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Towards operational modelling of flow and dispersion in urban areas with Computational Fluid Dynamics (CFD)

Thesis booklet

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Introduction

Urban air quality modelling is a multidisciplinary field of science shared by meteorology, where models are called microscale obstacle resolving models, and by a branch of engineering called Computational Wind Engineering. Both of these areas are dealing with numerical solution of the Navier Stokes equations and an additional scalar transport equation for the air pollutant. Urban air quality models become more and more popular as the computational resources are rapidly growing, and as at the same time the ratio of population living in urban areas is increasing as well. The main problem related to urban air quality modelling with Computational Fluid Dynamics resolving the buildings in an urban area is the complexity of the simulation process, and the time needed to give useful results to decision makers. This fact has been delaying the use of this kind of models in operational modelling, which in the thesis I define as modelling for everyday use in the design and regulatory phase of construction projects either by an architect or a government office. This topic is widely discussed in the literature, but the usual approach is from the model development point of view, not giving special emphasis to the constraints in operational modelling, namely the limited time and computational resources. Another point which is usually missed in the model development is the numerical discretization uncertainty quantification, while these building resolving models usually require complex and not ideal quality meshes, so this error is unavoidable.

Aim of the thesis and main topics covered

In this thesis I am focusing on these operational questions of air quality modelling with Computational Fluid Dynamics. The aim of my research is to provide a compromise between the limited resources and the accuracy of the computation, but taking care of the numerical uncertainties at the same time. For this I carried out a numerical experiment comparing four automatic meshing techniques and two different passive scalar transport models in a complex urban environment called Michelstadt (see Figure 1). For this geometry extensive wind tunnel measurements are available for both the flow field and the dispersion, which is essential for a proper validation process with well-defined boundary conditions. For the numerical uncertainty quantification I consider estimators based on Richardson extrapolation and one-mesh estimators which can be an alternative. As a step for using these kind of models for emergency response as well, short-term release sources, i.e. puffs were also considered. I used the steady state flow field to run the simulations for the puffs.

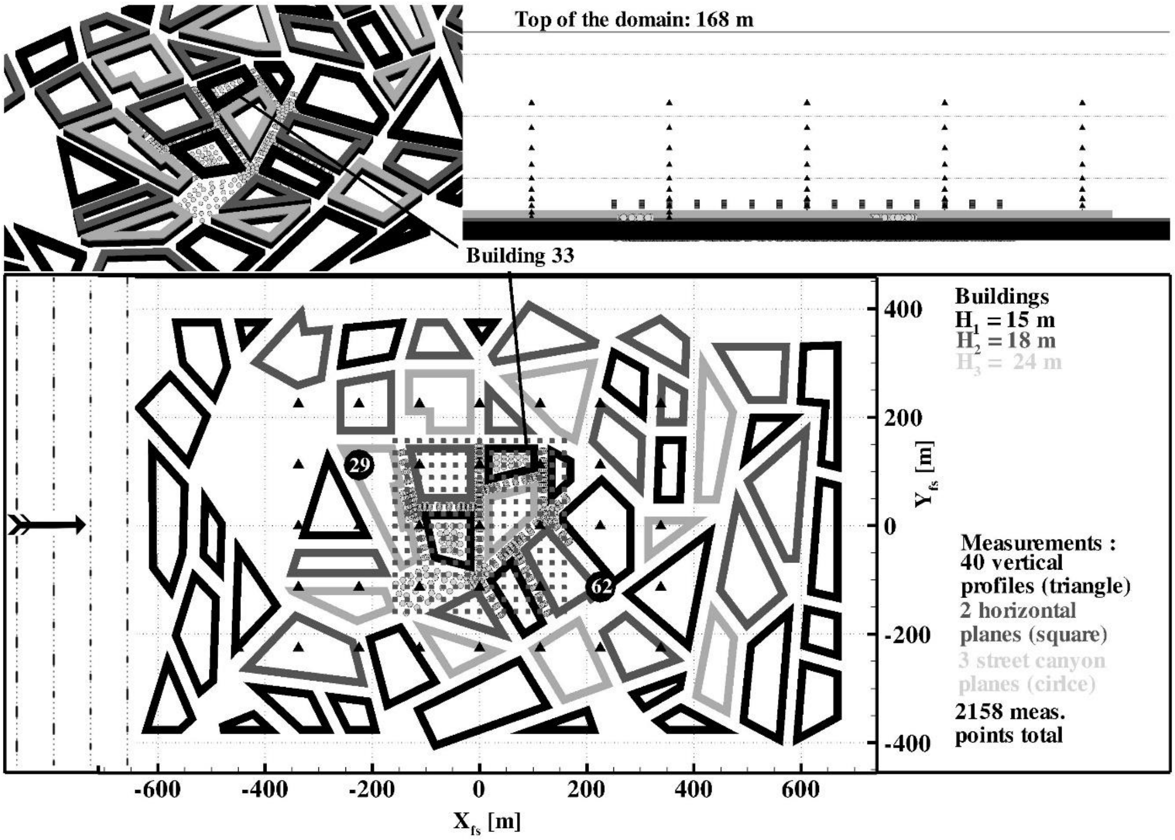

Figure 1: The computational model of the test case, Michelstadt, with the flow measurement points

What are the main challenges of urban flow and dispersion modelling?

