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

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Supervisor:
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The true delight is in the finding out rather than in the knowing.
Isaac Asimov
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Apart from the financial and technical support, a lot of people helped me during my work. The first to mention is Jörg Franke who I consider my honorary supervisor as he gave so many pieces of advice and suggestions not only during the months we worked together in Germany and Vietnam. He introduced me the test case I used for my research. My official supervisor Gergely Kristóf also helped me a lot and also let me follow my way in some occasions when I needed freedom. Special thanks to Tamás Lajos who always had some poetry in stock to overcome the difficulties and to celebrate success, to János Vad who does not let his department to sink to "honfibú" but brings rock&roll instead, and to the whole department. They provided a very pleasant and friendly working environment, not only during the office hours.

Last but not least I could not have finished without the support of my family and friends.

And thank you my dear reader for being interested in this story which spans through almost 5 years of my life. I enjoyed telling it so I hope you will equally enjoy reading it.
Abstract

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.

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. 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. The results show that the most suitable automatic meshing procedure for operational purposes is a body fitted nonconformal hexahedral mesh. I suggest a new metric based on numerical uncertainty, called validation rate, to be used for validation and model development studies. The results of the passive scalar modelling show that the generally used gradient diffusion hypothesis has a flow field dependent parameter, the turbulent Schmidt number, for which the optimal value if the source of the pollution is in an open square and the dispersion takes place in a complex urban canopy, is 0.7, but if the sources are in the urban canopy itself, the optimal value varies and the modelling has difficulties due to the underlying flow field modelling. I tried to go beyond the gradient diffusion hypothesis with anisotropic modelling, but I found that it is not suitable for operational purposes due to its numerical instability, however it can provide better statistical values in some cases. 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, and I found that the puff characteristics can be well defined even with this approach if the source volume is sufficiently small compared to the building and the geometry is well resolved.
Contents

Title page
Acknowledgement i
Abstract iii
Table of contents v
List of Symbols vii

1 Introduction 1
  1.1 Wind Engineering and Micro-Meteorology ........................................ 1
  1.2 What makes this thesis different? .................................................... 2
  1.3 Structure of the thesis ...................................................................... 2

2 Literature review 5
  2.1 Boundary Layer Meteorology, downscaling and upscaling ................. 5
  2.2 Errors, verification and validation ...................................................... 6
  2.3 Numerical uncertainty estimation in CWE ......................................... 7
  2.4 Investigation of modelling errors in CWE ......................................... 8
  2.5 Dispersion modelling .................................................................... 10
  2.6 International projects and best practice guidelines ............................ 11
  2.7 Validation test cases and their usage ............................................... 12

3 Theoretical background 15
  3.1 Governing equations ..................................................................... 15
  3.2 Discretization of the governing PDEs .............................................. 18
  3.3 Verification and validation .............................................................. 20

4 Test case – Michelstadt 31
  4.1 Wind tunnel experiment .................................................................. 31
  4.2 Computational model ...................................................................... 35

5 Results and discussion: flow field calculation 41
  5.1 Justification of the use of OpenFOAM® .......................................... 42
  5.2 A numerical experiment – tests for numerical discretization ........... 43
  5.3 Numerical uncertainty estimation and a new metric suggestion ........ 52
## Table of contents

6  Results and discussion: passive scalar dispersion calculation 63
   6.1 The key coefficient in passive scalar dispersion – the turbulent Schmidt number . . . . 65
   6.2 An attempt to go beyond the gradient diffusion hypothesis – anisotropic modelling . . . 79
   6.3 Towards emergency response – short-term releases, alias puffs . . . . . . . . . . . . . . 83
   6.4 More on numerical uncertainties: one mesh estimators . . . . . . . . . . . . . . . . . . 87

7  Conclusions 93
   7.1 Advice for operational modelers . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 93
   7.2 Thesis statements . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 94

8  Outlook 97

Index 99

Own references 101

References 103

   List of Figures 109

   List of Tables 115

A  Appendix A - Practical issues with OpenFOAM® 117
   A.1 Mesh generation . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 117
   A.2 Flow field calculation . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 118
   A.3 Passive scalar dispersion calculation . . . . . . . . . . . . . . . . . . . . . . . . . . . 120
   A.4 One-mesh error estimation for the passive scalar . . . . . . . . . . . . . . . . . . . . . 121
   A.5 Evaluation of the results . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 123

B  Appendix B - Additional figures and tables 125
# List of Symbols

Please note that in vector and tensor equations the Einstein summa convention is used.

## Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABL</td>
<td>Atmospheric Boundary Layer</td>
</tr>
<tr>
<td>ASME</td>
<td>American Society of Mechanical Engineers</td>
</tr>
<tr>
<td>COST</td>
<td>European Cooperation in Science and Technology</td>
</tr>
<tr>
<td>CF</td>
<td>Correction Factor</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>CPU</td>
<td>Central Processing Unit</td>
</tr>
<tr>
<td>CWE</td>
<td>Computational Wind Engineering</td>
</tr>
<tr>
<td>DNS</td>
<td>Direct Numerical Simulation</td>
</tr>
<tr>
<td>EWTL</td>
<td>Environmental Wind Tunnel Laboratory (of the University of Hamburg)</td>
</tr>
<tr>
<td>FS</td>
<td>Factor of Safety</td>
</tr>
<tr>
<td>GAM</td>
<td>Global Averaging Method</td>
</tr>
<tr>
<td>GCI</td>
<td>Grid Convergence Index</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>MMS</td>
<td>Method of Manufactured Solutions</td>
</tr>
<tr>
<td>MUST</td>
<td>Mock Urban Setting Test</td>
</tr>
<tr>
<td>RAM</td>
<td>Random Access Memory</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds Averaged Navier-Stokes</td>
</tr>
<tr>
<td>rms</td>
<td>root mean square</td>
</tr>
<tr>
<td>VKI</td>
<td>von Karman Institute</td>
</tr>
</tbody>
</table>

If no dimensional value is specified, the variable can have different dimensions, - means dimensionless quantity.

## Roman symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
</tr>
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<tr>
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<td>Model constants</td>
<td>-</td>
</tr>
<tr>
<td>$a_{t}$</td>
<td>Arrival time</td>
<td>$s$</td>
</tr>
<tr>
<td>$B_x$</td>
<td>Model constants</td>
<td>-</td>
</tr>
<tr>
<td>$c$</td>
<td>Passive scalar concentration</td>
<td>$kg/m^3$</td>
</tr>
<tr>
<td>$c'$</td>
<td>Variance of passive scalar concen</td>
<td>$kg/m^3$</td>
</tr>
<tr>
<td>$C$</td>
<td>Conservativeness of uncertainty estimation</td>
<td>-</td>
</tr>
<tr>
<td>$C_x$</td>
<td>Model constants</td>
<td>-</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td></td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td></td>
</tr>
<tr>
<td>$C^*$</td>
<td>Normalized passive scalar concentration</td>
<td></td>
</tr>
<tr>
<td>$D$</td>
<td>Mass transfer coefficient</td>
<td></td>
</tr>
<tr>
<td>$D_t$</td>
<td>Validation comparison error</td>
<td></td>
</tr>
<tr>
<td>$D_{jk}$</td>
<td>Turbulent mass transfer coefficient tensor</td>
<td></td>
</tr>
<tr>
<td>$dos$</td>
<td>Dosage $ppmVs$</td>
<td></td>
</tr>
<tr>
<td>$E$</td>
<td>Effectivity of uncertainty estimation</td>
<td></td>
</tr>
<tr>
<td>$E_i$</td>
<td>Experimental result</td>
<td></td>
</tr>
<tr>
<td>$E'$</td>
<td>Roughness wall function constant</td>
<td></td>
</tr>
<tr>
<td>$FAC^2$</td>
<td>Factor of two of observations</td>
<td></td>
</tr>
<tr>
<td>$FB$</td>
<td>Fractional bias</td>
<td></td>
</tr>
<tr>
<td>$FS$</td>
<td>Factor of safety</td>
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</tr>
<tr>
<td>$f_i$</td>
<td>Solution on a given spatial discretization</td>
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</tr>
<tr>
<td>$g_p$</td>
<td>Constant of power series expansion in Richardson extrapolation</td>
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</tr>
<tr>
<td>$h$</td>
<td>Average spatial discretization $m$</td>
<td></td>
</tr>
<tr>
<td>$HR$</td>
<td>Hit Rate</td>
<td></td>
</tr>
<tr>
<td>$k$</td>
<td>Turbulent kinetic energy $m^2/s^2$</td>
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</tr>
<tr>
<td>$L$</td>
<td>Reference length $m$</td>
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<tr>
<td>$L2$</td>
<td>L2 norm of difference between simulation and experiment</td>
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</tr>
<tr>
<td>$lt$</td>
<td>Leaving time $s$</td>
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</tr>
<tr>
<td>$m$</td>
<td>Skewness</td>
<td></td>
</tr>
<tr>
<td>$m_\phi$</td>
<td>Second moment of transported quantity</td>
<td></td>
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<tr>
<td>$MG$</td>
<td>Geometric mean bias</td>
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<tr>
<td>$NMSE$</td>
<td>Normalized mean square error</td>
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<td>Pressure $Pa$</td>
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<tr>
<td>$r$</td>
<td>Refinement ratio</td>
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<tr>
<td>$R_{ij}$</td>
<td>Reynolds stress tensor $m^2/s^2$</td>
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<tr>
<td>$S$</td>
<td>Face area vector $m^2$</td>
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<tr>
<td>$Sc_t$</td>
<td>Turbulent Schmidt number</td>
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<td>$S_i$</td>
<td>Simulation result (in Section 3.3)</td>
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</tr>
<tr>
<td>$S_{ij}$</td>
<td>Mean strain rate tensor $1/s$</td>
<td></td>
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<tr>
<td>$u$</td>
<td>fluctuating part of velocity $m/s$</td>
<td></td>
</tr>
<tr>
<td>$u_*$</td>
<td>friction velocity $m/s$</td>
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</tr>
<tr>
<td>$u_{fa}$</td>
<td>underrelaxation factor for velocity</td>
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</tr>
<tr>
<td>$u_{fp}$</td>
<td>underrelaxation factor for pressure</td>
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<tr>
<td>$U$</td>
<td>Estimated numerical discretization uncertainty</td>
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</tr>
<tr>
<td>$U_i$</td>
<td>Mean velocity components in tensorial equations $m/s$</td>
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<tr>
<td>$U,V,W$</td>
<td>Mean velocity components $m/s$</td>
<td></td>
</tr>
<tr>
<td>$U_E$</td>
<td>Experimental uncertainty</td>
<td></td>
</tr>
<tr>
<td>$U_{i,j}$</td>
<td>Mean velocity gradient tensor $1/s$</td>
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<tr>
<td>$u_{inst}$</td>
<td>instantaneous velocity $m/s$</td>
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</tr>
<tr>
<td>$U_{turb}$</td>
<td>turbulence intensity</td>
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<tr>
<td>$U_{num}$</td>
<td>Numerical uncertainty</td>
<td></td>
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<tr>
<td>$U_{ref}$</td>
<td>Reference velocity $m/s$</td>
<td></td>
</tr>
<tr>
<td>$u_T$</td>
<td>Wall friction velocity $m/s$</td>
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</tr>
<tr>
<td>$U_{val}$</td>
<td>Validation uncertainty</td>
<td></td>
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<tr>
<td>$VG$</td>
<td>Geometric variance</td>
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### List of Symbols

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<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
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<td>Validation Rate</td>
<td>-</td>
</tr>
<tr>
<td>$x_i$</td>
<td>Components of Cartesian coordinate in tensorial equations</td>
<td>m</td>
</tr>
<tr>
<td>$x, y, z$</td>
<td>Components of Cartesian coordinate</td>
<td>m</td>
</tr>
<tr>
<td>$y_+$</td>
<td>Nondimensional wall distance</td>
<td>-</td>
</tr>
<tr>
<td>$z_0$</td>
<td>Atmospheric roughness height</td>
<td>m</td>
</tr>
<tr>
<td>$z_{ref}$</td>
<td>Reference height</td>
<td>m</td>
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</table>

### Greek symbols

- $\alpha$: Non-orthogonality
- $\delta_{ij}$: Dirac delta
- $\partial_t$: time derivative
- $\partial_i$: space derivative
- $\epsilon_h$: Error of discretization
- $\varepsilon$: dissipation of turbulent kinetic energy: $m^2/s^3$
- $\kappa$: von Karman constant
- $\nu$: kinematic viscosity: $m^2/s$
- $\mu_t$: turbulent viscosity: $m^2/s$
- $\phi$: general conservative quantity
- $\rho$: density: $kg/m^3$
- $\sigma_x$: Model constants
- $\Omega_{ij}$: Vorticity tensor: $1/s$

### Sub- and Superscripts

- eff: effective
- $\varepsilon$: value referred to the dissipation of turbulent kinetic energy
- FS: full scale value
- $i$: component of Cartesian coordinate
- $k$: value referred to the turbulent kinetic energy
- $w$: value referred to the wall
Chapter 1

Introduction

In this thesis I am aiming to summarize the work that has been carried out during my PhD studies. Being an Environmental Engineer, my interest was in finding out to what extent Computational Fluid Dynamics (CFD) models can be used in solving everyday air quality problems. I use the term operational model to describe this everyday use, to show the difference between the applications in a government or design office and the academic research. It took me almost 5 years to carry out this work, which is unacceptably long time for an operational model. But I hope that based on this work, it will be possible to carry out air quality simulation within a much shorter time-frame in the future.

To get familiar with the topic, I introduce the two big fields of science which deal with air quality modelling.

1.1 Wind Engineering and Micro-Meteorology

Prognostic microscale obstacle resolving meteorological models and Computational Wind Engineering (CWE) models deal with the common fields of wind and pollutant dispersion modelling inside the urban canopy. Baklanov and Nuterman 2009 show that these models with increasing computational capacity can be the final scale in a nested multi-scale meteorological and dispersion model.

As we are considering two different fields of science, it is important to note some differences in terminology. In meteorology advection describes the predominantly horizontal, large-scale motions of the atmosphere, while convection describes the predominantly vertical, locally induced motions (from the glossary of the American Meteorological Society). In engineering for both directions the convection expression is used, describing the convective term in a general transport equation. In this thesis the engineering terminology is used.

Stull 1988 defines microscale in meteorology being a few kilometers or less where the typical phenomena include mechanical turbulence caused by the buildings. Britter and Hanna 2003 suggest the following length scales: regional (up to 100 or 200 km), city scale (up to 10 or 20 km), neighborhood scale (up to 1 or 2 km), and street scale (less than 100 to 200 m). The two last correspond to the microscale definition of Stull and are used in this work. These models deal with air quality forecasting and emergency response.

Computational Wind Engineering deals with engineering questions like wind load on buildings (Stathopoulos and Baniotopoulos 2007), wind comfort (Tominaga et al. 2004), and also with pollution dispersion and wind driven rain which can also be found in Micro-Meteorology.

This work deals with the intersection of the two described disciplines with the assumptions of quasi-stationary flow, neutral meteorological conditions and the pollutant is considered a passive scalar.
The focus is on the challenges of operational models. Limits for operational purpose are time con-
straints to find a solution, memory limits of general PCs, numerical stability, ease of meshing and the
quality requirement of the results. An idealized urban test case, Michelstadt, designed based on Cologne
and Hannover, is used to investigate these limits.

The main goal of the thesis: Evaluating the CFD flow and dispersion models from an operational
point of view with proper solution verification and validation to differentiate between the deficiencies of
the improper numerical resolution which is unavoidable for operational simulations and the deficiencies
of the modelling approach.

Throughout the thesis the terminology of ASME Standard for Verification and Validation in Com-
putational Fluid Dynamics and Heat Transfer (ASME 2009) will be used for verification, validation,
numerical errors and uncertainties, which will be introduced in Chapter 3.

1.2 What makes this thesis different?

To motivate the reader to continue on reading I 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 con-
  centration are of interest.

If any of these aspect is of interest, I suggest reading further to get familiar with the main chapters.

1.3 Structure of the thesis

It is not necessary to read through this work from the first until the last page if the reader is familiar with
the topic of air quality modelling with the help of CFD. I provide a short description of each chapter so
that the interesting topics can easily be chosen, and an Index can be found at the end of the thesis to help
finding definitions or clarify things during reading the main parts.

