CFD-RANS prediction of individual exposure from continuous release of hazardous airborne materials

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Abstract

One of the key issues of recent research on the dispersion inside complex urban environments is the ability to predict individual exposure (maximum dosages) of an airborne material which is released continuously from a point source. The present work addresses the question whether the Computational Fluid Dynamics (CFD) – Reynolds Averaged Navier Stokes (RANS) methodology can be used to predict individual exposure for various exposure times. This is feasible by providing the two RANS concentration moments (mean and variance) and a turbulent time scale to a deterministic model. The whole effort is focused on the prediction of individual exposure inside a complex real urban area. The capabilities of the proposed methodology are validated against wind tunnel data. The present simulations were performed “blindly” i.e. the modeler had limited information for the inlet boundary conditions and the results were kept unknown until the end of the COST Action ES1006. Thus a high uncertainty of the results was expected. The general performance of the methodology due to this “blind” strategy is medium. However the validation metrics fulfil the acceptance criteria. The reference data set was compiled by members of COST Action ES1006. The provision of reference data is gratefully acknowledged.

Objective

- To predict individual exposure (maximum dosages) using the CFD-RANS methodology in case of the continuous release of an airborne material from a point source in urban environments.

Methodology

The methodology for the prediction of individual exposure includes the following three steps:

1. Prediction of the turbulent flow and the concentration mean and variance using a CFD-RANS methodology.
2. Use of the results of the first step to the selected deterministic model for the prediction of individual exposure.
3. The selected deterministic model with the parameters calculated in the 2nd step is used to predict the individual exposure (maximum dosages) for various time intervals.

Mean concentration

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

Concentration variance

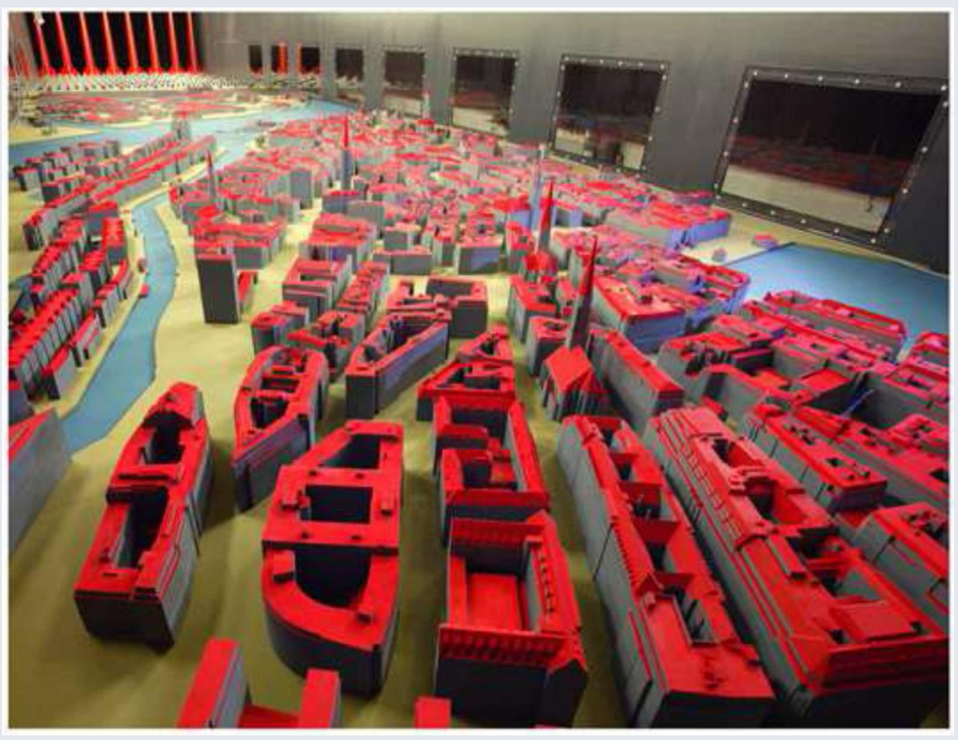
$$\frac{\partial}{\partial t}\left(\rho\overline{C'^2}\right)+\frac{\partial}{\partial x_i}\left(\rho\overline{u_i}\,\overline{C'^2}\right)=-2\rho\overline{u_i'C'}\frac{\partial\overline{C}}{\partial x_i}+\frac{\partial}{\partial x_i}\left(\rho D\frac{\partial\overline{C'^2}}{\partial x_i}-\rho\overline{u_i'C'^2}\right)-2\rho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

The deterministic model

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

The Complex Urban Terrain Experiment (CUTE)

The CUTE (Complex Urban Test Experiment) data set includes results from field and wind tunnel measurements. The data set is dedicated to test Emergency Response Tools/Atmospheric Dispersion Models predicting dispersion processes in urban areas.



