LANGRANGIAN MODELING EMBEDDED IN RANS CFD CODES FOR CONCENTRATIONS AND CONCENTRATION FLUCTUATIONS PREDICTIONS FROM AIRBORNE HAZARDOUS RELEASES IN URBAN ENVIRONMENTS

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MOTIVATION

- **<u>The Question</u>** : to what degree and under what parametrization the Lagrangian models can be successfully used in urban canopies to predict not only <u>concentrations</u> but more importantly <u>concentration fluctuations</u> as well.
- **The ambition** is such an approach to be widely adopted as an alternative dispersion model within CFD methodology and beyond
- The present work can be considered as a starting point addressing the above problem in the simplest way possible

OVERALL STRATEGY

- First explore relatively simple Lagrangian approaches based on Langevin Equation (Thomson, 1987) fully coupled with the detailed flow parametrization provided by the CFD codes.

I- Why Langrangian Models ?

<u>ADVANTAGES</u>

- They can produce concentration time series like LES, generating concentration statistics,
- The particle path geometry being independent on the flow grid, can theoretically recognize better the complex terrain subgrid features,
- The short time releases including instantaneous ones, can be directly simulated and
- The numerical diffusion error experienced in the corresponding Eulerian models are here non existent.

<u>DISADVANTAGES</u>

- The main disadvantage is that these simple approaches are not based on first principles making necessary the extensive testing on the specific type of problems to be addressed.

II-Why Langrangian Models ?

- The simple Lagrangian approaches have been approved quite successful at least in regional scale and/or mild topography (e.g. FLEXPART).
- Applications in build up domain have also been performed mainly in connection with diagnostic wind field (e.g. Kaplan and Dinar(1996), Tinareli et al (2007), Moussafir et al(2007)) with satisfactory results.
- Attempts also have been made to couple with the wind field produced by RANS-CFD approach using more complicated formulation of the Langevin Equation(e.g. Wilson et al, 2007).

NOTE

To the authors knowledge , the relevant effort up to now was on predicting concentrations and not concentration fluctuations

THE PRESENT MODELING APPROACH

- The basic equation (Kaplan and Dinar,1996):

$$\delta u_i(t+\delta t) = -\frac{\delta t}{T_{Li}} u_i + \frac{\delta t}{2}\frac{\partial \sigma_i^2}{\partial x_i}\left[1+\left(\frac{u_i}{\sigma_i}\right)^2\right] + \sigma_i\left(\frac{2\delta t}{T_{Li}}\right)^{\frac{1}{2}} \xi$$

The Langrangian time scale (T_L) has been assumed isotropic (Efthimiou and Bartzis,2011):

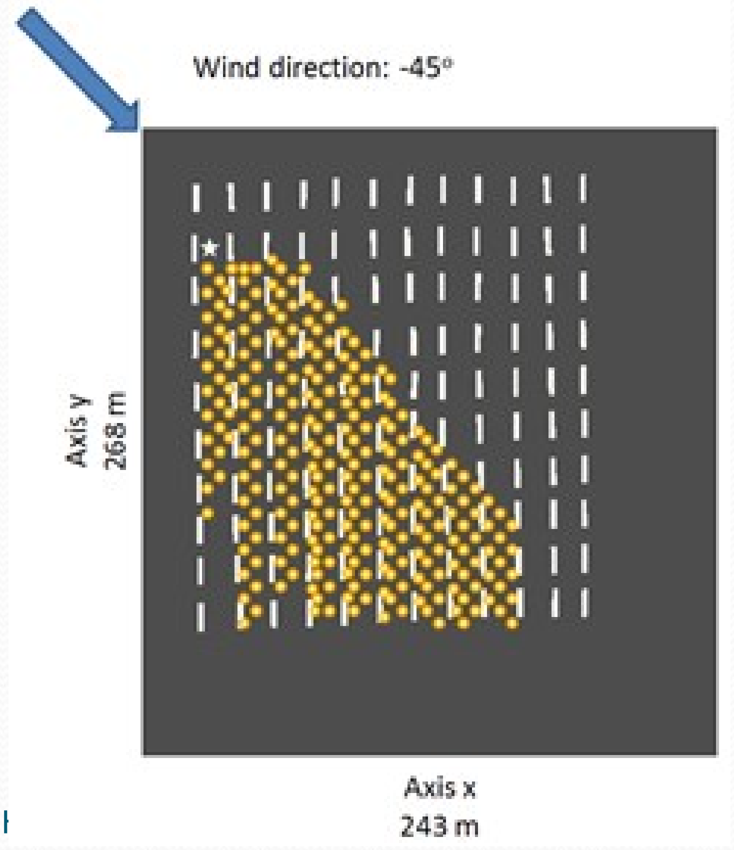
$$T_L = C_T\, k/\varepsilon\,, \qquad C_T = 0.5$$

The velocity fluctuations variance: $\sigma_i^2 \approx \frac{2}{3}\mathrm{k}$

$$\delta t \ll T_L,\ grid\ Courant\ time\ scale$$

THE MUST WIND TUNNEL EXPERIMENT

- The methodology has been validated against data of the MUST wind tunnel experiment (Bezpalcova and Harms, 2005) which have been scaled up for the conditions of the corresponding field experiment (Yee and Biltoft, 2004).