Chapter 2 reviews the current state of literature in the field of micrometeorology and CWE with a
focus on international projects and best practice guidelines, the most accepted methodology of verification
and validation and the most popular test cases used in this field. It is a very rapidly growing area where
new results appear every week, so I was trying to give an overview of the most influential papers I have read during my PhD studies.

Chapter 3 gives the most important equations and models used in the project and methodology of the evaluation of the great amount of results in a statistical way preceded by solution verification. I did not include every equation which can be found in every Computational Fluid Dynamics handbook, but I gave the reference of the ones which I have been using for each topic.

Chapter 4 introduces the test case used in this work and gives more detailed information about the experimental and numerical setups. As the Michelstadt case is a relatively new and very detailed test case, and its measurements have been carried out by several persons, I was trying to give sufficient detail about the measurements as well.

Results are shown in two separate Chapters. Flow field results with different meshing approaches, solution verification, validation of the code used in the thesis, OpenFOAM®, and a new statistical metric for validation, the validation rate, can be found in Chapter 5. It might be enough for a reader interested in only the flow field simulation for e.g. wind comfort studies. Additional results for the passive scalar dispersion calculations with details on turbulent Schmidt number dependency, anisotropic modelling, short-term releases and one-mesh numerical error estimators used for the scalar results can be found in Chapter 6.

Final conclusions are drawn in Chapter 7 with the list of the thesis statements resulting from the investigations. The thesis is closed in Chapter 8 with recommendations for future work and a list of questions that emerged in the scope of this PhD study but could not have been answered due to time restrictions.

Having familiarized with the topic and the structure, we can now go into more detail with the help of the literature review in the next chapter.
Chapter 2

Literature review

Modelling the flow and dispersion in a complex urban environment with CFD is a very challenging task due to several reasons. The literature review is built up so as to give an insight into these challenges and the most important contributions that have been carried out to solve them. These 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. This challenge is further addressed in Section 2.1.
- The improper spatial resolution results in numerical errors which are difficult to quantify and differentiate from the modelling errors. This aspect is detailed in Section 2.2 with an error topology applied in this thesis and Section 2.3.
- Modelling turbulent flow around bluff bodies, especially with a steady state approach, is difficult, this aspect is shown in Section 2.4.
- Modelling dispersion in an already probably not perfectly modelled flow field is another challenge to be faced, see in Section 2.5.

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.

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. These efforts are detailed in Section 2.6 and 2.7.

Keeping in my all these we can have a look at the literature to see what was already found to overcome these difficulties.

2.1 Boundary Layer Meteorology, downscaling and upscaling

The Atmospheric Boundary Layer (ABL) is defined by Stull 1988 as the approximately 1 km high layer above the earth surface below the free atmosphere, see Figure 2.1.
Phenomena interesting for both prognostic microscale obstacle resolving meteorological models and Computational Wind Engineering (CWE) models take place in this layer. As a high percentage of the population lives in urban areas, the description of flow and dispersion in the urban canopy gained high research interest from both research communities.

The extension of the urban canopy can reach up to 1 km in height and several kilometers in width. Meteorological phenomena which define the basic flow structures in the canopy can take even larger sizes. On the other hand the details of each building can also have a local effect on the flow field, which might be important to model.

From meteorological point of view Schlünzen et al. 2011 has shown that obstacles change the thermodynamic properties and influence mechanical properties in meteorological models. They show the parametric obstacle models used in the operational weather forecast models and the approaches to couple meso- and microscale models with their current limits and challenges. The main question which is still open according to them is the connection of the results of different scales and averaging assumptions. Yamada and Koike 2011 deals with the same issue also from meteorological point of view in a paper on downscaling meteorological models, stating that incorporating meteorology into CWE models becomes a more and more important issue.

Mochida et al. 2011 addresses the same topic from the opposite viewpoint, showing examples of up-scaling CWE models to include mesoscale meteorological influences. He states that to couple the meteorological models with CWE models, for which he suggests the use of Large Eddy Simulation (LES) which has a higher accuracy in CWE applications, the main problems to be solved are the associated computational load, the generation of instantaneous inflow turbulence and adjusting the differences in turbulence modelling.

At the moment all these suggestions about incorporating different scales have not reached a level which could be used in operational modelling for everyday use including the building obstacles explicitly. To run a calculation on a single PC in reasonable time, we have to use a steady state assumption and restrict our domain to the close environment of our urban geometry, with an assumed neutral temperature stratification to avoid solving for an additional energy equation.

### 2.2 Errors, verification and validation

When using any computational model, it is important to keep in mind that the result we find at the end of the simulation has several errors incorporated. Different communities have different error taxonomies, so for clarity the one used in this thesis is shown next.

The classification of error sources in CFD used in the Best Practice Guideline of the COST 732 Action Franke et al. 2007 is given and will be used throughout this work.
Modelling error sources:
• Simplification of physical complexity
• Usage of previous data
• Physical boundary conditions
• Geometric boundary conditions

Numerical error sources:
• Computer programming
• Computer round-off
• Spatial and temporal discretization
• Iterative convergence

The accepted approach to identify and differentiate these errors is verification and validation. This has been addressed in CFD by many authors, the most important being two recent books, Fundamentals of Verification and Validation by Roache 2009 and Verification and Validation in Scientific Computing by Oberkampf and Roy 2010 and the Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer of the American Society of Mechanical Engineers (ASME 2009). The book of Coleman and Steele 2009 discusses the same topic from the experimentation and measurement point of view giving an excellent overview of the whole validation process including measurement uncertainty estimation.

In the ASME standard, these definitions are given: "In V&V, the ultimate goal of engineering and scientific interest is validation, which is defined as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. However, validation must be preceded by code verification and solution verification. Code verification establishes that the code accurately solves the mathematical model incorporated in the code, i.e. that the code is free of mistakes for the simulations of interest. Solution verification estimates the numerical accuracy of a particular calculation."

Initial code verification with the Method of Manufactured Solutions for the simpleFoam solver of OpenFOAM®, the one used in this thesis, was carried out by Fisch et al. 2012.

This approach of V&V is not widely used in CWE but has been addressed in a detailed paper of Franke 2010a. In general the validation exercises in CWE used the concept of validation without the preceding verification steps, so the code verification and numerical uncertainty estimation was not discussed. In the following the few examples where numerical error sources were dealt with are discussed.

2.3 Numerical uncertainty estimation in CWE

As it was stated before, numerical uncertainty estimation is not widely used in CWE. However there are some examples of their usage. Mostly uncertainties are addressed as grid sensitivity analysis and checking the difference between the solutions, as in Blocken and Gualtieri 2012, while Parente et al. 2010 also quantifies solution uncertainty.

Numerical uncertainty can be interpreted as a grid sensitivity, where the different grid types are also important. Franke et al. 2012b and Hefny and Ooka 2009 are the only ones to my knowledge who compared different mesh types when investigating microscale meteorological or air quality models. Franke et al. 2012b compared a block-structured hexahedral meshing approach to an unstructured hexahedral and an unstructured hybrid mesh which consists of tetrahedral and prism elements, the latter comprising of 3 layers around the geometries. They investigated simple block geometries and rows of blocks, thus
Literature review

simpler urban arrangements than the one presented here. Their findings about the quality of the results of mean velocity components compared to experiments showed that the unstructured meshes yield often better metrics which they attributed to the higher resolution of those meshes. For the geometry of rows of blocks Franke et al. 2012b found that second order simulations with unstructured meshes are unstable. Hefny and Ooka 2009 compared hexahedral and tetrahedral elements only for a simple block geometry, and they compared the results of dispersion to each other. In their findings the hexahedral mesh had the best performance regarding estimated numerical error, but they did not compare the results to experimental values. There is no comparison for the flow field in their paper either, which determines the results of the dispersion essentially.

More detailed analysis is given for flow around buildings in Franke and Frank 2006, for a street intersection in Franke and Frank 2008, a 2D street canyon in Franke 2010b and for an array of obstacles in Schatzmann et al. 2009. Another interesting study is given by Gousseau et al. 2013 who evaluates numerical error contribution of LES computations around a high-rise building.

These examples use a relatively simple geometry compared to the one in this thesis, which makes a large difference as those geometries can have very high quality meshes. Here automatically generated meshes will be used, which are essential for operational purposes, but which call for more careful numerical uncertainty quantification.

The examples below use a Richardson extrapolation based numerical error quantification, which is the standard method suggested by ASME 2009. The problem of this approach which probably reduces the number of its users is that three different mesh densities are needed for its calculation. In academic applications this should not discourage a researcher, but for operational use a simpler method could be advantageous. The methods described in Jasak 1996, Jasak and Gosman 2003 and Juretić and Gosman 2010, namely the residual error estimator and moment error estimator are mainly used for mesh adaptation during the solution but could have a potential to be used in everyday calculations, as they require only one mesh, and can be included in the calculation itself. Roache 2009 says that single grid methods cannot be used for the verification of a code, but can be used with verified codes for the verification of individual simulations. He recommends their inclusion in all commercial codes, which is currently not the case. However they are included in the OpenFOAM® 1.7 version so they are investigated in this thesis.

2.4 Investigation of modelling errors in CWE

This is the error type that has been addressed in much more detail in the literature.

One of the greatest challenges in CWE and obstacle resolving models is that buildings act as bluff bodies, which results in the stagnation point anomaly in the turbulence modelling described by Durbin 1996. Franke et al. 2004 has shown that several ad-hoc modification of the standard $k - \varepsilon$ model have been proposed as a remedy of this problem but in general they only improved the pressure coefficients in front of the buildings but led to worse predictions of the velocities, especially in the wake of obstacles.

The most promising workaround of the stagnation point anomaly and the overestimation of the building wake was from one part overstepping the isotropic turbulence assumption of the linear eddy-viscosity approach by using nonlinear models. The models used in CWE applications are by Shih et al. 1996 and Craft et al. 1995, two examples of the modelling of flow around a single obstacle with improved results is shown in Wright and Easom 2003 and Ehrhard et al. 2000.

The stagnation point anomaly was reproduced with OpenFOAM® and turbulence model variations by Rakai 2012. Results are shown here to clarify the difficulties.

Cross section contour plots are provided about the streamwise velocity and streamlines in Figure 2.2a, 2.2b, 2.2c and 2.2d to have a better look at the phenomena. Results for the RNG $k - \varepsilon$ model with the same boundary conditions are provided to see how a linear model reacts which is modified to reduce the high turbulent kinetic energy ($k$) production in the stagnation point. The $k$ results show better
agreement with the measurement values as seen in Figure 2.3a, 2.3b, 2.3c and 2.3d but on the cost of an overestimated recirculation zone.

These model developments have been only used for simple geometries where grid generation is not problematic and high-quality structured grids can be used so solution stability is more ensured. For more complicated geometries where the users are more likely to use unstructured grids the convergence of these more complicated models is more questionable. Tominaga and Stathopoulos 2013 also state that differences between turbulence model variations are smaller in building complexes where turbulence is mainly produced by the surrounding buildings.

Another deficiency of these tests with different turbulence models is that the solution verification step was not carried out, so the numerical uncertainties are not estimated. So it is not clear how much the differences between the solution and the comparison data are due to numerical errors. To justify a model choice and its improvements the numerical uncertainties has to be excluded as much as possible with solution verification. This approach will be followed in this thesis.

Another possible way is to turn to unsteady calculations. Iaccarino et al. 2003 has shown that averaged URANS (unsteady RANS) has better results than steady RANS, especially for the reattachment region. This behaviour stems from the fact that these flows behind buildings are essentially unsteady flows with vortex shedding. Menter 2012 defines them as the classical example of globally unstable flows. Tominaga and Stathopoulos 2013 find also the URANS a promising possibility for urban simulations.

There are several examples in using unsteady calculations in CWE, but it is still too computationally demanding to be used for operational purposes. As the main goal of this work is to assess the numerical uncertainties and carry out a validation together with the solution verification for operational purposes, steady approach is used.

For air quality modelling the pollutant dispersion has to be addressed as well.
2.5 Dispersion modelling

So far we have only looked at the modelling of the flow field, which serves as a constant field in the dispersion modelling if the steady approach is used, providing the velocity vector field for the convective term of the transport equation, and the turbulence field for the turbulent diffusion term.

The general approach in CWE for air pollution dispersion modelling is adding a passive scalar transport equation decoupled from the solution of the flow field, or modelling Lagrangian particle dispersion in the computed flow field. Although this is essentially less effort than computing the flow field itself, if there are errors already in the mean velocity field, e.g. reattachment length overestimation or in the turbulent fields, e.g. stagnation point anomaly, those errors are propagated in the pollutant transport modelling. Especially the turbulent fields which are not always vital for the flow field are equally important in the dispersion model as they are responsible for the turbulent diffusion.

On the other hand in air quality forecasting models in meteorology outwash, sedimentation and reaction kinetics are usually included, with a high emphasis on pollution source inventory. These additional effects add further modelling challenges and uncertainties at the same time. The present work employs the CWE approach and only passive scalar dispersion is considered and the pollutant source is well defined.

A comparison of the Eularian additional transport equation approach and the Lagrangian approach in a single building configuration is given in Gorlé et al. 2010. They find no great difference between the two approaches, but the additional transport equation has slightly better statistical results. However the shape of the plume is significantly different between simulations and experiments. It must be added that the test case they are using has a pollutant source in the wake of the building, where the flow field modelling is already problematic, and they focus on the different modelling approaches of the flow field. Gorlé et al. 2008 has investigated the effect of turbulent kinetic energy inlet boundary conditions on the dispersion results and compared to analytical Gaussian solutions. The test case in that case was a simple boundary layer case, while in urban environments the effect of the inlet turbulent kinetic energy is smaller due to its extensive production in the shear layers around buildings.

Tominaga and Stathopoulos 2007 investigated the effect of turbulent Schmidt number on the dispersion results. The test cases they used are a free jet, a plume in the boundary layer and dispersion around
a single building. They found that a smaller value of turbulent Schmidt number, 0.3 provides better predicted results on concentration distribution around plumes in open country and around a single building, where the turbulent momentum diffusion is often underestimated when using RANS models.

In a review article Tominaga and Stathopoulos 2013 show the difficulties of near-field pollution dispersion in urban areas, where the interaction of the plume and the perturbed flow field is important. They show that in some cases in streamwise dispersion counter gradient mechanisms also appear. Gousseau et al. 2011 also focus on the details of transport, namely the different role of convective and turbulent mass fluxes and their ratio, but they focus on an isolated building which can have different important features than a complex urban area where building wakes interact.

Due to the analogy existing between transport of momentum, heat and scalar concentration, improvement methods similar to the ones for the momentum equations, and heat transfer model developments can also be applied. Anisotropic models were developed for passive scalar dispersion problems focusing on heat transfer applications and are getting more and more popular in turbomachinery, see Younis 2010. It was used in Yee et al. 2009 and Izarra 2009 for pollutant dispersion problems in atmospheric applications. Yee et al. 2009 did not compare it to isotropic models while Izarra 2009 found improvement in some cases but worse results in others, not showing clearly only advantages of the model. Both of them used the approach for more simple geometries. Yee et al. 2009 also solve an additional equation for the variance of the concentration, which has significance in emergency response modelling. Rossi et al. 2010 compare also the simple gradient diffusion hypothesis to more complex models with significant improvement, but their test case is a simple wall-mounted cube. None of these studies comment on the stability of the models though, and all of them used simple block geometries where the mesh generation is rather easy.

Similarly as Iaccarino et al. 2003 has shown that unsteady simulations can provide improved results of the flow field around a single building, Tominaga and Stathopoulos 2010 has shown that with unsteady calculations the dispersion patterns around a cube improve also substantially, even if the mean velocity field is not so different between the steady and unsteady calculations. They compare convective and turbulent diffusion fluxes for a steady RANS and an LES computation as well, and conclude that the large difference between the turbulent fluxes in the two model suggests that the accuracy of turbulent diffusion modelling is very important in predicting the mean concentration distribution. The improved results are obtained on the cost of approximately 25 times more CPU time. This is still too much for operational purpose applications, so this work deals with the possibilities of the steady approach.