Modelling the flow and dispersion in a complex urban environment with CFD is a very challenging task due to several reasons. The main challenges are:

- In the topic of urban air quality, the range of scales is very wide, both in space and time. It is not possible with the current computational resources to solve for all these scales. And what makes things even more difficult, all these scales reside in the atmosphere, a continuously changing environment incorporating complex physical phenomena.
- The improper spatial resolution results in numerical errors which are difficult to quantify and differentiate from the modelling errors.
- Modelling turbulent flow around bluff bodies, especially with a steady state approach is difficult due to flow separation and reattachment, possible vortex shedding and overprediction of turbulent kinetic energy in high shear flow.
- Modelling dispersion in an already probably not perfectly modelled flow field is another challenge to be faced.

All the previously mentioned challenges reduce the confidence in these type of models. One of the greatest concern of the use of flow and dispersion models in urban areas is given by Schatzmann and Leitl 2011. They state that these models have not been the subject of systematic evaluation but are used in the preparation of decisions with profound economic and political consequences. They also add that much more powerful computers than presently available and substantial research efforts will still be needed before the first reliable unsteady obstacle-resolving predictions for urban scale dispersion problems will become available. This thesis is therefore focusing on the steady approach.

There were and are substantial international research efforts to justify the use of CFD models for flow and dispersion modelling in urban areas and to help to better understand and resolve these challenges. One that must be mentioned here is the ongoing COST ES1006 Action "Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments" as the work of this PhD study is strongly related to the Action.

What makes this thesis different?

I would like to highlight the aspects of this thesis which make it different from a lot of papers and studies that can be found in the literature of Computational Wind Engineering and microscale obstacle resolving Meteorology:

- The operational viewpoint: There are a lot of papers which give very accurate results for a simple geometry and a structured mesh, which cannot be obtained if we are facing a real urban flow and/or air quality problem. This thesis focuses on the everyday use solutions.
- Test case with a complex urban geometry: One or a few ordered blocks are the usual test cases investigated in CWE. Michelstadt, the test case used here has sharp angles, squares, like in reality, but on the other hand has very detailed and reliable flow field and passive scalar dispersion results from several source locations.
- Focus on numerical uncertainties: There are a lot of papers suggesting model improvement without taking into consideration numerical uncertainties. For simple block geometries one can hope that due to the structured mesh they are low, but for real life applications that is not acceptable.
- Automatic meshing approaches: Usually papers in CWE use only one type of mesh, which sometimes takes more effort to generate than the calculation afterwards. If we

consider operational modelling, being able to mesh any urban geometry automatically is a must.

- Short term emissions: This aspect in CWE is starting to be considered, to enable giving results suitable for emergency response modelling. Here quantities like dosage, arrival time or peak concentration are of interest.

Summary of the new scientific results in the form of thesis statements:

Thesis 1

I used a new test case for the validation of modelling flow and dispersion in urban environment with the help of computational fluid dynamics, which enables the investigation of more complex urban geometry than the previously used test cases, with the help of detailed wind tunnel measurements. I carried out a numerical experiment with steady Reynolds Averaged Navier Stokes (RANS) modelling, which incorporates operative, everyday engineering/government usage aspects that have not been detailed in literature before.

1.1: I elaborated an evaluation method which incorporates not only the accuracy of the simulation results but also the following: cost of calculation, stability of calculation, ease of automatic meshing.

1.2: With the help of the evaluation method I deduced that the meshing technique which has been newly used in the PhD studies, a body fitted, automatic hexahedral cell based technique, which refines the mesh around the geometry with cell halving, and after snaps the refined mesh to the body, is the most suitable for operational modelling of urban flow and dispersion with computational fluid dynamics, based on the criteria of 1.1.

In the thesis this topic is covered in Section 5.2

Related publication: Rakai and Franke 2012b and Rakai et al 2014b

Thesis 2

I introduced a new statistical metric, the validation rate (VR), which as opposed to the metrics used in the literature, incorporates the numerical discretization uncertainty of the simulation, when comparing the simulation and experimental results with statistical methods. For its calculation the difference between experimental and simulation results (D_i) is compared to the validation uncertainty (U_{val}) and averaged over the number of measurement points (N) in the database.

$$VR = \frac{1}{N}\sum_{i=1}^{N}\delta_i \quad \delta_i = \begin{cases} 1 & D_i \leq U_{val} \\ 0 & \text{for} \quad \text{else} \end{cases}$$

With the help of this metric, both the experimental and numerical discretization uncertainty is taken into consideration. I compared four methods based on Richardson extrapolation, which enable the calculation of numerical discretization uncertainty from the numerical discretization error with the help of a safety factor. I presented the usage of the new metric on an example of comparing two turbulence models, the standard and the realizable k-ε to evaluate and compare the model performance including the numerical discretization uncertainty.