THE MUST WIND TUNNEL EXPERIMENT

- Obstacles were arranged in 12 rows, each consisting of 10 obstacles. The obstacles were nearly identical and had average length, width and height 12.2 m × 2.42 m × 2.54 m respectively in field scale
- A 256-detectors array arranged along obstacle rows in the part of the domain covered by the plume, placed at the same height equal to 1.28 m in field scale.
- *Wind speed at the roof level* $U_{ref} = 8$ m/s
- Wind direction -45^o
- The release strength 3.3×10^{-6} m^3s^{-1}.

The CFD-RANS SIMULATIONS

- The CFD ADREA-HF code (Venetsanos et al., 2010) has been setup for the simulation in the field scale
- The standard k-ε model has been used for turbulence closure
- A 85 x 95 x 26 non uniform grid is used with 209,950 active cells

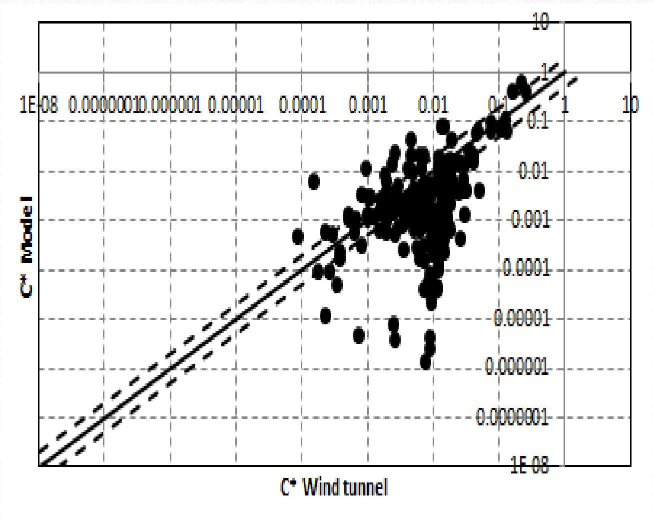
THE DISPERSION SIMULATIONS

LANGRANGIAN

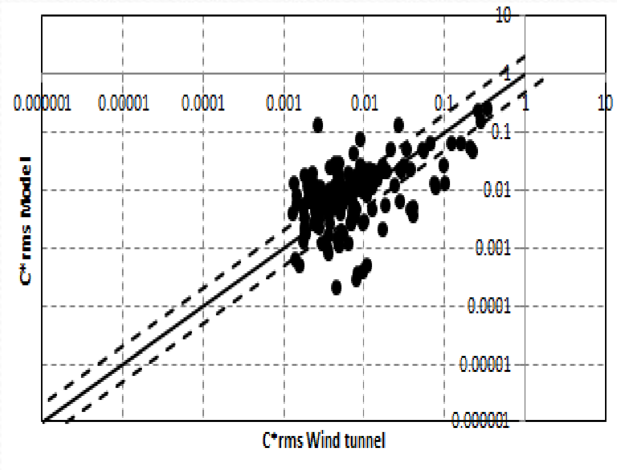
- The continuous release has been simulated by 1,000,000 particles [one particle released every (600/1000000) sec i.e. total release time 600sec)
- $\Delta t=0.1$ sec