A very new aspect in Computational Wind Engineering and Microscale Meteorology is short-term release, i.e. puff. It has a very important aspect in emergency response and preparedness, where the different characteristics of the puffs can have an effect on the action taken. For this kind of modelling usually more simple and less time consuming models are used, like Gaussian models, but in the future with the increasing computing resources the approach based on resolving the flow field can also gain more interest. At the moment there are only a few pioneering results on puff modelling and validation by Harms et al. 2011. The COST ES1006 Action "Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments” has a specific working group focused on this kind of model. The author of this thesis is one of the members of this group. The approach of the wind tunnel investigation of the Michelstadt case describing also short term release measurements can be found in Berbekar et al. 2013, Harms et al. 2013 and Lübcke et al. 2013.

2.6 International projects and best practice guidelines

It is a generally accepted view that CFD is a highly user sensitive and knowledge based field of modelling and to avoid the modelling errors of inexperienced users as much as possible it has been a general means
to publish best practice guidelines.

The CFD modelling community in general has issued a best practice guideline in 2000, ERCOFTAC 2000 on how to use the CFD models properly.

The COST C1-4 Action on ”Impact of Wind and Storms on City Life and Built Environment”, 2000-2004 has given recommendations on the use of CFD in Wind Engineering (Franke et al. 2004) based mostly on comprehensive literature review.

COST 732 Action on ”Quality Assurance of Microscale Obstacle Resolving Meteorological Models”, 2005-2009 issued a Best Practice Guideline (Franke et al. 2007) which also contained the experiences gained during the action.

An 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” has also plans to publish best practice guidelines based on the modelling activities of its working groups.

The Architectural Institute of Japan (AIJ) has also published a best practice guideline for practical applications of CFD to pedestrian wind environment around buildings (Tominaga et al. 2008) based on exhaustive sensitivity studies carried out.

The Association of German Engineers (VDI) has also a guideline for prognostic microscale wind field models for the evaluation of flow around buildings and obstacles (VDI 2005).

The guidelines all show the best practices to be followed if one wants to use models to define the flow in the urban canopy with obstacle resolving models. The dispersion modelling is less addressed, in Franke et al. 2007 it is stated that dispersion modelling is not addressed because specific guidelines or recommendations on that topic are not yet available from the literature. However even the accuracy of the flow models used is still an open question not only in CWE but in CFD in general, the typical CWE validation test cases to investigate this issue are shown next.

2.7 Validation test cases and their usage

Well defined boundary conditions and high-quality measurement data with low uncertainty are of vital importance for validation purposes. Schatzmann and Leitl 2011 shows that although it is a common belief that field data represent the "truth", in many cases wind tunnel data are best suited for validation purposes. So the test cases shown below are from wind-tunnel measurements.

2.7.1 Atmospheric Boundary Layer

As Atmospheric Boundary Layer properties are different from the general boundary layers, reproducing them has been in the focus in many studies. The main problem was to gain horizontal homogeneity with the synchronization of the inlet and wall boundary conditions. The most widely used boundary conditions were defined by Richards and Hoxey 1993. The efforts for lateral homogeneity are shown in Blocken et al. 2007a, Yang et al. 2007, Parente et al. 2010, O’Sullivan et al. 2011, Sumner and Masson 2010, Richards and Norris 2011 and Balogh et al. 2012.

2.7.2 Single block

There are several wall mounted cube experiments which are used for validation. The two most famous databases which are publicly available, and were carried out in an atmospheric boundary layer with tunnel, thus providing realistic boundary conditions, are from the Environmental Wind Tunnel Laboratory of the University of Hamburg. (the data can be found at

http://www.mi.uni-hamburg.de/CEDVAL-Valid.427.0.html and
http://www.mi.uni-hamburg.de/CEDVAL-LES-V.6332.0.html)
Most model evaluations were carried out for this test case, they were discussed in detail in Section 2.4.

### 2.7.3 Array of blocks

Both datasets mentioned in the previous section also contain regular array of blocks. This is an increase in complexity but is still not the real challenge for meshing due to the ease of adding blocks to the regular arrays. The most famous test case of this type is MUST (Mock Urban Setting Test) which has been used in COST 732 Action.

### 2.7.4 More realistic urban geometries

For an extensive list of field and wind tunnel test cases the reader is referred to Britter and Schatzmann 2007 and *COST ES1006 Background and Justification Document* 2012. In the COST 732 Action the Joint Urban 2003 test of Oklahoma city was modelled in wind tunnel by the EWTL of Hamburg. The other comprehensive database, AIJ also contains real urban test cases, Niigata and Shinjuku.

One of the conclusions in the COST 732 Action was that a complexity between the regular blocks and a real city is needed, which encouraged the completion of a new test case, the one also used in this work, Michelstadt, a geometry based on Cologne and Hannover, but idealized. More details are given in Chapter 4.

This concludes the most important aspects of the literature of flow and dispersion modelling in urban environment. In the next chapter we will go through the theoretical background of this field listing the most important equations and relations.
Chapter 3

Theoretical background

Before we move on to the interesting part of the thesis, it is important to clarify the used equations and methods. This is a rather dry part which can be skipped if the reader is familiar with the topics, and can be used as a reference when reading the results of the simulations. There are however some important definitions of the used terminology in Section 3.3 which might be used differently in certain scientific communities. This includes verification, validation, the difference between numerical error and uncertainty. This terminology I suggest to refresh before reading the main part to avoid misunderstandings.

Symbols and parameters are defined in the text with the equations when they first appear, but the reader can always find them in the List of Symbols chapter of the thesis if they come across them at a later point.

3.1 Governing equations

When describing turbulent flows the following Reynolds decomposition is used.

\[ u_{\text{inst}} = U + u \]  

(3.1)

Where the instantaneous velocity \( u_{\text{inst}} \) is decomposed to a mean value \( U \) and a fluctuating value \( u \). See Wilcox 1993 for further reference on statistical averaging of variables and the equations.

3.1.1 Transport equations and closure problem

Incompressible turbulent flows are governed by the Reynolds averaged continuity and Navier-Stokes equations:

\[ \partial_t U_i = 0 \]  

(3.2)

\[ \partial_t U_i + \partial_j (U_j U_i - \nu U_{i,j} + \overline{u_i u_j}) = \frac{\partial p}{\rho} \]  

(3.3)

The closure problem is caused by the fact that when averaging the equations, new correlation terms of the fluctuating velocities emerge, what are called the Reynolds stresses, \( R_{ij} = \overline{u_i u_j} \) (Wilcox 1993).

The constitutive relations used for the closure of the models for the \( k - \varepsilon \) two equation models are as follows:

For the turbulent kinetic energy, \( k \):
\[
\partial_t k + \partial_j (U_j k) = -\nu_i \nu_j U_{i,j} + \partial_j \left( \frac{1}{\sigma_k \varepsilon} \frac{k}{\nu_i \nu_j} \partial_j k \right) - \varepsilon \quad (3.4)
\]

For its dissipation rate, \( \varepsilon \):

\[
\partial_t \varepsilon + \partial_j (U_j \varepsilon) = -C_1 \varepsilon \frac{k}{\nu_i \nu_j} U_{i,j} + \partial_j \left( \frac{1}{\sigma_\varepsilon \varepsilon} \frac{k}{\nu_i \nu_j} \partial_j \varepsilon \right) - C_2 \varepsilon^2 \frac{\varepsilon}{k} \quad (3.5)
\]

In case of modelling a quasi-stationary flow with a steady state approach, the time dependent terms in Equation 3.3-3.5 disappear.

### 3.1.2 Linear closure

The equation for the Reynolds stresses in the linear eddy viscosity models is the following.

\[
R_{ij} = \nu_i \nu_j = \frac{2}{3} k \delta_{ij} - \nu_t (U_{i,j} + U_{j,i}) \quad (3.6)
\]

where the turbulent viscosity is modelled as:

\[
\nu_t = C_\mu k^2 \frac{\varepsilon}{k} \quad (3.7)
\]

\( C_\mu = 0.09 \) is constant in the standard \( k - \varepsilon \) model, the other model coefficients are \( C_1 \varepsilon = 1.44 \), \( C_2 \varepsilon = 1.92 \), \( \sigma_k = 1.3 \), \( \sigma_\varepsilon = 1.0 \). For more explanation on different closure types and turbulence models the reader is referred to Wilcox 1993 for a comprehensive explanation and ERCOFTAC 2000 for a short overview.

### 3.1.3 Realizability constraints and stagnation point anomaly

The non-realizability of the standard \( k - \varepsilon \) model means that it can produce negative values for the diagonal of the Reynolds-stresses as defined if

\[
\nu_t (U_{i,j} + U_{j,i}) \geq \frac{2}{3} k \delta_{ij} k \quad (3.8)
\]

which is not physical as they are squares. This suggests problem in high shear flows.

The stagnation point anomaly means that the two-equation models predict a too large growth of \( k \) in stagnation point flows also due to high shear.

From the model equations Durbin 1996 found that in case of high velocity gradients the production of \( k \) grows, and the production of \( \varepsilon \), basically the same term multiplied by a constant \( C_1 \varepsilon \) and the reciprocal of the turbulent time scale \( \frac{k}{\varepsilon} \) (see Equation 3.5), cannot follow this production as the turbulent time scale becomes also very large and reduces the production of \( \varepsilon \).

This phenomena is important in urban flow simulations as the flow around buildings has high shear areas due to separation and reattachment.

### 3.1.4 Passive scalar dispersion

The Eulerian approach is considered for the calculation of passive scalar dispersion. This means that we are solving an additional transport equation for a scalar quantity that has no feedback to the flow field. Due to this passive behaviour this equation can be decoupled from the main flow equations.

The transport equation for mean passive scalar concentration \( c \):

\[
\partial_t c + \partial_j (U_j c) = f \quad (3.9)
\]

where \( f \) is the source or sink term.
\[
\partial_t c + \partial_j (u_j \cdot c) = \partial_j(D \cdot \partial_j c) - \partial_j(\overline{u_j c'}) + Q \tag{3.9}
\]

The closure of the turbulent scalar flux term, which emerges due to the averaging of the instantaneous equation just like the Reynolds stress tensor term in the momentum equation, has a general form:
\[
\overline{u_j c'} = -D_{jk} \partial_k c \tag{3.10}
\]

In most of the cases in CWE \(D_{jk}\) is defined as a scalar field computed from the turbulent viscosity with \(Sc_t\) turbulent Schmidt number. This is the simple gradient diffusion hypothesis, where the direction of the diffusion is driven only by the gradient of the pollutant.
\[
D_{jk} = \frac{\nu_t}{Sc_t} \tag{3.11}
\]

But it can also be defined as a tensor using an anisotropic approach as in Yee et al. 2009.
\[
D_{jk} = C_{s1} k^2 \delta_{jk} + C_{s2} k^3 (U_{j,k} + U_{k,j}) \tag{3.12}
\]
\[
C_{s1} = 0.134, \quad C_{s2} = -0.032 \tag{3.13}
\]

This is the tensor form used in this thesis, but several other closures are possible, with different coefficients as well, see other variations in Izarra 2009.

For the passive scalar transport equation a time dependent solution can be used in the constant flow field. For continuous release a steady solution is looked for by monitoring the change of the passive scalar concentration in certain points. For short-term releases the time evolution of the passive scalar concentration is the property that we are interested in. For the stability of the time marching solution of the transport equation the Courant-Friedrichs-Lewy criteria has to be monitored in the cells with a typical size \(\Delta x\) and a typical velocity \(U\) and the time step \(\Delta t\) must be chosen to keep the CFL ratio defined in Equation 3.14 under 1.
\[
CFL = \frac{U \Delta t}{\Delta x} < 1 \tag{3.14}
\]

For the comparison of experimental and simulation results a normalized concentration, \(C^*\) is defined in Equation 3.15.
\[
C^* = \frac{e \cdot U_{ref} \cdot L^2}{Q_{source}} \tag{3.15}
\]

It is \(Q_{source}\), the source strength which is a function of the cell volume which is set as volume source.

In case of short-term emission, it is more difficult to compare the resulting puffs. The comparison at the same location is then more demanding due to time dependence. The puffs are characterized based on their dosage as suggested by Harms et al. 2011. The parameters such as arrival time (at), peak time (pt), leaving time (lt), dosage (dos) and peak concentration (pc) are explained in Figure 3.1. The arrival time is defined as the time after release when the dosage exceeds the threshold of 5%. The leaving time is defined as the time when 95% of the total dosage is reached.
3.1.5 Initial and boundary conditions

To be able to solve the governing equations, initial and boundary conditions are very important. They are discussed in detail for the test case in Section 4, here only the wall boundary condition is discussed to clarify the meaning of wall functions.

Wall functions are used if the wall region cannot be resolved due to cell number limitations for example. In urban applications where large scales are addressed and the extension of the computational domain is in the order of kilometers, this is the only operationally feasible approach. An important parameter to see if the wall resolution is sufficient to use wall functions is the nondimensional wall distance, $y^+$, defined in Equation 3.16 with the help of the wall friction velocity $u_τ$ and the normal distance from the wall $y$. Usually a minimum value of $20 − 30$ is required to justify the use of wall functions (ERCOFTAC 2000).

$$y^+ = \frac{y \cdot \rho \cdot u_τ}{\mu} \quad \text{(3.16)}$$

For more details on wall functions and other boundary conditions in CFD the reader is directed to Wilcox 1993 and ERCOFTAC 2000.

3.2 Discretization of the governing PDEs

As was stated before, numerical discretization has an effect on the results of the solution due to numerical discretization error. In complex geometries its exact quantification is difficult as no analytical solution of the governing equations exists, but with a numerical experiment the effect can be investigated. In the following the mesh type, spatial resolution and the convective term discretization is explained. All the meshes considered are generated automatically which is a necessity for using this model for operational purposes and general building configurations.

3.2.1 Spatial discretization

Four mesh types are considered:

- unstructured full tetrahedral Delaunay mesh generated with ANSYS® Icem
- unstructured full polyhedral mesh created by ANSYS® Fluent from the tetra mesh
Theoretical background

- Cartesian hexahedral mesh created with snappyHexMesh of OpenFOAM®
- Body fitted hybrid mesh with mostly hexahedral elements meshed with snappyHexMesh of OpenFOAM®

More details on the generation of the meshes are given in Chapter 4.

3.2.2 Mesh quality

If we would like to resolve complex geometries properly, a compromise in mesh quality is unavoidable. This can cause a decrease both in the numerical accuracy and the stability of the computations, for more detail see Jasak 1996.

Some general measures on mesh quality to keep in mind when creating a mesh are the following:

- Cell aspect ratio
  Ratio of longest to shortest edge length is best to keep close to 1.

- Expansion ratio/cell volume change
  Ratio of the size of two neighbouring cells is best to keep under 1.3 in regions of high gradients (Franke et al. 2007).

- Non-orthogonality
  Angle $\alpha$ between the face normal $\vec{S}$ and $\vec{PN}$ vector connecting cell centers $P$ and $N$ is best to keep as low as possible, see in Figure 3.2.

![Figure 3.2: Graphical representation of non-orthogonality ($\alpha$) and skewness ($m$) in a 2D nonconformal grid](image)

- Skewness
  Distance between face centroid and face integration point (where flux is evaluated by weighting cell centroid values) is best to keep as low as possible, see $m$ in Figure 3.2. In OpenFOAM® this value is normalized by the magnitude of the face area vector $\vec{S}$. 
3.2.3 Discretization of the convective term

The discretization of the convective terms of the transport equations solved is an important source of numerical discretization error. Upwind schemes use the value of the upwind cell as face value for the flux calculation (Jasak 1996).

Central differencing uses a linear interpolation of the upwind and downwind cell value for the face value, which is of higher accuracy but may be unstable. Other schemes are defined as combination of the two for an optimal compromise between accuracy and stability (Jasak 1996), like linearUpwind (a first/second order, bounded scheme (OpenCFD Limited 2011)) in OpenFOAM® or second order upwind in ANSYS® Fluent (Ansys 2009).

It is important to note here that using higher order schemes of the convective terms for meteorological models is not straightforward. E.g. in the MISKAM® model (version 5), which is a microscale operational model for urban air pollution dispersion problems only upwind-differences are used for the discretization of the advection terms in the momentum equations (Eichhorn 2008). Janssen et al. 2012 also shows that for certain meshes the use of higher order terms can cause convergence problems so users may be forced to use lower order discretization. He suggests a not automatically generated hexahedral mesh to avoid this problem.