In the thesis this topic is covered in Section 5.3

Related publication: Rakai and Franke 2012a, Rakai and Franke 2013 and Rakai and Franke 2014a

Thesis 3

I added the aspect of sensitivity to source location to the available literature on passive scalar dispersion modelling in a complex urban geometry. The investigated locations are an open square, a street canyon and a street intersection.

3.1: I analysed the most important parameter of the passive scalar dispersion model, the turbulent Schmidt number, and I found that for a source location in an open square, its optimal value is 0.7, which is different from the values suggested in the literature for simple urban geometries.

3.2: For the other two locations, the street canyon and street intersection, this value is not optimal anymore, in the street canyon no optimal value can be defined, while for the street intersection 0.5 is found to be optimal. This means that in the same wind field a location dependent parameter definition has to be given even for the same flow field.

In the thesis this topic is covered in Section 6.1

Related publication: Rakai and Kristóf 2013, Rakai and Franke 2014, Rakai et al. 2014a

Thesis 4

I investigated the use of an anisotropic model for the passive scalar dispersion (Yee et al. 2009) in a complex urban flow field, for which I implemented the model in the used computational fluid dynamics code.

4.1: Comparing the results with statistical metrics, I found that the anisotropic model can help to take into consideration the directional dependence of the dispersion, and can help to improve the results, but in case of the used test case, improvement was found only for the source in the open square. There the value of the L2 norm for the difference of the experimental and simulation results of the measurement points reduced from 0.29 to 0.23. For the sources in the street canyon and street intersection, the value of the L2 norm increased.

4.2: Based on the aspects of an operative, everyday engineering/governmental usage this model is not suitable due to numerical stability problems. Properly converged results could only be obtained for the coarsest hexahedral mesh investigated for the comparison.

In the thesis this topic is covered in Section 6.2

Related publication: Rakai and Kristóf 2011, Rakai and Kristóf 2013

Thesis 5

I extended the urban dispersion modelling with the help of computational fluid dynamics to consider not only air quality problems but also emergency response modelling, where short-term release modelling is also necessary, for the complex urban test case, investigating three different source locations. I solved the problem in a constant flow field with time dependent passive scalar transport model. I carried out sensitivity studies to spatial resolution and I found that in the more difficultly modelled street canyon and street intersection source locations the results of the dispersion simulations are very sensitive to the spatial resolution, for a too coarse mesh the plume does not reach the receptor points. With finer mesh, with a resolution of 1 m^2 cell or smaller on the surface of the buildings the simulation results with this method agree well with the experimental results of dosage based short-term release parameters. The investigated dosage and peak time for the 8 receptor points does not differ more than 65% from the experimental results except for one point, which is considered good agreement for a comparison in both space and time.

In the thesis this topic is covered in Section 6.3

Related publication: Rakai et al. 2014a

Thesis 6

I included two one-mesh error estimators in the investigation on numerical discretization error of passive scalar dispersion, which has not been used before for urban geometries. The advantage of these estimators compared to the Richardson extrapolation based methods is that there is no need to generate three different mesh densities. I compared the results of the residual and moment error estimates to the standard method based on Richardson extrapolation. The residual method estimates the numerical discretization error based on the difference of volume and cell face integrals; the moment method based on a transport equation for the second moment of the investigated variable (Jasak 1996). Comparing the estimated numerical discretization error and uncertainty of the methods I found that the one-mesh estimators give smaller values, but the moment error estimate shows similar trends to the Richardson extrapolation based method. With a suitable method to calculate the safety factor, the moment error estimate can ease the use of numerical discretization uncertainty estimation in the everyday use, which is not widespread in the literature of urban flow and dispersion modelling with computational fluid dynamics.

In the thesis this topic is covered in Section 6.4

Related publication: Rakai and Franke 2014a

Related publications:

A. Rakai and J. Franke (2014a). "*On quantification of numerical discretization uncertainty in urban flow and dispersion modelling*". In: Journal of Atmospheric Environment, in preparation

A. Rakai, E. Berbekar and J. Franke (2014a). "*RANS Passive Scalar Transport Modelling in a Complex Urban Area – Effect of Source Location on the Results*". In: 6th International Symposium on Computational Wind Engineering, June 8 - 12, 2014 - Hamburg, Germany

A. Rakai and J. Franke (2014). "*Validation of two RANS solvers with flow data of the flat roof Michelstadt case*". In: Journal of Urban Climate. DOI: http://dx.doi.org/10.1016/j.uclim.2013.11.003

A. Rakai, G. Kristóf and J. Franke (2014b). "*Sensitivity analysis of microscale obstacle resolving models for an idealized Central-European city centre, Michel-Stadt*". In: Időjárás, Journal of the Hungarian Meteorological Society 118/1, p 53-77, **IF: 0.289**

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A. Rakai and J. Franke (2013). "*Numerical error quantification of RANS modelling in an idealized Central European city centre*". In: International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes 6-9 May 2013, Madrid, Spain

A. Rakai and J. Franke (2012a). "*Validation of RANS flow models with flow data of an idealised Central-European city centre, Michel-Stadt*". In: Proceedings of Conference on Modelling Fluid Flow. Budapest, Hungary, 04/09/2012-07/09/2012

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