- EULERIAN
- The model embedded to ADREA-HF

The MUST Wind Tunnel Experiment : Langrangian Model vs Experiment comparisons



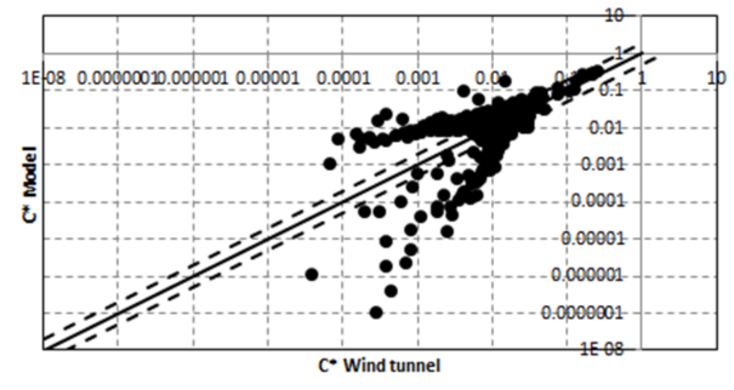
(a) Mean concentrations

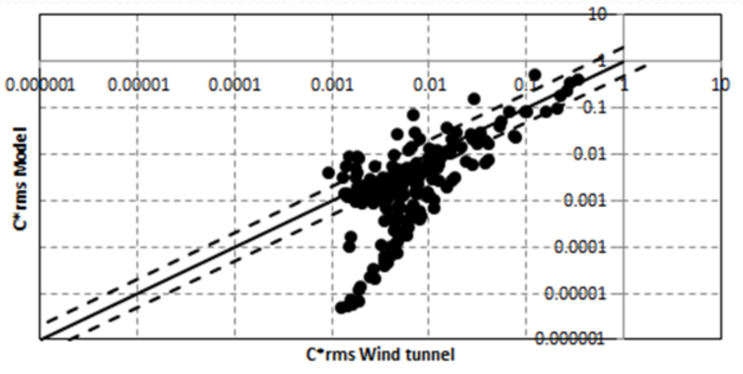


(b) concentrations standard deviation

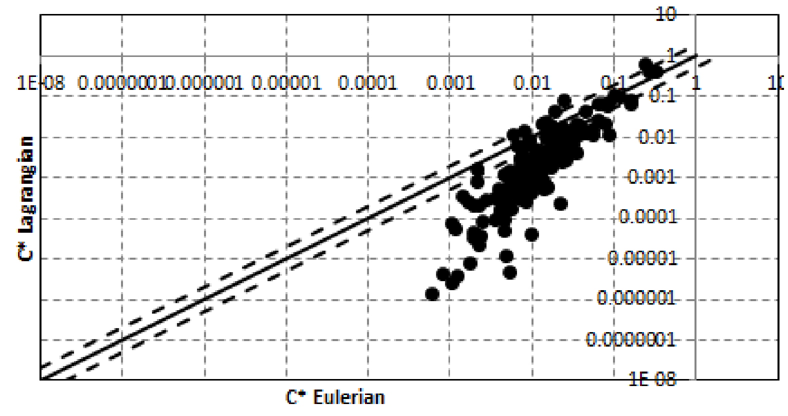
Figure 2. Experiment and model concentration comparisons (a) mean (b) standard deviation.

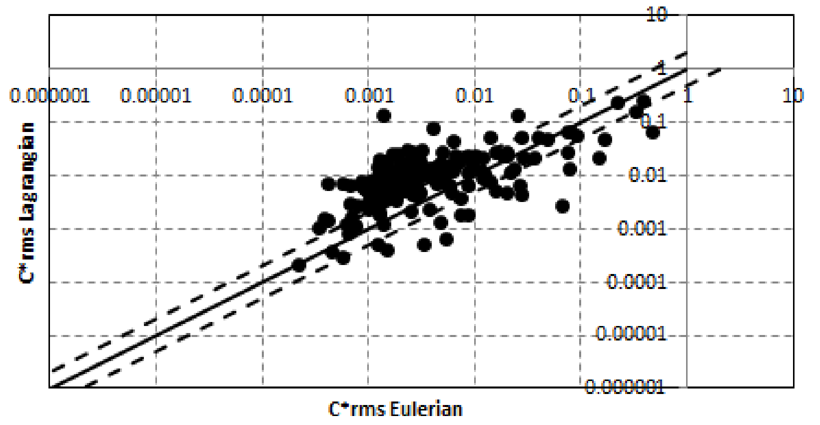
The MUST Wind Tunnel Experiment : Eulerian Model vs Experiment comparisons





The MUST Wind Tunnel Experiment : Langrangian vs Eulerian Model comparisons





The MUST Wind Tunnel Experiment : Modeling Statistical Comparisons

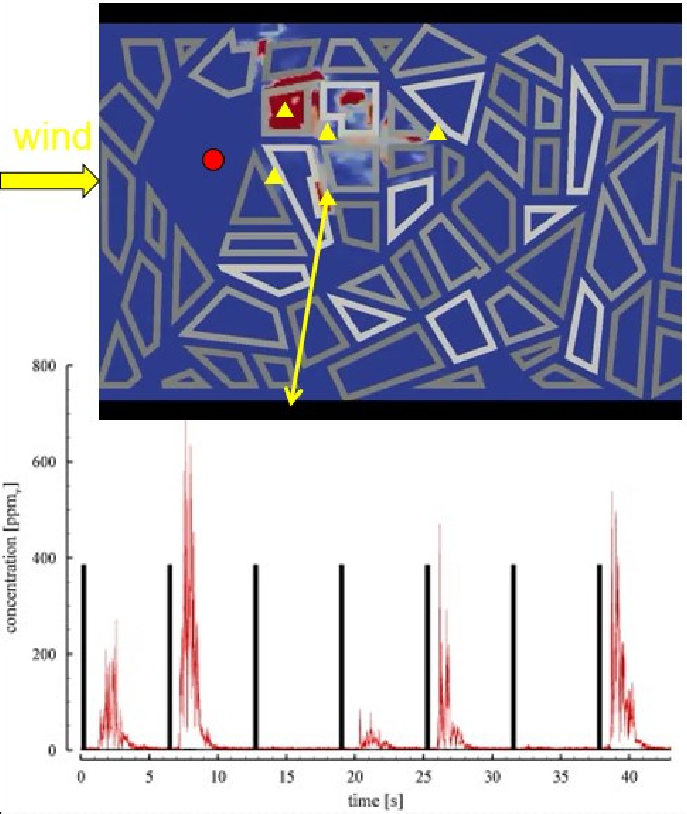
Table 1. Experiment and model comparisons. The statistical indicators for the Langrangian and the Eulerian model .