3.3 Verification and validation

To gain confidence in any kind of numerical model verification and validation is unavoidable. The definition given earlier in Chapter 2 by the Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer of the American Society of Mechanical Engineers is repeated here for convenience: "In V&V, the ultimate goal of engineering and scientific interest is validation, which is defined as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. However, validation must be preceded by code verification and solution verification. Code verification establishes that the code accurately solves the mathematical model incorporated in the code, i.e. that the code is free of mistakes for the simulations of interest. Solution verification estimates the numerical accuracy of a particular calculation.”

3.3.1 Code verification

Code verification is suggested to be carried out by the Method of Manufactured Solutions (MMS). It is designed to investigate whether the code solves the intended equations. The simpleFOAM solver of OpenFOAM® was verified in Fisch et al. 2012 so this is not addressed here in more detail.

3.3.2 Solution verification

Solution verification estimates the numerical error and/or uncertainty of a particular solution (ASME 2009). There are several possible methods to carry out this task. The standard method based on Richardson extrapolation and its variants will be shown as well as methods which require only one mesh to estimate numerical error, which are less accepted. But first a very important definition have to be clarified.

Difference between error and uncertainty

Before going into details about the numerical uncertainty estimation, it is important to differentiate between error and uncertainty. The explanation from the book of Oberkampf and Roy 2010 is used here: "In cases where numerical errors cannot be estimated with a great deal of reliability (as is often the case
Theoretical background

in scientific computing), while they are still truly errors, our knowledge of these errors is uncertain. Thus when numerical error estimates are not reliable, they can correctly be treated as epistemic uncertainties. That is, they are uncertainties due to a lack of knowledge of the true value of the error.”

This is important to keep in mind that quantifying the numerical discretization error is not a goal of this work. We aim only to estimate the uncertainty of the numerical discretization of the different meshes to show the users of CWE models (i) to what extent it is possible, (ii) that it gives additional information.

Standard method

The most widely used and established methods are based on Richardson extrapolation. The basic idea of the Richardson extrapolation is that from a power series expansion around an exact value ($\tilde{f}$) with at least two different spatial discretization ($h$) the error of the discretization ($\epsilon_h$) can be calculated with a system of algebraic equations. For this the order of the discretization ($p$) must be known and $h$ must be small enough so that its higher order powers are substantially smaller (e.g. $h^{p+2}$ in Equation 3.17), which is regarded as the asymptotic range of the refinement. This will be discussed in more detail but for now the estimated error by the generalized Richardson extrapolation (Roy 2010):

$$\epsilon_h = f_h - \tilde{f} = g_p h^p + g_{p+1} h^{p+1} + g_{p+2} h^{p+2} + ... \quad \text{(3.17)}$$

The greatest difficulty of this method is that the order of discretization, $p$ cannot be guaranteed to have the theoretical order until the refined meshes are in the asymptotic range. To check this three systematically refined meshes (this will be discussed in detail later) are used and the observed order of accuracy is calculated.

For that calculation refinement ratios need to be defined (Celik et al. 2008):

$$r_{12} = \frac{h_2}{h_1}$$

$$h = \left[ \frac{1}{N} \sum_{i=1}^{N} (\Delta V_i) \right]^\frac{1}{3} \quad \text{(3.18)}$$

For cases where $r_{12} = r_{23} = r$ (1 means the finest mesh) the observed order can be calculated from this equation (Phillips and Roy 2011):

$$\hat{p} = \frac{\ln \left( \frac{f_3 - f_2}{f_2 - f_1} \right)}{\ln (r)} \quad \text{(3.19)}$$

With $f_1$, $f_2$ and $f_3$ being the numerical solution on the finest, medium and coarsest grid, respectively. The different behaviour of the solutions and the problem of order calculation with this method can be seen in Figure 3.3. On the left side three different behaviour of the results from mesh refinement can be observed (i.e. results as a function of grid spacing), on the right the calculation of the observed order from their ratios as defined by Equation 3.19.

Looking at the graph on the left hand side the impression is that all three types of points are approaching a similar exact value. However, if we want to calculate the observed order for an oscillatory point (defined by $(f_3 - f_2)/(f_2 - f_1) < 0$) we can see that the logarithm is not defined for negative values in Equation 3.19 so no order can be given. This is denoted by the black area on the right hand side. Divergent points (defined by $0 < (f_3 - f_2)/(f_2 - f_1) < 1$) are also problematic as they result in negative values for the order calculation, see the dark gray area in the right hand side of Figure 3.3. To include these points in the numerical uncertainty estimation special treatment of these types is needed.
Theoretical background

Even if we consider the convergent points \((1 < (f_3 - f_2)/(f_2 - f_1))\) some problems can be observed. The formal order of accuracy \(p_f\) and a limit for accuracy \(p_l\) is also shown, marking the borders of the area which is the theoretical solution for the order. To understand this look at Equation 3.20 for the estimated error.

\[
\hat{\epsilon} = \frac{|f_2 - f_1|}{r^\hat{p} - 1}
\]  
(3.20)

As the order approaches zero, the error approaches infinity. To avoid unrealistically large error estimates Phillips and Roy 2011 determined a lower limit by looking at error estimates from cases with analytical solution. They also give an upper limit to avoid vanishingly-small discretization error estimates.

No special treatment for converged nodes is applied. If the ratio of the solutions \((f_3 - f_2)/(f_2 - f_1)\) gave 0 result at machine accuracy it is treated by adding a small number to avoid division by 0 in later calculations.

Before explaining in detail the methods used to define an uncertainty from the different types of points, the assumptions for Richardson extrapolation by Roy 2010 are given here, with comments on how this can be maintained for a realistic urban geometry calculation:

- Results in the asymptotic range
  "Definition": where the dependent solution variables converge at the formal order of accuracy.

This is investigated by the three mesh densities. If \(r_{12}\) and \(r_{23}\) are not equal, iteration is necessary.

\[
\hat{p} = ln \left[ \left( r_{12}^{\hat{p}} \right) \left( \frac{f_2 - f_1}{f_2 - f_3} \right) + r_{12}^{\hat{p}} \right] \\
ln(r_{12}r_{23})
\]  
(3.21)
In real problems it is not likely that all the points will converge with the formal order of accuracy, e.g. Schatzmann et al. 2009 for the MUST case found 30 – 50% total divergence depending of the investigated variables.

It can also be argued that point to point order estimation should not be used. One of the methods described later suggests global order values. Another approach could be to calculate order from integral quantities of the flow field like average or maximum values. However in this work those methods were chosen which have already been tested with a comparison to analytical values, so their performance in estimating the numerical error is known for at least simple test cases.

- **Uniform mesh spacing**
  The theory is based on a typical length, $h$, which should be constant. In real problems it is used as in Equation 3.18:

- **Systematic mesh refinement**
  Two criteria are available:
  - UNIFORM: refined by the same factor over the whole domain. In urban geometries with automatic grid generation this cannot be fully fulfilled but was kept as much as possible.
  - CONSISTENT: mesh quality remains or improves with refinement.

- **Smooth solution**
  Richardson extrapolation is based on solution derivatives, so it breaks down in the presence of discontinuities. For this case no discontinuities are expected.

- **Other numerical error sources**
  Be at least two order of magnitudes smaller.

### From estimated error to uncertainty

Grids in the asymptotic range are often difficult to achieve for practical engineering applications. In such cases Phillips and Roy 2011 suggest to account for the uncertainty of the discretization error estimate by converting it to an uncertainty estimate which is considered as a $+/-$ range centered about the fine grid solution usually multiplied with a factor of safety. They describe several methods but all are based on the following (note that the only difference between Equation 3.20 and 3.22 is $FS$ the factor of safety):

$$U = FS\frac{|f_2 - f_1|}{r^p - 1}$$

The difference between the methods is mainly the treatment of solutions outside of the asymptotic range with the choice of $p$ and $FS$, see details in the descriptions and collected in Table 3.1.

After Phillips and Roy 2011 diverging points are treated as oscillatory in all calculations to obtain numerical uncertainty estimation for them as well. For oscillatory points if no special treatment is mentioned when describing the methods, the order of accuracy is set to the lower limit $p_l$. If not stated otherwise the suggested limit is $p_l = 0.5$.

1. **Grid Convergence Index (GCI-Roy)**
   This method was developed by Roache 1994, and is used with the recommendations of Oberkampf and Roy 2010. They suggest $FS = 1.25$ if $\hat{p}$ within 10% of $p_f$, otherwise $FS = 3.0$ and $p = \min(\max(p_l, \hat{p}), p_f)$. 
24 Theoretical background

### Table 3.1: Choice of factor of safety ($FS$) and order of grid convergence ($p$) for the different methods to estimate numerical uncertainty from the estimated numerical error

<table>
<thead>
<tr>
<th>Method</th>
<th>Conditions</th>
<th>$FS$</th>
<th>$p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Roy GCI</td>
<td>$\hat{p}$ within 10% of $p_f$ otherwise</td>
<td>$FS = 1.25$</td>
<td>$p = p_f$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$FS = 3.0$</td>
<td>$p = \min(\max(p, \hat{p}), p_f)$</td>
</tr>
<tr>
<td>Global Averaging</td>
<td>$(f_3 - f_2)(f_2 - f_1) &gt; 0$ otherwise</td>
<td>$FS = 1.25$ same</td>
<td>$p = \frac{1}{N} \sum_{i=1}^{N} \min(\max(0.05, \hat{p}_i), p_f)$</td>
</tr>
<tr>
<td>Factor of Safety</td>
<td>$0 &lt; \hat{p}/p_f \leq 1$</td>
<td>$FS_1 \cdot \hat{p}/p_f + FS_0 \cdot (1 - \hat{p}/p_f)$</td>
<td>$\hat{p}_{FS} = \max(p, \hat{p})$</td>
</tr>
<tr>
<td>Correction Factor</td>
<td>$0 &lt; CF \leq 0.875$ and $CF \geq 1.125$</td>
<td>$9.6(1 - CF)^2 + 1.1$</td>
<td>$\hat{p}$</td>
</tr>
<tr>
<td>Oscillatory and divergent nodes</td>
<td>$\hat{p}/p_f &gt; 1$</td>
<td>$2[1 - CF] + 1$</td>
<td>$\hat{p}$</td>
</tr>
<tr>
<td></td>
<td>$U_{CF} = 0.5(S_U - S_L)$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

$p_f = 2$, $p_t = 0.5$, $\hat{p}$ computed order, $CF = \frac{n^{p_f-1}}{n^{p_t-1}}$, if not specified oscillatory nodes taken with $p = 0.5$

2. **Global Averaging (GA) Method**

This method, suggested by Cadafalch et al. 2002, uses an averaged order of accuracy for the investigated domain. The global observed order of accuracy is calculated by averaging the observed orders of accuracy at the Richardson nodes, which they define as $(f_3 - f_2)(f_2 - f_1) > 0$. Note that this includes the divergent nodes in Figure 3.3 so the negative observed orders of accuracy are also averaged. To avoid this Phillips and Roy 2011 expanded the averaging as $p = \frac{1}{N} \sum_{i=1}^{N} \min(\max(0.05, \hat{p}_i), p_f)$. They also included the oscillatory points in the numerical discretization uncertainty estimation with the same order of accuracy as used for the Richardson nodes. $FS = 1.25$ is used for all points.

3. **Factor of Safety (FS) Method**

Developed by Xing and Stern 2010, this method changes the factor of safety as a function of the observed order of accuracy (see in Table 3.1). No lower or upper limit was specified by them, but Phillips and Roy 2011 used the lower limit given before for consistency. The variation of $FS$ can be seen in Figure 3.4.

4. **Correction Factor (CF) Method**

Similarly to the previous method here also a function is defined (see in Table 3.1). The lower limit $p_t$ is also used here. Oscillatory and divergent nodes are treated by $U_{CF} = 0.5(S_U - S_L)$ where $S_U$ and $S_L$ are the upper and lower bounds of the solution for more than three solutions. Here only three solutions were available but the same method was used. The variation of $FS$ can also be seen in Figure 3.4.

To evaluate these uncertainty estimators Phillips and Roy 2011 compared $U$ to the real numerical error $\epsilon_{total}$ on test cases with the exact analytical or a very fine numerical solution available. They used effectiveness index (Eqn. 3.23) and conservativeness ratio (Eqn. 3.24) to find an optimal uncertainty estimator:

$$ E = \frac{||\epsilon_{total}||_{L2}}{||U||_{L2}} \quad (3.23) $$

$$ C = \frac{N}{n} = \frac{1}{n} \sum_{i=1}^{n} N_i \quad \text{with} $$

$$ N_i = \begin{cases} 1 & \text{for } \frac{\epsilon_{total}}{U} \leq 1 \\ 0 & \text{else} \end{cases} \quad (3.24) $$
They found that no optimal estimator is available, so I decided to investigate the behaviour of all of them in my thesis. In complicated cases, like our case-study, where exact solution is not available, which happens very often in engineering practice and is the main goal of these numerical applications, the estimated uncertainty can be used as an additional information for validation to compute validation uncertainty (Eça and Hoekstra 2008a) or can give additional information about the reliability of the solution. There is still active ongoing research in this area which will expectedly increase the acceptance of the numerical error and uncertainty estimation methods.

**Non standard method: one-mesh error estimators**

Generating three different mesh resolutions to have an idea about the numerical discretization uncertainty is a tedious work and is very often overlooked, especially in industrial applications. As the aim of this research is to give guidance for operational modelling, being used for everyday urban design problems, it can be useful to investigate one-mesh estimators, which might be less accurate or accepted, but do not put the burden of three mesh generation and calculation on the practitioner.

The methods chosen here are the residual error estimate and the moment error estimate from Jasak 1996. It is important to note, that these are only error estimates, no safety factor is incorporated and to the knowledge of the author there were no efforts to derive safety factors for these methods. So they differ in this point from the uncertainty estimates worked out based on the Richardson extrapolation which are the standard method described before. For a possible comparison a safety factor have to be defined.

The description of these error estimators follows:

- Residual error estimate is based on the difference of the linear change inside a cell for volume integration (in case of second-order discretization) and the linear interpolation between two cells, see Figure 3.5 (Jasak and Gosman 2003). The face value $\phi_f$ can be defined based on the neighbouring cells of cell $P$, see solid line parallel with the dashed line connecting the neighbours. But it can also be defined based on the value of the cell center of $P$ and $N$. If the variation of the transported quantity is higher than second order, the two values will not be the same. This is the main idea of the residual error estimate, for more details and the normalization procedure see Jasak 1996.

- Moment error estimate is based on the investigation of conservation properties of the second moment ($m_\phi$) of transported conservative quantities ($\phi$), writing a transport equation for them as well. More details can equally be found in Jasak 1996.

\[ m_\phi = \frac{1}{2} \phi^2 \]  

(3.25)
Theoretical background

Figure 3.5: Inconsistency between face interpolation and the integration over a cell, the basis of residual error estimation method (from Jasak 1996)

The disadvantage of this method, is that although the same second moment equation can be written for vector quantities as well, the resulting estimated error is scalar also for vector quantities.

For this reason these methods will only be investigated for the passive scalar transport equation and its numerical discretization errors emerging in the simulations\(^1\).

3.3.3 Validation metrics

Three levels of validation metrics are shown. One without considering either the experimental or the numerical uncertainties, based on \(L^2\) norm, one taking into account only the experimental uncertainty, the most widely used hit rate metric and finally a new validation metric which incorporates both experimental and numerical discretization uncertainty, implemented in this thesis, the validation rate.

\(L^2\) norm

Using matrix norms for comparison is the simplest approach. With \(L^2\) norm the negative values of velocity components are not problematic. This metric can be seen as a normalized relative error of the whole investigated dataset.

\[
L^2 = \frac{\sqrt{\sum_{i=1}^{n}(E_i - S_i)^2}}{\sqrt{\sum_{i=1}^{n}E_i^2}}
\]  

(3.26)

\(E_i\) and \(S_i\) are the corresponding experimental data and simulation results in the \(i\)th experimental point.

