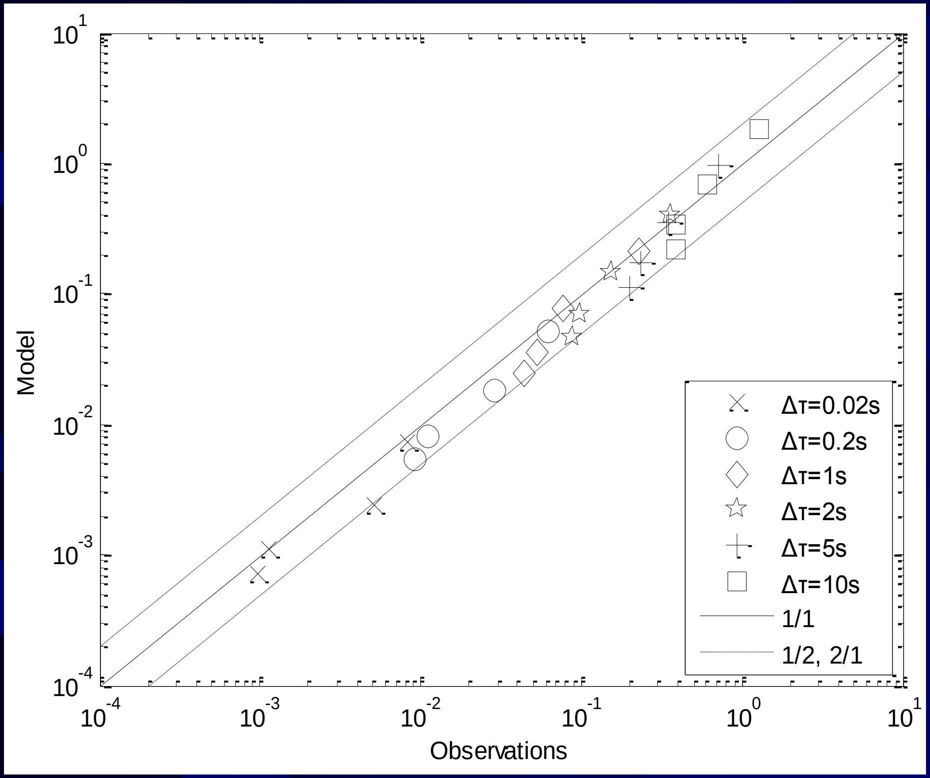
$NMSE < 4$

$FAC2 > 0.5$

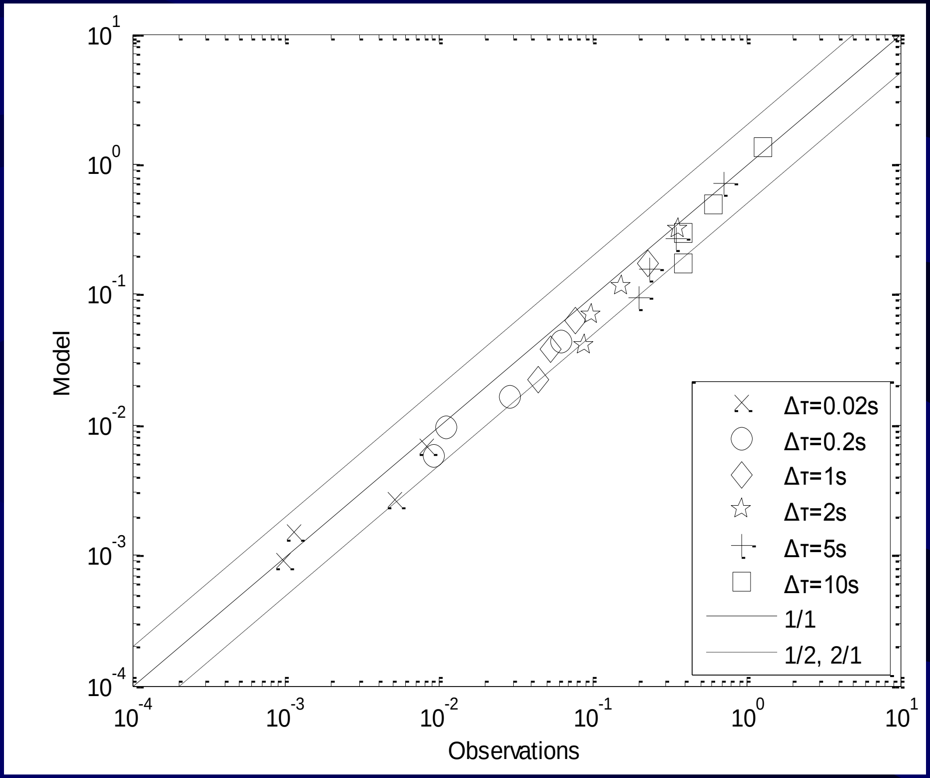
	Validation metrics		
	FAC2	FB	NMSE
Near ground measurements			
Trial 11 (k-ζ / k-ε)	0.63 / 0.60	0.21 / 0.37	0.22 / 0.35
Trial 12 (k-ζ / k-ε)	0.82 / 0.67	0.075 / 0.19	0.088 / 0.17
Total measurements			
Trial 11 (k-ζ / k-ε)	0.59 / 0.69	-0.33 / 0.12	1.39 / 0.26
Trial 12 (k-ζ / k-ε)	0.76 / 0.68	-0.35 / -0.047	1.20 / 0.34

Individual exposure

Trial 11



Trial 12



Conclusions

- The proposed approach on concentration time scale dependency on pollutant travel time seems to be a valid approximation in predicting plume dispersion from a point source in CFD RANS modeling using the k-ζ and standard k-ε turbulence models.

- In case of k-ε model a new value for c_{dc} 1.7 allowed a good insight into the fluctuation results.

- The validation study was performed against MUST field experimental data under neutral conditions.

- An overall better performance for concentration mean and standard deviation was observed when the k-ζ model was used.

- More validation and intercomparison studies are planned by the authors.