		FAC2	FB	NMSE
mean	eulerian	0.283	-0.303	1.43
	langrangian	0.307	-0.206	6.89
std	eulerian	0.357	0.129	4.09
	langrangian	0.332	-0.058	3.98

The next step : Puff releases

- Puff release : a stochastic phenomenon
- The Langrangian modelling characteristic of 'randomness' might allow for direct treatment of multiple puffs to extract the statistics of this stochastic behavior

Successive puff releases in wind tunnel: The measured concentration time series at a specific sensor(Michelstadt Experiment)



Harms F. et al. (2011), Validating LES-based flow and dispersion models, J. Wind Eng. Ind. Aerodyn., 99, p. 289-295.

Berbekar E. et al., (2015), Dosage-based parameters for characterization of puff dispersion results, J. Hazard. Mater., 283, p.178-185.

The black vertical lines correspond to the beginning of the release of a single puff.

The **actual short time exposure is stochastic** .

Successive puff releases in wind tunnel: Mean dosage variability

(Source: COST ES1006, Model Evaluation Protocol(2015))

Many repetitions to estimate the ensemble average exposure

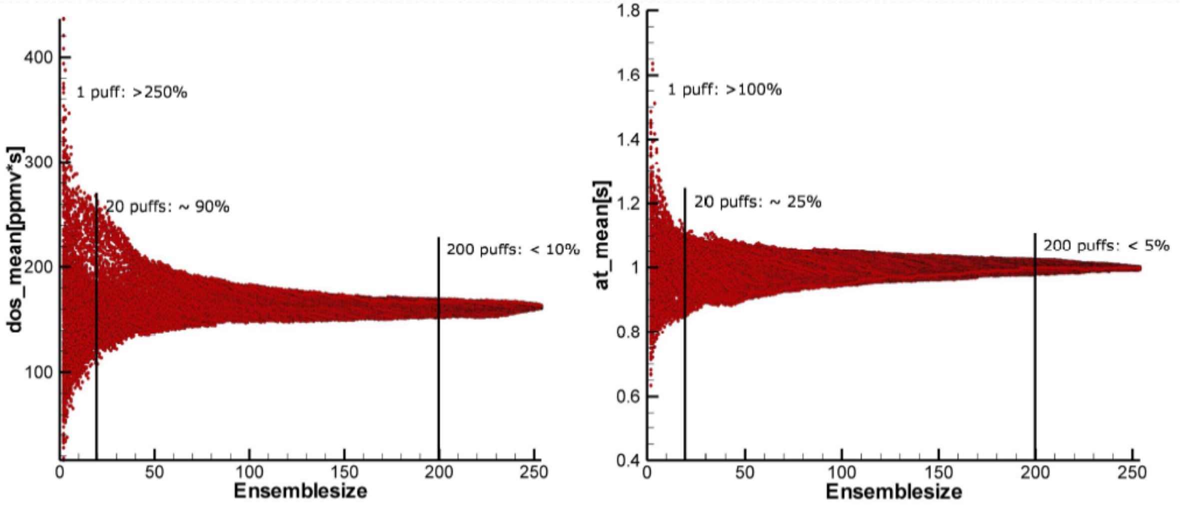


Figure 2: Exemplary diagrams about the variability of the mean dosage and puff arrival time at a certain sensor calculated from different ensemble averages for an instantaneous release scenario in "Michelstadt" urban dispersion test case (University of Hamburg, Environmental Wind Tunnel Laboratory)

Concluding Remarks

- The results in this particular application show that it is possible to estimate concentration fluctuations with Langrangian models based on Langevin Equation.
- The obtained results for mean concentration and concentration fluctuations standard deviation are comparable with the Eulerian ones.
- However further testing is needed before definite results can be drawn
- Priority for short time/instantaneous releases

ARISTOTELES

Ευχαριστώ

Thank you