Hit rate

The most widespread metric in CWE (see e.g.: VDI 2005, Parente et al. 2010, Schatzmann et al. 2009) for wind velocity data is hit rate, which can be defined as in Equation 3.27, where \(S_i\) is the prediction of the simulation at measurement point \(i\), \(E_i\) is the observed experimental value and \(W\) is an allowed absolute deviation, based on experimental uncertainty. \(N\) is the total number of measurement locations.

\[
HR = \frac{1}{N} \sum_{i=1}^{N} \delta_i
\]

\(^1\)For more details on OpenFOAM® implementation settings see Appendix A
The theoretical background

$$\delta_i = \begin{cases} 1 & \text{for } \left| \frac{S_i - E_i}{E_i} \right| \leq 0.25 \text{ or } |S_i - E_i| \leq W \\ 0 & \text{else} \end{cases}$$ (3.27)

The allowed relative deviation in Equation 3.27 was used as 25% first in the VDI guideline (VDI 2005) and from thereon this value is used by the CWE community.

A disadvantage of the hit rate metric is that it takes into consideration only the experimental uncertainty and it is sensitive to the used allowed experimental uncertainty (W) value. More detail on this can be found in COST ES1006 Background and Justification Document 2012. When comparing different simulations with the same allowed threshold values, differences can equally be seen.

**Metric based on validation uncertainty: validation rate**

Validation uncertainty, based on both experimental and numerical uncertainty is proposed for the 3\textsuperscript{rd} Workshop on CFD Uncertainty Analysis (Eça and Hoekstra 2008b) and adapted in the ASME standard for verification and validation (ASME 2009). The procedure compares two quantities:

- the validation uncertainty, an estimate of the standard deviation of the parent population of the combination of all errors except the modelling error in S and E (Equation 3.28 can only be used if the uncertainties are effectively independent, and parameters in simulation and experiment are not shared. For shared error sources the propagation equations of the discrete uncertainties has to be combined, see ASME 2009 for more detail)
  \[ U_{val} = \sqrt{U_{\text{num}}^2 + U_{\text{input}}^2 + U_E^2} \] (3.28)

- validation comparison error
  \[ D_i = S_i - E_i \] (3.29)

The strong model concept is used, i.e. \( U_{\text{input}} = 0 \), see Eça and Hoekstra 2008b. This concept is explained in Roache 2009: Model in a general sense, often termed as weak model, is the general mathematical formulation, e.g. the incompressible Navier Stokes equations. Model in a specific sense, often termed as strong model, includes all parameter values, boundary and initial conditions needed to define a particular problem.

The procedure identifies deficiencies in the modelling when:

\[ D_i > U_{val} \] (3.30)

The concept is illustrated in Figure 3.6. Here the offset of a comparison point from the 45° line in a scatter plot is the validation comparison error, and a point is declared "validated" with the given experimental and numerical settings, if this offset is smaller than the validation uncertainty, i.e. when the circle around the point touches the line.

If the aim of a project is model development, Equation 3.30 is necessary to carry on with the development, otherwise improved experimentation or numerical discretization is necessary.

I suggest a new metric, the validation rate, which is defined for several comparison points similar to the hit rate metric:

\[ VR = \frac{1}{N} \sum_{i=1}^{N} \delta_i \]

\[ \delta_i = \begin{cases} 1 & D_i \leq U_{val} \\ 0 & \text{else} \end{cases} \] (3.31)

}\}
3.3.4 Validation metrics exclusively used for air quality models

The following metrics suggested by Chang and Hanna 2004 are widely used for air quality model evaluation, not only for CFD models but also for more simpler models, like Gaussian plume models.

- **FAC2**: factor of 2 of observations
  \[
  FAC2 = \frac{N}{n} = \frac{1}{n} \sum_{i=1}^{n} N_i \quad \text{with}
  \]
  \[
  N_i = \begin{cases} 
  1 & \text{for } 0.5 \leq \frac{S_i}{E_i} \leq 2.0 \\
  0 & \text{for otherwise}
  \end{cases}
  \]

- **FB**: fractional bias
  \[
  FB = \frac{E - S}{0.5(E + S)}
  \]

- **MG**: geometric mean bias
  \[
  MG = \exp \left( \ln \tilde{E} - \ln \tilde{S} \right) \quad \text{with } \tilde{E} = \max(W, E) \quad \text{and } \tilde{S} = \max(W, S)
  \]

- **NMSE**: normalized mean square error
  \[
  NMSE = \frac{(E - S)^2}{E \cdot S}
  \]
• VG: geometric variance

\[ VG = \exp \left[ \left( \ln \tilde{E} - \ln \tilde{S} \right)^2 \right] \quad \text{with} \quad \tilde{E} = \max(W, E) \quad \text{and} \quad \tilde{S} = \max(W, S) \quad (3.36) \]

With these we reached the end of definitions and equations which I found necessary to be familiar with, to understand the rest of the thesis, the more interesting part. So now we can start to deal with a complex urban area, Michelstadt, and the flow and dispersion inside its urban canopy.
Chapter 4

Test case – Michelstadt

Simulating atmospheric flow and dispersion phenomena in an urban environment is a very complex challenge, which I already addressed in Chapter 2 listing the main problems involved. When choosing the Michelstadt test case, my motivation was to find something which is reliable not only for a general evaluation of my model, but also for a validation in the sense that was shown in Section 3.3, which involves the quantification of experimental uncertainty. Using a wind tunnel measurement campaign for this purpose is often criticized, stating that I am not comparing to the real problem. However, as the real problem is extremely complex, using a field measurement campaign for validation purposes is problematic due to the question of experimental uncertainty quantification. Schatzmann and Leitl 2011 have shown in their paper the statistical variability of field measurement data, and they show that for the field measurements reproducibility of a measurement is more of concern than the inaccuracy of the instrument, which is often used exclusively for the uncertainty quantification. As the RANS simulations represent ensemble averaged values, I believe that for proper point-to-point comparison at the first stage it is best to compare to an average value of the measurement which is calculated from a statistically representative ensemble of measurements, or from long enough time series for the time average. This is difficult to obtain in a field campaign where the wind speed and direction may vary rapidly, so I am using a wind tunnel dataset which has been generated for time dependent model evaluation, so contains sufficiently long time series. As a next step, comparison to field data is planned for urban flow and dispersion modelling, but not in the scope of this thesis. So now I will introduce the complex urban geometry, Michelstadt.

4.1 Wind tunnel experiment

Michelstadt is an idealized Central European city centre inspired by Hannover and Cologne, a complex urban geometry with non-parallel streets, different building heights. In the COST Action 732 (Schatzmann et al. 2009) the more simple MUST case and a more complex (a part of Oklahoma city) test-case was used, and it was found that an in-between complexity would be beneficial. See the increasing complexity of the wind tunnel models in Figure 4.1. In the COST Action ES 1006 on the Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments (http://www.elizas.eu/) the Michelstadt case is used for the first evaluations.

Two component LDV (Laser Doppler Velocimeter) measurements were carried out in the Environmental Wind Tunnel Laboratory of the University of Hamburg to investigate the flow field. They are part of the CEDVAL-LES database (http://www.mi.uni-hamburg.de/Data-Sets.6339.0.html) which consists of different complexity datasets for validation purposes. This case, Michelstadt, is the most complex case of the dataset. There are two versions of it, one with flat roofs and another
with slanted roofs, in this work the flat-roof case is used.

A detailed description of the flow measurements can be found in Hertwig et al. 2012, here only the most relevant details are summarized. 2158 measurement points are available for the flow field, they can be seen in Figure 4.2. They consist of 40 vertical profiles (10-18 points depending on location for each), 2 horizontal planes (height 27m and 30m, 225 measurement points for each) and 3 so-called street canyon planes.
planes (height 2m, 9m and 18m, 383 measurement points for each), which are located inside the urban canopy.

The two available components are the streamwise and lateral velocity component, and time series are available for each of them. The dataset also contains the statistically evaluated mean, rms and cross-correlation values for comparison with steady state computations.

Dispersion measurements were carried out in the framework of COST Action ES 1006. Different source locations were used, from which here results for source S2, S4 and S5 (see Figure 4.4) are calculated. 58 measurement locations were measured for source S2, 25 for S4 and 22 for S5, which can also be seen in Figure 4.4. A constant plane at height z = 7.5m was measured and at three locations for S2 vertical profiles are also available. More details on the dispersion measurements can be found in Berbekar 2013 and Berbekar et al. 2013.

The source is built in the wind tunnel’s floor, see Figure 4.3. From operational point of view to model the source geometry is not very likely to be used, so this was not included in the mesh generation.

![Figure 4.3: Source geometry in the wind-tunnel (from EWTL)](image)

(a) Source mounted in the wind tunnel
(b) Design of the source geometry

For the continuous emission all the measurement points (Figure 4.4) were used to measure time series of the concentration, which were evaluated by the measurement team to provide mean concentration value for the comparison.

For the short-term release emission, i.e. puff measurements only a limited number of the measurement points were used, as for them around 200 repetitions per measurement point are necessary to have an acceptable mean value for the puff characteristics. The points where puffs were also measured are shown in Figure 4.5 for the three source locations separately.

The duration of the continuous release measurements and the number of the released puffs ensure the statistical representativeness of the results.

Approach flow data are provided from 3 component velocity measurements. The approach flow is modelled as an atmospheric boundary layer in the wind tunnel with the help of spires and roughness elements.

For the investigated Michelstadt case, the allowed absolute uncertainty $W$ (see Equation 3.27 in Chapter 3) was defined by Hertwig et al. 2012 for the streamwise and lateral normalized velocity component (0.0165 for $U/U_{ref}$ and 0.0288 for $V/U_{ref}$), and 0.00434 is used for $U_{rms}/U_{ref}$ and 0.00874 for $V_{rms}/U_{ref}$) as was given by the experimental team. For the concentration the uncertainty is given in percentage due to the wide scale of the possible values, it is given as 11.16% for a confidence interval of 90% based on repetition measurements.

It must be noted that in earlier publications different values were used (see Efthimiou et al. 2011, Franke et al. 2012a and Rakai and Franke 2012b) which were double checked and reconsidered by the
Figure 4.4: Michelstadt with dispersion measurement points coloured differently for all used sources (2, 4 and 5), profile locations P7, P11 and P32 for source 2 highlighted.

experimental team.
4.2 Computational model

The computational domain was defined to correspond with the COST 732 Best Practice Guideline (Franke et al. 2007) (Fig. 4.2), which resulted in a $1575 \times 900 \times 168$ m domain, with a distance of the buildings of $11H_3$ from the inflow, $9.4H_3$ from the outflow and at least $6H_3$ from the top boundaries, where $H_3 = 24$ m is the highest building’s height. The computations were done in full scale, while the experiment was done at a scale of 1:225. The dependence of the results on this scale change was investigated by Franke et al. 2012a using both full scale and wind tunnel scale simulations and only a small difference in the statistical validation metrics was observed.

As Roache 1997 explains, the governing partial differential equations (PDE) and their numerical solution both add up to the total error of the simulation. For the estimation of the numerical uncertainty, the governing PDEs were kept the same during all the numerical experiments and are as follows.

As inflow boundary condition, a power law profile (exponent 0.27, with a reference velocity $U_{ref} = 6.11$ m/s defined at $z_{ref} = 100$ m) fitted to the measured velocity values was given. This corresponds to a surface roughness length $z_0 = 1.53$ m. Britter and Hanna 2003 define this as a very rough or skimming approach flow. The turbulent kinetic energy and its dissipation profiles were calculated from the measured approach flow values by their definition and equilibrium assumption. At the top of the domain the measurement values corresponding to that height were fixed. The lateral boundaries were treated as smooth solid walls, as the computational domain’s extension is the same as the wind tunnel width. The floor, roughness elements and buildings were also defined as smooth walls. Standard wall functions were used. As the roughness elements are included in the domain there is no need to use rough wall functions for the approach flow and also the problem of maintaining a horizontally homogeneous ABL (Atmospheric Boundary Layer) profile, which is reported (Blocken et al. 2007b) to be problematic for this kind of modelling, is avoided. Franke et al. 2012a have shown in a further investigation that this is not necessary as the flow is governed by interacting with the first buildings. They compared modelling the roughness elements explicitly and implicitly and found little influence on the results. The same conclusion was found by An et al. 2013. For the sake of using the same computational setup throughout the thesis, I did not remove the roughness elements from my model even after these findings.
The steady Reynolds Averaged Navier Stokes Equations were solved with standard k-ε turbulence model and the SIMPLE (Semi-Implicit Method for Pressure Linked Equations) method was used for pressure-velocity coupling (Jasak 1996).

The solution of the passive scalar dispersion was decoupled from the flow modelling. It was carried out according to Equation 3.9 with both the traditional gradient diffusion hypothesis closure of Equation 3.11 and the anisotropic closure of Equation 3.12. A constant volume source of one cell was defined as the closest point to the centre of the source in the wind tunnel. This results in different sizes of volume source depending on the resolution of the mesh, as will be discussed later. Calculations were run with the time dependent solver passiveScalarFoam of OpenFOAM®, modified for the turbulent dispersion equations1. Runs were carried out with the Courant number always smaller than 1, until a converged dispersion field was reached.

Four mesh types are compared, their visual appearance is illustrated always for Building 33, highlighted in Figure 4.2. All the meshes were generated automatically which is a necessity for using this model for operational purposes and general building configurations:

- unstructured full tetrahedral Delaunay mesh generated with ANSYS® IceM
  For the creation of the Delaunay volume cells, first an Octree mesh was created and kept only at the surfaces, the Delaunay mesh was grown from that surface mesh. The coarsening of the meshes was carried out by scaling the defined minimum length scales in ANSYS® IceM by 1.6. Resolution of buildings was given by the minimum face and edge size on each building. The maximum allowed expansion ratio was given for the Delaunay algorithm.

- unstructured full polyhedral mesh created by ANSYS® Fluent from the tetra mesh
  The polyhedral meshes were converted from the original tetrahedral meshes by ANSYS® Fluent. Each non-hexahedral cell is decomposed into sub-volumes called duals which are then collected around the nodes they belong to in order to form a polyhedral cell (see Ansys 2009 for more details). The refinement ratio is thus kept very similar to the one in case of the tetra meshes.

- Cartesian hexahedral mesh created with snappyHexMesh of OpenFOAM®
  As the main research tool for these investigations is OpenFOAM®, its open-source meshing tool is also used for mesh generation. This is done first by creating a Cartesian castellated mesh by refining around a given .stl file and deleting cells inside the geometry. This mesh was also investigated in the studies, as the generation process for this one in much faster than for any of the other meshes mentioned. Building resolution cannot be given explicitly only the resolution of the starting domain and the number of refinement iteration cycles.

- body fitted hybrid mesh with mostly hexahedral elements meshed with snappyHexMesh of OpenFOAM®
  The Cartesian mesh is snapped to the edges of the geometry as a next step, which takes approximately 10 times more time as the creation of the original source mesh. 2

The grid convergence performance of the meshes was also investigated, at least 3 different resolutions were used for each mesh type. This makes it possible to use them for numerical uncertainty estimation with Richardson extrapolation.

The cell numbers of the investigated meshes can be found in Table 4.1. The size of the volume sources for source S2 used for the dispersion calculations can be found in Table 4.2. As the non-dimensional concentration, $C^*$ (see Equation 3.15) is used for comparison, the different size of source volume causes no problem if we are far away from the source.

---

1see more practical details in Appendix A
2For some practical OpenFOAM® issues see Appendix A
Another important property of the meshes is the $y^+$ value (see Equation 3.16), the dimensionless distance from the wall in the center of the first cell, which is important to monitor when we want to use wall functions. For this test case, only in case of the finest meshes was $y^+$ below the value of 30, the theoretical limit for the validity of the wall function (see ERCOFTAC 2000), reached in a limited number of cells. The average value of $y^+$ varies from 5000 for the fine meshes to 20000 for the coarsest hexahedral meshes.