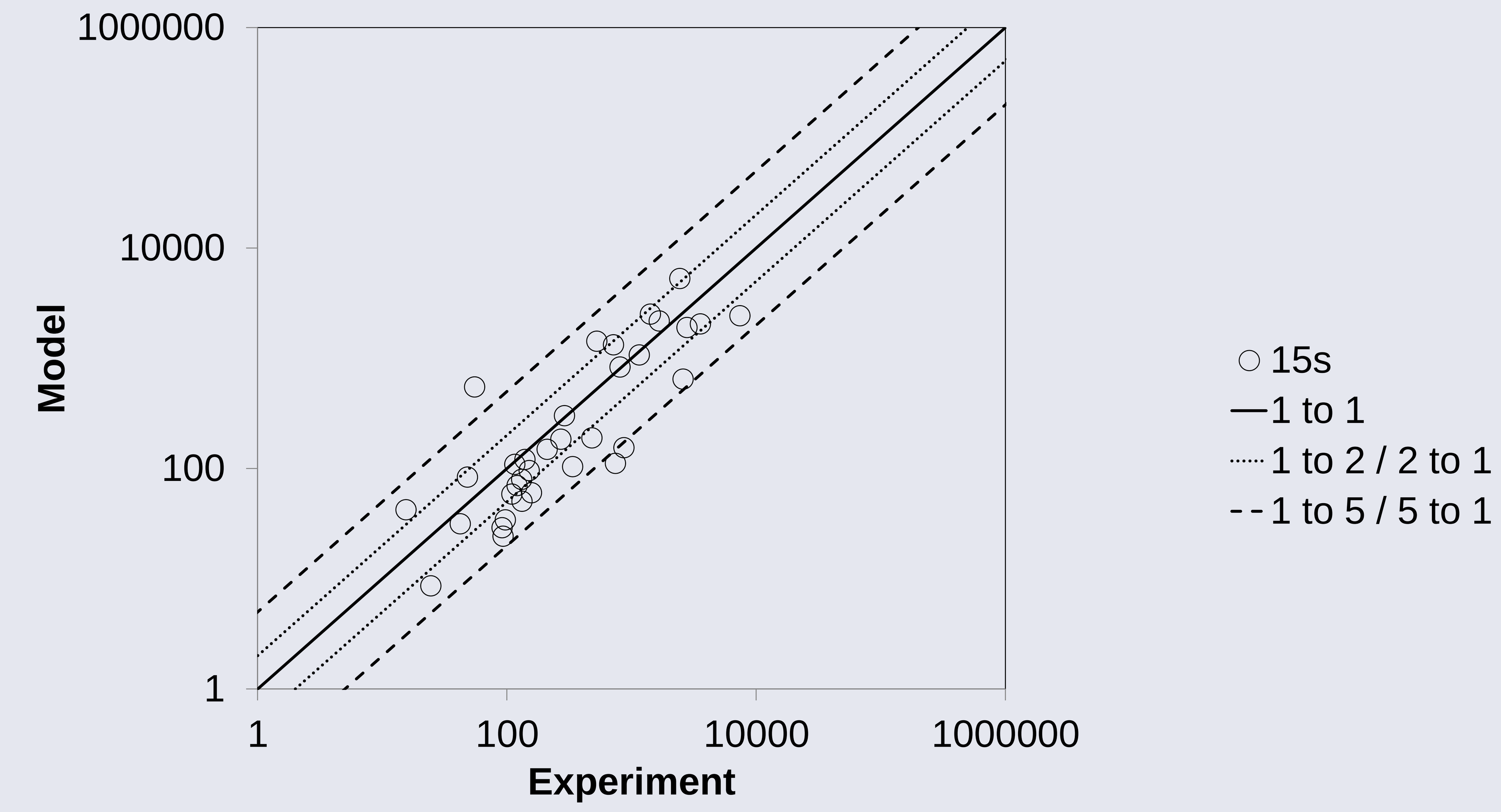
http://www.elizas.eu

The CFD-RANS numerical simulations

Concerning the CUTE experiment the computational domain for simulating the developing flow and dispersion within and above the three-dimensional obstacle array extended in the streamwise direction from x = −540 m to 2105.02 m, with the upstream wall of the first obstacle at x = 0 m. The simulations were conducted with a domain height of 6H_{max} (H_{max} is the maximum building height equal to 108 m), which was sufficiently deep to ensure that the flow changes near the surface (within and above the obstacles) were not being moulded (or influenced) by the boundary conditions imposed at the top of the computational domain. In the spanwise (or y) direction, the computational domain spanned −540 m ≤ y ≤ 1755.02 m. The vertical x-z centre plane at y ≈ 300 m contained the ground-level source at location of the red star. In this coordinate system, the source at the red star is located at $\mathbf{x}_s \equiv (x_s, y_s, z_s)$ = (229 m, 295 m, 0).
Due to the limited time no sensitivity of the solution to the discretization of the computational domain was performed. A coarse grid of 157 × 129 × 25 control volumes (in the streamwise, spanwise and vertical directions, respectively) were used for the simulations. Partial views for the discretizations of the computational domain, in the (x, z) (vertical) and (x, y) (horizontal) planes, are displayed in Fig. 6b and c, respectively. The grid is equidistant between the buildings and increases logarithmically outside the urban area.

Results

Modelled maximum dosages have been calculated for the time intervals Δτ = 15 s, 10 min, 30 min, 1 hour as obtained by the present model and for b = 2.88. The experimental maximum dosages were provided by COST Action ES1006.



Metric	15 s	10 min	30 min	1 hour
FAC2	0.529	0.500	0.529	0.500
NMSE	2.04	2.21	1.94	1.79
FB	0.198	-0.254	-0.362	-0.383

Conclusions

- Half of the majority of points lie in the factor-of-two range, which is a positive sign of the model performance.
- The differences in dosages are related to the discrepancies between calculated and experimental wind velocity, as well as concentration and concentration variance.
- Generally all the metrics fulfilled the quality acceptance criteria.

References

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