<table>
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<tr>
<th></th>
<th>coarsest</th>
<th>finest</th>
</tr>
</thead>
<tbody>
<tr>
<td>polyhedral</td>
<td>1.73 (P3)</td>
<td>6.17 (P1)</td>
</tr>
<tr>
<td>tetrahedral</td>
<td>6.65 (T3)</td>
<td>26.79 (T1)</td>
</tr>
<tr>
<td>Cartesian hexahedral</td>
<td>2.39 (H4,C)</td>
<td>14.23 (H1,C)</td>
</tr>
<tr>
<td>body fitted hexahedral</td>
<td>2.4 (H4)</td>
<td>27.52 (H0)</td>
</tr>
</tbody>
</table>

Table 4.1: Cell numbers (million cells) of the investigated meshes

For source S2, the size of the volume sources $[m^3]$ is as follows:

<table>
<thead>
<tr>
<th></th>
<th>coarsest</th>
<th>finest</th>
</tr>
</thead>
<tbody>
<tr>
<td>polyhedral</td>
<td>46.98</td>
<td>1.014</td>
</tr>
<tr>
<td>tetrahedral</td>
<td>4.321</td>
<td>0.514</td>
</tr>
<tr>
<td>Cartesian hexahedral</td>
<td>6.59</td>
<td>0.202</td>
</tr>
<tr>
<td>body fitted hexahedral</td>
<td>5.74</td>
<td>0.176</td>
</tr>
</tbody>
</table>

Table 4.2: Size of the volume sources $[m^3]$ for source S2
Figure 4.7: Mesh sections in street canyon at ground level for the coarsest meshes

What was discussed in this Chapter about the test case experiments and the details of computations is sufficient to turn eventually to the results of the research project on the modelling of flow and dispersion in urban areas within the scope of operationally feasible models.
Figure 4.8: Mesh cross sections at $y_{FS} = 0m$
Chapter 5

Results and discussion: flow field calculation

After all the introduction to the literature, theoretical background and the test case, the discussion of the results can start at last. I will deal with the flow field calculations in this chapter, while the dispersion results are in a separate one, Chapter 6. The reason for this is that they have essentially different aspects in their evaluation, although the dispersion relies on the flow field. The flow field can be considered as a vector field of velocity and a symmetric tensor field of the Reynolds stress tensor, which means a large amount of data, even if we only consider the 2158 measurement points.

For this reason I will rely on statistical quantities of the computations, showing pure flow data in profiles or vectors only in a few cases. Qualitative comparison is important to understand the characteristics of the flow field, but to draw any conclusions, I think that quantitative comparison is a must.

In the first section of the flow field results, 5.1, the justification of the use of OpenFOAM® will be given. One may say that any CFD code should give the same results for a Fluid Dynamics problem, so the choice of the program is just a personal preference, but in my opinion it is important to compare with other codes, especially with an open source code, like OpenFOAM®. It was important for this reason to carry out not only model validation, but a model-model intercomparison to have sufficient confidence in the code OpenFOAM®, which has not been widely used for atmospheric flow simulations at the time when I started my PhD.

After this part I will explain the details and results of the numerical experiment in Section 5.2, carrying out the simulations on four different mesh types and at least three resolutions for each, comparing their performance from an operational point of view. That means I focus not only on the accuracy of the results, but also on the memory and CPU time need, numerical stability and the ease of the meshing, all aspects that are interesting for a model which aims to be used in everyday design or regulatory procedures.

Finally in Section 5.3 I will finish the flow field investigations with the numerical uncertainty estimation. I implement a new statistical metric, validation rate, to broaden the validation process with the result of the numerical uncertainty estimation. To understand the added value of this estimate and the new metric, I will show results from a model change from standard to realizable $k-\varepsilon$.

Before going further I would like to remind the reader to the convention of symbol use in figures introduced in Figure 4.6. It is also important to keep in mind that experimental results are available for only two components of the velocity vector, so the compared quantities are always derived from them: streamwise and lateral mean velocity, in some cases their root mean squares and cross-correlation terms, i.e. Reynolds stress components. Without having experimental results for the third component of the velocity, any assumption to calculate the turbulent kinetic energy, $k$, for comparison would add an additional uncertainty to the comparison, which is avoided.
5.1 Justification of the use of OpenFOAM®

For operational modelling an open source general purpose CFD code without limitation in parallelisation is more suitable than a commercial software. However before using the results for decision making it is a must to check the quality of the results. To gain confidence in the OpenFOAM® code I was comparing the flow field results to the results of ANSYS® Fluent, a code which has already been widely used and validated for atmospheric urban flow modelling (see Schatzmann et al. 2009 and Franke et al. 2012b). The comparison was done in cooperation with Jörg Franke who provided the Fluent results. We also compared to the wind tunnel experiments. The final conclusion was that OpenFOAM® can be used for building resolving urban simulations, published in Rakai and Franke 2012b, Rakai and Franke 2012a and Rakai and Franke 2014b.

All possible effort was made to have the same numerical and model settings for the two codes used, ANSYS® Fluent and OpenFOAM®, described in Section 4.1. Due to the convergence problems which will be analyzed later, those result were compared which use second order differential schemes for the momentum equation and upwind for the turbulent equations. The fully converged results are used as well later with OpenFOAM® but with Fluent no special effort was made as it was not the aim of the model intercomparison.

<table>
<thead>
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<th>medium</th>
<th>fine</th>
</tr>
</thead>
<tbody>
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<td>0.68/ 0.68</td>
</tr>
<tr>
<td></td>
<td>tetrahedral</td>
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</tr>
<tr>
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<td>0.78/ 0.78</td>
<td>0.79/ 0.78</td>
</tr>
<tr>
<td></td>
<td>tetrahedral</td>
<td>0.82/ 0.80</td>
<td>0.82/ 0.82</td>
</tr>
</tbody>
</table>

Table 5.1: Hit rates for OpenFOAM® / Fluent

In Table 5.1 the hit rate metrics ¹ are compared for all the tetrahedral and polyhedral meshes described in Table 4.1. It can be seen that taking real care of the settings gives almost identical metric values for the two different code. Not all numerical settings could be matched due to different discretization schemes available in the two codes, but these results with this complex geometry justify the choice of OpenFOAM®.

In Figure 5.1 a vertical profile comparison is also shown to prove the good agreement between the two codes. The location of the profile can be seen in Figure 4.2.

This profile is in the courtyard of a building, so recirculation modelling problems can also be observed for the streamwise velocity profile. For the lateral velocity close to the ground another problem appears, a wrong flow direction is predicted by the results. However as these properties appear for both numerical codes the final conclusion of this part of the research was to carry out all further simulations and investigations with OpenFOAM®.

¹Here the values 0.033 for $U/U_{ref}$ and 0.0576 for $V/U_{ref}$ were used as at the time of the first publication those were the official values. This does not effect the model intercomparison.
Results and discussion: flow field calculation

5.2 A numerical experiment – tests for numerical discretization

The next part of the investigation was to evaluate the numerical modelling from an exhaustive list of viewpoints for operational modelling. These were chosen to be mesh quality with an effect on numerical stability, the computational cost with regards to RAM and CPU time, and quality of the results compared to experiments. I found that the body fitted hexahedral mesh which has not been used before for these kind of application gives the best compromise taking into considerations all the operational requirements, and the main factor responsible for numerical instability is the mesh non-orthogonality.

5.2.1 Mesh quality: result on numerical stability and iterational convergence

The grid quality measures explained in Chapter 3 are investigated first for the mesh types used for the computations. The values of the mesh quality metrics are shown in Figure 5.2 as a function of the number of cells. They were computed by the checkMesh utility of OpenFOAM®.

Maximum aspect ratio is highest for the polyhedral mesh, the tetrahedral and body fitted hexahedral one is approximately half of it, while the Cartesian hexahedral mesh has an average aspect ratio of 1 as can be expected.

The non-orthogonality is highest for the tetrahedral meshes, followed by the polyhedral ones, while all hexahedral based meshes have a constant value of $10^\circ$. Although these meshes are mainly Cartesian where $0^\circ$ value is expected, by halving the cells this rule is broken for different sized neighbours. In Figure 3.2 it can be observed how this effects the non-orthogonality. The angle for a transition of this kind in 2D can be computed, as the ratio of the edges is $1 : 3$, as can be seen in the Figure. This results in an angle of approximately $20^\circ$, which is averaged with the rest $0^\circ$ values resulting in this $10^\circ$ average.

Maximum skewness is the highest for the body fitted hexahedral mesh. For this metric no average value is given by the utility, it shows only the values of the worst quality cells. In that mesh cells with skewness vector 3 times greater than the face area vector occur.

Minimum cell volume and face area decrease vary rapidly with the increase of resolution. The creation of polyhedral mesh is done by splitting the tetrahedral first, so smaller volumes and face areas occur in case of the polyhedral meshes. This can also be seen in Figure 4.6.

About the expansion ratio it can be said that it was set to maximum 1.3 in case of the tetrahedral meshes. For the snappyHexMesh meshes neighbouring cells can differ by a factor of 2 in edge length due
Results and discussion: flow field calculation

Figure 5.2: Different mesh quality metrics plotted as a function of cell number for the four different mesh types (recall labelling in Figure 4.6)

to halving cells when refining locally. For unstructured meshes the cell volume change in neighbouring cells is a more useful indicator of the smoothness of transition between smaller and larger cells. In case of the tetrahedral meshes the majority of this cell volume change is below 2, while for the polyhedral meshes 6-8% of the neighbours have a cell volume change more than 10. For the hexahedral meshes the cell volume change is below two in 90% of the neighbours and a jump appears around 7-8 due to the refinement method of cell halving which is expected in 3D.

These properties are far from defining an ideal mesh, so they effect substantially the iterative convergence behaviour and the numerical stability of the computations. Reaching convergence in complicated geometries and low quality meshes is not always trivial, and in case of this test case, the first computations were often not successful. The best way to reach convergence for all of the cases was found to be the following: the case was initialized with a potential flow solution, and first the calculation was run in first order for all convective term of variables (denoted -11 later) until convergence. After the mean velocity was changed to second order, the turbulence remaining first (denoted -21 later), until the convergence of this setup. Finally all convective terms were set to the second order version to reach the final convergence (denoted -22 later).

In cases of tetra- and polyhedral meshes the simulations were unstable also with the described method with default relaxation factors (0.3 for \( p \) and 0.7 for the other variables). The cases had to be drastically underrelaxed to reach convergence (0.1 for \( p \) and 0.3 for the other variables). As in the Best Practice Guideline for ERCOFTAC (European Research Community On Flow, Turbulence and Combustion) special interest group “Quality and Trust in Industrial CFD” (ERCOFTAC 2000) it is suggested to increase the relaxation factors at the end of the solution to check if the solution holds, we checked it for one of the converged underrelaxed simulations. It is also important because Ferziger and Perić 2002 has shown that the optimum relation between the underrelaxation factors for velocities \( (u_f) \) and pressure \( (u_f) \) is...
$u_f p = 1 - u_f u$. With raising the relaxation factors each time by 0.1 the combination of 0.2 for $p$ and 0.6 for the other variables were reached but with the default combination the computation crashed again. For this reason results with the low relaxation factors were investigated.

The difference between the convergence behaviour of the hexahedral and polyhedral based meshes is not only their stability. Residual history is smoother for the hexahedral meshes, which makes them a more suitable tool for operational modelling, where robustness is a big advantage and can save a lot of time for the user.

It is an important question what may cause the instability of the tetrahedral and in one case also the polyhedral simulations. Looking at the quality metrics of the meshes one similar behaviour was found for the non-orthogonality of the meshes, which can be seen in Figure 5.2. It is clear that the tetrahedral meshes have the highest non-orthogonality followed by the polyhedral meshes, what can cause the instabilities. This indicates that gradient discretization can also be problematic. Ferziger and Perić 2002 show that in the discretization of non-orthogonal grids of the general transport equation mixed derivatives arise for the diffusive term. They say that if the angle between gridlines is small and aspect ratio is large the coefficients of these mixed derivatives may be larger than the diagonal coefficients, which can lead to numerical problems. The checkMesh utility of OpenFOAM® reports the number of cells above the non-orthogonality threshold, which is given as 70° as a default. Although the tetra meshes have higher averages of non-orthogonality, their maximum values never reached this threshold. For the polyhedral ones on the other hand there were around 10 highly non-orthogonal cells in each mesh.

<table>
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<tr>
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</tr>
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</tr>
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<td>2500</td>
</tr>
<tr>
<td>Cartesian hexahedral-21</td>
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<td>Cartesian hexahedral-22</td>
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</tr>
<tr>
<td>body fitted hexahedral-22</td>
<td>+1000</td>
<td>+1000</td>
</tr>
</tbody>
</table>

Table 5.2: Necessary iterations for convergence of the steady state flow field calculations (full upwind-11/mixed-21/full linearUpwind-22)

The convergence behaviour of the meshes in general is explained in Table 5.2 where the necessary number of iterations is shown for each mesh, separately for the first order initialization (full upwind-11)/linearUpwind for momentum, first order for turbulence variables (mixed-21)/all higher order (full linearUpwind-22) variations. Convergence is considered when a plateau is reached in the residuals for all variables. For the meshes where the residuals were not smooth, other variables were also checked to stay stable.

What can be observed is that more iteration is necessary for more cells to reach the first converged state what can be expected for linear solvers. The outstanding value of 5000 for the medium poly mesh can be explained by the instability of the computation which made heavy underrelaxation necessary.

In general the iteration numbers are of the same order of magnitude for all of the meshes. The most orderly results are given by the body fitted hexahedral meshes, which underlines again their robustness for operational simulations.

No big difference can be seen between the body fitted and Cartesian hexahedral meshes, but in some
Cases with the last some periodic oscillation occurred. This oscillation reduced for the higher order computations, see Figure 5.3.

![Figure 5.3](image_url)  
**Figure 5.3**: Residual behaviour of a Cartesian mesh: first jump in residuals is caused by changing from full upwind to second order for only mean values, second jump by changing to full second order.

Turning to the value of the residual norm and its drop from the beginning of the computation it was observed that this case is too complex and values do not reach the machine accuracy in single precision mode. The lowest drop is found in each case for the Poisson equation for the pressure, followed by the lateral and vertical mean velocity component. Another general observation is that all values drop below $10^{-5}$ for the first order calculations except for the pressure, while for the linearUpwind only for the momentum equation this drop is usually smaller, followed by a drop below $10^{-5}$ again for the full linearUpwind computations. The continuity error had a similar behaviour, but the first drop was usually below $10^{-8}$ (see Figure 5.3 for graphical explanation).

This behaviour can be explained by the categorization of Menter 2012 who states that the classical example of a globally unstable flow is the flow past bluff bodies (like the buildings). Because of this unsteadiness periodical changes in the residuals are appearing even if the boundary conditions are steady, like in our case.

### 5.2.2 Computational cost: memory need and CPU time

One of the main goals is to compare the models from an operational purpose point of view. When carrying out simulations for e.g. a government, it is usually not possible to wait several days until the simulation is finished on a cluster and numerical stability is of high importance. For this reason the computational costs are also evaluated.

The results of this analysis for all of the meshes can be seen in Figure 5.4. What is apparent is that the memory usage scales linearly for all of the meshes, and the difference in the mesh types can be explained by the relative number of cell faces, i.e. the poly mesh uses more memory for a given number of cells, while the tetrahedral mesh uses less. There is no significant difference between the two kinds of hexahedral meshes, but it is important to note that the solver itself takes no benefit from the fact that one
of them is Cartesian.

![Graph](image)

Figure 5.4: Computational cost (memory usage - left and CPU time - right) of the simulations for the full upwind simulations, 4000 iterations

For the comparison of the CPU time only the relative values are interesting, and it can be seen that the CPU time demand scales linearly with the number of cells, and there is no significant difference in the mesh types. These comparative simulations were carried out on the new cluster of the University of Siegen (http://www.uni-siegen.de/cluster/index.html?lang=en), run for 4000 iterations with first order upwinding for all variables on 24 cores. As a rule of thumb for this setup it can be said that a simulation result can be obtained in 1 hour/1 million cells. Those meshes which were unstable with the default relaxation factors are omitted from the CPU-time graph.

5.2.3 Accuracy of the solution: Sensitivity to discretization in view of different metrics

Metrics are unavoidable when comparing a lot of different variations, but it is better to check with different metrics to reveal if one of them is biased. The metrics described in Chapter 3 are used to compare the performance of 4 mesh types, 3-5 spatial resolutions and 3 discretization scheme combinations for the convective term of the transport equations.

Hit rate results for all the cases investigated are shown in Figure 5.5 as a function of the number of cells, the underlying values can be found in Appendix B in Table B.1 if the reader is interested, as here the figure helps to evaluate the trends. The metric based on L2 normalization can be seen in Figure 5.6 also as a function of the number of cells.

Comparing the hit rate metric results in Figure 5.5 and the L2 norm metric results in Figure 5.6 it is important to note that in case of the hit rates a "1 - HR" is shown to make them visually similar. Thus on both figures the smaller is the better. However, the interpretation is very different. In case of the hit
rate figure a smaller value means that more points became "hits", the difference between simulation and experiment getting to the acceptable range. Once a point is in this range, the hit rate will not improve even if the results get closer to each other. On the other hand, for the L2 norm metric a smaller value means that the difference between simulation and experiment got smaller.

For the absolute value of the hit rate metric for the mean velocity values it can be said that these high hit rates are good results for this complex case. Similar values were found by Efthimiou et al. 2011 for two other codes, Andrea® and Star-CD®, and by Franke et al. 2012a and Rakai and Franke 2012b for the ANSYS® Fluent code for the mean velocities. In the VDI guideline (VDI 2005) an acceptable HR value is given for certain test cases, thresholds and measurement points, but it is not easily transferable to a totally different case.

The absolute value of the L2 norm metrics can be interpreted as a kind of relative error, showing that for the streamwise velocity results, where the values are essentially higher, the metric is smaller than for all the other variables. For the conclusions drawn later the absolute value of this metric is not considered.

The conclusions which can be drawn from Figure 5.6 of the L2 metric norm:

1. For streamwise velocities, tetrahedral meshes perform outstandingly better.

   From theoretical point of view the smallest numerical error is expected from the hexahedral meshes (Juretić and Gosman 2010). The reason for this is shown by Juretić and Gosman 2010 to be because the hexahedral mesh is aligned with the flow, so the errors in fluxes are cancelled. Explanation for the superior performance of the same mesh size for the tetrahedral meshes in this case can be that those were made with the Delaunay algorithm, so they are not "wasting" so many cells in the middle of the domain where there is no geometric feature to disturb the flow, so the gradients
Results and discussion: flow field calculation

Figure 5.6: Sensitivity to discretization evaluated with the L2 metric for four flow variables, streamwise and lateral mean velocities and their rms values (full upwind-11/mixed-21/full linearUpwind-22).

are small and do not make high mesh resolution necessary. In case of the hexahedral meshes the underlying original mesh block has a quite high density. This can be seen in the two coarse meshes compared in Figure 5.7. Also seen is that the transition of tetrahedral cells is smoother from the fine to the coarse cells, and above the canopy where shear layers are present, the hexahedral meshes are not fine enough. See Figure 5.8 for the visualization of these gradients above the urban canopy. A line is shown in Figure 5.7 below which high gradients occur in the solution.

Franke et al. 2012a used also a block-structured hexahedral mesh for their investigations with ANSYS® Fluent and had better performance also in the mean velocities. That mesh is not automatically generated and has very different mesh quality metrics than the automatic snappy-HexMesh meshes (Average non-orthogonality 2.64, maximum skewness 1.47 and smooth cell volume transition). The worse result of the automatic hexahedral meshes can be explained by their larger and lower quality cells in the most important regions shown in Figure 5.7.

2. This is not so apparent for lateral velocity, and disappears for the rms values.

To understand better this phenomenon Figure 5.8 shows the profiles compared at location 29 (see Figure 4.2) which is in the yard of a 18 m high building. In the non-dimensional scale 0.18 is the top of the building and it can be observed that changes in streamwise mean velocity reach 0.4, while for the other values the maximum is 0.3. So the smoother transition of the tetra mesh can help to resolve better the streamwise velocity but for the other values it is not so important. The oscillations on the profiles for the tetra meshes can be found on other profiles computed with OpenFOAM® as well. They may be a consequence of the instability of the simulations, however for the ANSYS® Fluent results they not appear. This phenomenon needs further investigation.
50 Results and discussion: flow field calculation

Figure 5.7: Tetra (6.65 \cdot 10^6 cells) and hexa (8.0 \cdot 10^6 cells) mesh cross sections (diagonal lines are just visualization tool specific features in the hexa mesh), red horizontal lines indicate the height up to which high shear occurs.

Figure 5.8: Profile 29 (recall location in Figure 4.2) of one tetra (6.65 \cdot 10^6) and hexa (8.0 \cdot 10^6) mesh (full second order discretization for the convective scheme), results for all measured flow variables.
3. Full second order solutions perform better already for the mean values, but that difference competes with the CPU-time cost of the results. For the turbulent quantities however, full second order solutions are outstanding.

Theoretically this is obvious as higher order terms are more accurate but on the other hand this can amplify the errors in the modelling assumptions. In the Michelstadt case the higher order results for the simulation always compare better to the experimental values. It must be kept in mind that not all micrometeorological models use higher order advective terms. As the turbulent quantities are used for the dispersion calculations it can have a significant effect and higher order terms are suggested.

4. Polyhedral meshes have very low performance compared to all the other cases if not full second order discretization is used.

This can be a result of the larger volumes in those meshes and the large cell volume changes explained, strengthening the numerical errors. It is suggested to use polyhedral meshes only with higher order convective terms, as those metrics are comparable with the other mesh types.

5. The Cartesian hexahedral meshes have lower performance in the mean velocities but this disappears for the turbulent statistics.

More comparable results for rms value prediction needs further investigation. This can be caused by the generally wrong rms predictions for all mesh types and the numerical errors canceling the modelling errors.

6. There is a jump of low performance for the second coarsest hexahedral meshes which is visible both in the hit rate metric and in the L2 norm metric.

This is a sign that mesh refinement does not always lead to improved solutions because of the error cancellation explained above. Also the importance of investigation of mesh dependency on more meshes must be noted.

5.2.4 Discussion

For operational modelling not only the highest quality results are necessary, an optimum in computational time, numerical stability and result quality has to be reached so a trade-off is necessary, a decision to be made by the consulting engineer. A summary of the four mesh types and their behaviour is given in Table 5.3. This table shows the method of evaluating the meshing procedure from operational point of view, giving a poor value to the parameter if that meshing procedure is not advised for operational modelling, OK if that behaviour is sufficient, and very good if that was remarkable during the evaluation procedure. From the results shown here it can be concluded that for complex geometries where automatic meshing is a difficulty and necessity at the same time, the hybrid body fitted hexahedral meshes generated by snappyHexMesh prove to be the most stable choice. At the same time their quality in the flow field computation is not considerably worse than that of the tetrahedral meshes. The CPU-time needed is a similar function for both kind of meshes and for fast what-if scenario comparisons even the coarsest meshes can give an acceptable solution provided that they resolve the building blocks properly.
Results and discussion: flow field calculation

<table>
<thead>
<tr>
<th></th>
<th>polyhedral</th>
<th>tetrahedral</th>
<th>Cartesian hexahedral</th>
<th>body fitted hexahedral</th>
</tr>
</thead>
<tbody>
<tr>
<td>numerical stability</td>
<td>OK</td>
<td>poor</td>
<td>very good</td>
<td>very good</td>
</tr>
<tr>
<td>meshing time and ease</td>
<td>poor</td>
<td>OK</td>
<td>very good</td>
<td>OK</td>
</tr>
<tr>
<td>PC memory need</td>
<td>OK</td>
<td>very good</td>
<td>very good</td>
<td>OK</td>
</tr>
<tr>
<td>CPU time need</td>
<td>very good</td>
<td>OK</td>
<td>OK</td>
<td>OK</td>
</tr>
<tr>
<td>accuracy of result</td>
<td>OK</td>
<td>very good</td>
<td>poor</td>
<td>OK</td>
</tr>
</tbody>
</table>

Table 5.3: Summarizing the behaviour of the different meshing approaches

The following thesis statement is suggested from this Section:

**Thesis statement 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 study, 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.

Results were published in Rakai and Franke 2012b and Rakai et al. 2014b.

### 5.3 Numerical uncertainty estimation and a new metric suggestion

After the conclusion in Section 5.2 about the most suitable mesh type for operational use, it would be possible to investigate only the body fitted hexahedral mesh further. But as three different resolution results are available for all mesh types, it is interesting to compare them from the numerical discretization error point of view as well. It is important to keep in mind, that on all of the meshes the same equations are solved, so the differences in the results are essentially due to numerical discretization error.

In this section I will carry out a proper solution verification as suggested by the ASME 2009 standard. The whole procedure was described in Section 3.3.2. I suggest a new metric for validation, taking into consideration this value as well. At the end of the section I show a possible use of this new metric in validation, as opposed to the simple concept what was used in the previous chapter, and what is used most of the time in validation studies, as there are only a few examples of solution verification in the literature.

#### 5.3.1 Grid convergence and observed orders

As a starting point of the Richardson-extrapolation based error estimation, it is interesting to see the grid convergence behaviour of the considered points. As more than 2000 measurement points are available, it was logical to investigate those points. The mesh refinement was not obtained by grid doubling so it would anyway be problematic to define the exact points for the investigation and interpolation is anyway unavoidable, so it is straightforward to investigate the point where experimental data is also available.
Results and discussion: flow field calculation

Table 5.4: Observed order of grid convergence with the global averaging method \((p_{GA})\) and grid convergence ratios of the investigated meshes, shown separately the ratio of theoretically correct orders \((0.5 < p < 2)\) for streamwise and lateral mean velocity components.

<table>
<thead>
<tr>
<th>Mesh Type</th>
<th>(p_{GA})</th>
<th>Monotone</th>
<th>(0.5 &lt; p &lt; 2)</th>
<th>(p_{GA})</th>
<th>Monotone</th>
<th>(0.5 &lt; p &lt; 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polyhedral</td>
<td>1.27</td>
<td>37%</td>
<td>5%</td>
<td>1.18</td>
<td>35%</td>
<td>6%</td>
</tr>
<tr>
<td>Tetrahedral</td>
<td>1.13</td>
<td>27%</td>
<td>4%</td>
<td>1.14</td>
<td>25%</td>
<td>5%</td>
</tr>
<tr>
<td>Cartesian hexahedral</td>
<td>1.35</td>
<td>17%</td>
<td>2%</td>
<td>1.21</td>
<td>13%</td>
<td>1%</td>
</tr>
<tr>
<td>Body fitted hexahedral</td>
<td>1.07</td>
<td>25%</td>
<td>4%</td>
<td>1.18</td>
<td>24%</td>
<td>4%</td>
</tr>
</tbody>
</table>

The method of order calculation in discrete points can be debated as discussed in Chapter 3 but was accepted as taken from the ASME standard (ASME 2009).

The reason for not using grid doubling for the refinement is twofold:

1. Grid doubling would result in meshes with a ratio of 64 in cell number, in which case unrealistic meshes would be used for the problem, either by not resolving the geometry or by having a computation which needs considerable computer resources. In the present study even the finest meshes could run on the strongest available 16 GB single machine in single precision.

2. Phillips and Roy 2011 showed that smaller refinement factors result in a better estimate of the observed accuracy as it is more likely to be in the asymptotic region.

Results for the tetrahedral, polyhedral, body fitted hexahedral and Cartesian hexahedral grid triplets are investigated. As a first impression on grid convergence the ratio of monotone convergent results are shown, where the grid convergence was evaluated at the measurement points only, as stated earlier. In Table 5.4 the ratios are shown for the two measured mean velocity component, \(U\) and \(V\), together with the ratio of those points which fall in the realistic \(0.5 < \hat{p} < 2\) range. Additionally the estimated global order of grid convergence averaged from all of the points given by the Global Averaging Method is also given in Table 5.4. It can be concluded that the investigated points are mostly not in the asymptotic range, with the best grid convergence ratio of the polyhedral mesh where almost 40\% of the points are monotone convergent. However as it was shown in Chapter 3 convergent behaviour can also result unrealistic observed orders of grid convergence, it happens also in this case. Realistic order estimation (i.e. \(0.5 < \hat{p} < 2\)) happened for only 1-6\% of the more than 2000 investigated points. This underlines the decision to estimate the numerical discretization uncertainty instead of the error which would only be possible for those points. As it was already mentioned in Chapter 3 in real problems it is not likely that all the points will converge with the formal order of accuracy, e.g. Schatzmann et al. 2009 for the MUST case found \(30 - 50\%\) total divergence depending of the investigated variables, which is similar to the here observed value, and that is a simpler geometry.

It was also mentioned that calculating order of grid convergence from single point to point comparison is questionable, and Phillips and Roy 2011 state that in most cases the behaviour of integrated quantities and averages are better behaved and converge more rapidly with mesh refinement than local quantities. In Table 5.5 the averaged values for the mean streamwise velocity are shown for three of the investigated meshes in the street canyon planes. The experimental value is also given. It can be observed that in this test case in the street canyon planes the convergent behaviour of the averaged velocity is not better than for the point to point comparison values, in a large number of cases the averages are diverging with mesh refinement. So it was decided to use the methods described in Chapter 3 and not to deal with averaged quantities.

After this it is interesting to have a look at the observed order of the discretization calculated for the four different mesh types, seen in Figure 5.9 in all the measurement points based on a point to point
Table 5.5: Grid convergence of mean velocity magnitude in the street canyons an example of evaluating integrated quantities, not point-to-point comparison values.

<table>
<thead>
<tr>
<th></th>
<th>tetrahedral</th>
<th></th>
<th>polyhedral</th>
<th></th>
<th>body fitted hexahedral</th>
<th></th>
<th>exp.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>coarse</td>
<td>medium</td>
<td>fine</td>
<td>coarse</td>
<td>medium</td>
<td>fine</td>
<td>coarse</td>
</tr>
<tr>
<td>2 m</td>
<td>0.191</td>
<td>0.208</td>
<td>0.205</td>
<td>0.208</td>
<td>0.217</td>
<td>0.222</td>
<td>0.197</td>
</tr>
<tr>
<td>9 m</td>
<td>0.189</td>
<td>0.187</td>
<td>0.183</td>
<td>0.191</td>
<td>0.192</td>
<td>0.191</td>
<td>0.182</td>
</tr>
<tr>
<td>18 m</td>
<td>0.328</td>
<td>0.326</td>
<td>0.322</td>
<td>0.329</td>
<td>0.338</td>
<td>0.334</td>
<td>0.335</td>
</tr>
</tbody>
</table>

Figure 5.9: Observed difference between experiment and simulation, order of accuracy for all non-oscillatory points and used order by the method of Roy.
number of monotonic ratios and the highest orders. This is due to the high ratio of oscillatory points which are excluded from the averaging, for the Cartesian hexahedral cells 20% more nodes are excluded than for the other meshes. It must be kept in mind to check the oscillatory node ratio for this numerical uncertainty estimator.

### 5.3.2 Numerical uncertainty

The estimated uncertainties by the different methods are also shown in Figure 5.10 with the probabilities to have an idea about the magnitudes of the uncertainties estimated by the different methods. In the first row the absolute value of the difference between simulation and experiment $|S - E|$ is shown, as the estimated uncertainties are always positive, and the highest difference of the mesh pairs multiplied by 3 also appears ($3 \times |S_{\text{min}} - S_{\text{max}}|$).

![Figure 5.10: Difference between experiment and simulation ($|S - E|$) and estimated absolute uncertainties of nondimensionalised velocity](image)

The first impression when looking at the graphs in Figure 5.10 is that for the tetra meshes smaller uncertainties are estimated, which results from the fact that the differences between the different meshes are smaller, as can be seen from the second row. The comparison with the total errors of the first row is difficult graphically, but earlier it was shown that the statistical results for the tetra meshes are better in all cases. From these two facts it can be concluded that the performance of the tetra meshes is indeed better because the numerical errors are lower, and this can be shown with all of the numerical uncertainty estimators. This would be the best choice of mesh type for model development from this point of view, however later this will be compared point-by-point with the validation rate to reveal if the numerical uncertainties are low enough for model development or not.

Comparing the uncertainty estimators it can be observed in Figure 5.10 that the rows with the simple difference multiplied by 3, the global averaging method and the correction factor method are more similar to each other. This is due to their definition which can be recalled from Table 3.1. Global averaging uses...
Results and discussion: flow field calculation

$FS = 1.25$ which is a low value, and it is using a constant $p$ that is why the shape is so similar to the $3 \cdot |S_{\text{min}} - S_{\text{max}}|$. Only there $3$ is replaced by $\frac{1.25}{r}$, see in Equation 3.22. Similarity of the correction factor method can be explained by the relatively low $FS$ used by that, see in Figure 3.4 compared to the factor of safety method and the GCI Roy method. The orders where the correction factor method uses also high $FS$ (above $p = 3$) do not have a high probability in our test case, see Figure 5.9.

The similarity of the estimated uncertainties by the GCI Roy method and the factor of safety method are caused by different properties, but both result in higher estimated uncertainties than with the other methods. The GCI Roy method uses $FS = 3$ for most of the nodes, see the probability distribution of the orders used by them in Figure 5.9 in the second row. And as they are forcing most of the order to 0.5, an almost constant value of $\frac{3}{4} \cdot r$ can be considered the $FS$, which in our meshes is about 20 due to the small refinement ratio $r$. The factor of safety method does not limit the orders but has higher $FS$ values as can be seen in Figure 3.4.

![Image](a) Wind tunnel measurement, mean streamwise velocity

![Image](b) Finest tetrahedral, mean streamwise velocity

![Image](c) Estimated uncertainty of mean streamwise velocity – Roy

![Image](d) Estimated uncertainty of mean streamwise velocity – GAM

Figure 5.11: Estimated numerical discretization uncertainties with the actual values in the 2m street canyon streamwise velocities

Estimated numerical discretization uncertainties are also shown in Figure 5.11 so that it is possible
Results and discussion: flow field calculation

to pair the values in space. On the top the measured and calculated values are shown. It can be seen that the highest numerical discretization uncertainties are generally occurring at the street intersections with both methods shown in Figure 5.11, the GCI Roy and the GAM method, however the first estimates higher values as was seen already in Figure 5.10. It can also be observed that there are regions where the experiment and the simulation is clearly different, for example in the lower right street canyon with measurement points, but there the estimated numerical discretization uncertainties are the lowest of all values. These are the regions where the model development can be focused on, as there we can clearly say that if there is a change in the result, that is not caused by the numerical uncertainty. The same can be said about the two streamwise street canyons on the top.

It is useful to quantify somehow the result of these numerical uncertainties as well when making comparisons in the statistical metrics, to draw objective conclusions. For this reason I suggest a new metric, the validation rate.

5.3.3 The validation rate metric

The validation rate metric I suggest for proper comparison of validation results containing the effect of numerical discretization error was defined in Chapter 3 in Equation 3.31. Results for the Michelstadt test case can be seen in Table 5.6 for the finest meshes of each mesh type. The reason for this is that the estimated numerical discretization uncertainty is calculated for the finest mesh and the new metric incorporating that, the validation rate ($\text{VR}$) is also shown. Superscripts denote the different estimation methods, see Chapter 3.

<table>
<thead>
<tr>
<th></th>
<th>$L_2$</th>
<th>$HR$</th>
<th>$VR_{\text{GCI-Roy}}$</th>
<th>$VR_{\text{GA}}$</th>
<th>$VR_{\text{FS}}$</th>
<th>$VR_{\text{CF}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>polyhedral</td>
<td>0.21</td>
<td>69%</td>
<td>63%</td>
<td>44%</td>
<td>63%</td>
<td>28%</td>
</tr>
<tr>
<td>tetrahedral</td>
<td>0.15</td>
<td>72%</td>
<td>65%</td>
<td>39%</td>
<td>62%</td>
<td>27%</td>
</tr>
<tr>
<td>Cartesian hexahedral</td>
<td>0.18</td>
<td>66%</td>
<td>75%</td>
<td>41%</td>
<td>72%</td>
<td>22%</td>
</tr>
<tr>
<td>body fitted hexahedral</td>
<td>0.17</td>
<td>71%</td>
<td>68%</td>
<td>43%</td>
<td>65%</td>
<td>26%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$L_2$</td>
<td>$HR$</td>
<td>$VR_{\text{GCI-Roy}}$</td>
<td>$VR_{\text{GA}}$</td>
<td>$VR_{\text{FS}}$</td>
<td>$VR_{\text{CF}}$</td>
</tr>
<tr>
<td>polyhedral</td>
<td>0.47</td>
<td>66%</td>
<td>84%</td>
<td>72%</td>
<td>85%</td>
<td>65%</td>
</tr>
<tr>
<td>tetrahedral</td>
<td>0.39</td>
<td>68%</td>
<td>86%</td>
<td>72%</td>
<td>85%</td>
<td>65%</td>
</tr>
<tr>
<td>Cartesian hexahedral</td>
<td>0.57</td>
<td>60%</td>
<td>89%</td>
<td>71%</td>
<td>87%</td>
<td>57%</td>
</tr>
<tr>
<td>body fitted hexahedral</td>
<td>0.45</td>
<td>66%</td>
<td>85%</td>
<td>70%</td>
<td>84%</td>
<td>63%</td>
</tr>
</tbody>
</table>

Table 5.6: Different validation metrics ($L_2$ norm, hit rate $HR$ and validation rates $VR$ evaluated with the four numerical uncertainty estimation methods) compared for the streamwise and lateral velocity components for all mesh types

It can be observed that with the Roy method hit rates and validation rates are close to each other for the mean streamwise velocity, showing that the experimental uncertainty has an important role in accepting certain points as well. The lower value of validation rate is due to the exclusion of the 25 % limit of difference which appears in the hit rate.

It is interesting to note that with also the Roy method the validation rates are higher for the lateral mean velocity. This is caused by the generally smaller values of lateral velocity, while the numerical discretization uncertainties are larger.

The ASME standard for verification and validation (ASME 2009) says that from a practical standpoint, in case the difference is bigger than the validation uncertainty, $U_{\text{val}}$, one has information that can
possibly be used to improve the model (reduce the modeling error). In case of equal or smaller differences, however, the modeling error is within the "noise level" imposed by the numerical, input, and experimental uncertainties, and formulating model "improvements" is more problematic.

In the following the regions with points where \(|E - S| > U_{val}\) will be shown, to reveal the regions which can be used for model development.

To go further with investigations it is favourable to choose one estimator which is the best for the goals. In case of a validation study which will possibly further on continue with model development, the main goal is to have an estimator which is rather effective than conservative (see Equation 3.23 and 3.24, respectively), since a very conservative estimator will hide the non-numerical errors. Based on the paper of Phillips and Roy 2011 the most effective estimator is the Global Averaging Method. They compared their uncertainty estimations to the known real numerical error in three simple test cases where they were analytically available. In our case it is also shown that that method is the "least conservative", which can be interpreted as the least hiding the total errors.

However as the acceptance of estimating numerical discretization uncertainty is not widespread, it is an important factor to use the most tested estimator. Roache 2009 states that the only uncertainty estimator methods that have been subject to statistically significant database are the GCI (Grid Convergence Index) and least-squares GCI. The Roy method used in this work is a version of the GCI, while the other one is not used here, so I decided to focus on the GCI Roy method results for the graphical comparison.

In Figure 5.12 the validated and not validated points can be seen as was defined in Equation 3.30 using the GCI Roy method for numerical discretization uncertainty estimation. Black dots denote the locations where the difference between experiment and simulation is higher than the validation uncertainty. What is black on the figures can now be exactly related to the deficiency of the physical model, e.g. the turbulence model. In case of the tetrahedral results it is clearly the two more or less streamwise street canyon and the one in the right bottom corner. The reason for this not showing so clearly is not that this deficiency does not exists with the other meshes, but that their the numerical uncertainties are higher so they hide the true behaviour of the model. It is important to keep in mind that on all of the meshes the same equations are solved, so without the numerical errors result have to be the same.

These figures can be different if we use the hit rate as a method for comparison, this is shown in Figure 5.13. This is natural as the numerical uncertainty is purely a property of the mesh. This is why it is important to differentiate between the numerical and modelling uncertainties before starting to develop a certain turbulence model with an experimental dataset for example. In Figure 5.13 results for the standard and the realizable \(k - \varepsilon\) closure (see Wilcox 1993 for difference) are shown evaluated by the hit rate and the validation rate metric in the 2m street canyon. The global results are for HR are 75 % for standard and 65% for realizable, while VR with the GCI Roy method is 65 % and 63% respectively. It can be seen that the VR results are closer to each other, as they excluded the differences caused by the numerical discretization uncertainty. Both methods give better result for the standard method however.

In the Figure 5.13 on the top the hit rate evaluations are shown, on the bottom the validation rate ones. It is apparent that there are less non-validated point in the bottom, showing that the numerical uncertainties are quite high, which is not surprising in this complex urban geometry. The critical regions which can be used for model development look similar, but what is important to note is that with the validation rate method these results are justified from the numerical uncertainty point of view as well, so we can be sure that only the modelling errors are present in the Figure.

It is interesting to note that however the statistical metrics gave clearly better results for the standard \(k - \varepsilon\) closure, in Figure 5.13 the realizable method has improvement for the street canyons in the bottom. This shows that different turbulent closure my have advantages in some regions and disadvantages in others, and their interpretation also depends on the location of the measurement points for validation.

To have a visual view of the the flow in the street canyons vectors are shown in Figure 5.14 for all of the mesh types for the standard \(k - \varepsilon\) closure, still for the fine meshes. This way the difference in the critical locations, i.e. the streamwise street canyons can be investigated. What we can see is that there is
Results and discussion: flow field calculation

Figure 5.12: Non validated points in the 2m street canyon
Results and discussion: flow field calculation

Figure 5.13: The usage of the method for model development justification with tetrahedral mesh ske – standard $k - \varepsilon$ closure, rke – realizable $k - \varepsilon$ closure
Results and discussion: flow field calculation

(a) tetrahedral
(b) polyhedral
(c) body fitted hexahedral
(d) Cartesian hexahedral

Figure 5.14: Vectors of the flow in the 2m street canyon, arrows: experiment – black hollow, simulation – gray full
not much difference in the behaviour of the four mesh types in that location. The same can be expected for the realizable \( k - \varepsilon \) closure as the non-validated points were in that location as well.

If we compare the plots with the same vector plots given in Hertwig et al. 2012 in Figure 6, it can be seen that the vectors of the Star-CD computations in the street canyons are similar to the results here, while the ANDREA vectors differ a bit more. Although they made no numerical uncertainty estimation, this may be a sign that in this location the turbulence model can have an important influence, as the Star-CD simulations were done with the standard \( k - \varepsilon \) model while the ANDREA used a different turbulence model.

### 5.3.4 Discussion

Solution verification, or in other words numerical discretization error and uncertainty estimation is a very important part of quality assurance of the CFD results. This exercise is becoming more popular but till now was used typically only on simple Fluid Mechanics academic test cases. The method based on Richardson extrapolation is well established thanks to these evaluations and comparisons to analytical results. Here it was shown that the methods already collected in the ASME standard give an additional possibility for practising engineers to check their results. For the given Wind Engineering problem in most part of the domain where measurement results are available, the estimated validation uncertainty is in the same order of magnitude than the difference between experiments and simulations. A new metric, validation rate was developed to show the ratio of the measurement points where experimental and numerical discretization uncertainties can hide the real behaviour of the model, where no model development is possible with the current level of experimental and numerical accuracy. However the positions where the difference between experimental and numerical results is higher that the validation uncertainty, which were shown to be the streamwise and a \( 45^\circ \) street canyons can be used for model development even with the available rather coarse meshes.

The following thesis statement is suggested from this Section:

**Thesis statement 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.

\[
VR = \frac{1}{N} \sum_{i=1}^{N} \delta_i
\]

\[
\delta_i = \begin{cases} 
1 & D_i \leq U_{val} \\
0 & \text{for else} 
\end{cases}
\]

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 \( k - \varepsilon \) to evaluate and compare the model performance including the numerical discretization uncertainty.

Results were published in Rakai and Franke 2012a, Rakai and Franke 2013 and Rakai and Franke 2014a.
Chapter 6

Results and discussion: passive scalar dispersion calculation

In the previous chapter I showed the difficulties of the flow field simulations from an operational point of view. We have seen that the best mesh to use in everyday application is a body fitted hexahedral mesh which is very robust but provides good accuracy results. But we have also seen that with complex urban geometries the numerical discretization error can be in the same order of magnitude as the modelling error, so it is very important to make the effort to quantify it.

Now I will turn to the dispersion calculations, keeping in mind that the underlying flow field is already not perfectly modelled, and can have an effect on the dispersion. I investigated three different source locations, one in an open square, S2, another in a street canyon, S4, and finally one in a street intersection, S5. For a reminder on their location see Figure 4.4.

Given the four different mesh types used for flow simulations I will start with an overview of the performance and sensitivity of the dispersion results to grid type and resolution in Section 6.1. First I will show mean concentration comparison for continuous release. I performed also an optimization for the turbulent Schmidt number, \( Sc_t \), which is a highly argued parameter in urban dispersion calculations, as it was discussed in Section 2.5. I will show that depending on the source location different values can be optimal, which means the value may be locally depending on the flow field.

In Section 6.2 I will show results from an anisotropic closure of the turbulent scalar flux model, which can take into consideration the direction dependence of the turbulent diffusion. It is an alternative of the simple gradient diffusion hypothesis using \( Sc_t \). The variation I used was numerically unstable, so it is not yet suitable for operational modelling. However the results obtained for the coarsest hexahedral mesh show improvement in the statistical results for source S2, so this model can be considered for further development and evaluation.

RANS based urban flow and dispersion simulations can not only be used for air quality assessment, but they have a potential to be involved in emergency response applications. They have rarely been evaluated for these kind of modelling before, where short-term releases are more important, with more complex puff parameters than simply the mean concentration what was compared so far. In Section 6.3 therefore I carry out a comparison for puff parameters looking at their sensitivity to source location and grid resolution. I found that these results are more sensitive to the resolution, but with a sufficiently fine grid the RANS approach can be a useful tool for emergency response with the increase of computational capacity. It can already be used for the preparatory or post-accident investigations.

I will end the discussion of the results in Section 6.4 with a possible extension of numerical discretization error estimation with one-mesh estimators. Two methods, the residual and the moment error method is compared to the traditional Richardson extrapolation based methods. These methods have a
potential as they can make the numerical discretization error estimation more widespread, not demanding three different grid resolutions. However, it was found that they estimate lower errors than the standard method, and there is not yet literature on a suitable safety factor used for them to be converted to uncertainty estimates, so they need further investigation.

In this chapter there is only one variable, the mean concentration, which is a simple scalar field, and some post-processed values of its time evolution for the puff simulations, so it is easier to follow the discussion. Also as there are fewer measurement points, more profiles and qualitative plots can be shown to understand the general behaviour of the transport equation and the evolution of the plume in the urban canopy. It is important to keep in mind, that the results of concentration can take over a range of several orders of magnitude, so often logarithmic diagrams are used.

With this in mind we can start our tour of the pollution field.
6.1 The key coefficient in passive scalar dispersion – the turbulent Schmidt number

I was investigating several factors, like the effect of the flow field (Section 6.1.3), grid type and grid resolution (Section 6.1.4), and their effect on the results of the dispersion simulation of source S2, using two different statistical metrics to avoid bias in their results. I will show that the most significant effect on the metrics performance is caused by changing the turbulent Schmidt number, $S_C$. An optimization for this parameter was carried out for all investigated sources showing that depending on the location of the source different optimal values are obtained (Section 6.1.5). This means that this parameter has a local flow field dependency, and a more elaborate modelling approach would be necessary.

6.1.1 Convergence

Before going into details about the results I would like to discuss the monitoring of convergence, as for the solution of the transport equation it is slightly different. Instead of monitoring the residuals and finally checking some field values, here field values are monitored in some chosen receptor points during the whole simulation, until they reach a constant value. This is because time dependent simulations were carried out until a steady state was reached. Convergence was monitored in 5 measurement points in case of source S2, highlighted in Figure 6.1. Point 9 is the closest to the source while point 37 is further away from it. 3 more points were chosen in-between, so steady behaviour was checked all over the domain of measurements. The same process was used for source S4 and S5, not detailed here.

As second order simulations were unstable in case of some meshes, all calculations were started with upwind differencing for the convective term and only after convergence was it changed to the linearUp-wind scheme. For steady calculations it is not a problem.

Figure 6.1: Location of points where convergence was checked for the steady state passive scalar dispersion simulations for source 2
6.1.2 Metric evaluation

For the dispersion evaluation fewer measurement points are available so a more detailed location dependent analysis is also possible. However metrics are necessary to check the overall performance of the transport model. We can recall from Chapter 4 that 58 measurement locations were measured for source S2, 25 for S4 and 22 for S5. See Figure 4.4 for exact locations. As source S2 has the more measurement points, those results are used for the statistical evaluation of all grid types.

$L^2$ norm is used again as it is already familiar from Section 5.3, and the $FAC^2$ metric (Equation 3.32) is used here instead of the $HR$ used for the flow field values, as that is used more often in air quality modelling. This metric has very similar behaviour to $HR$ so also here $1 - FAC^2$ results are plotted for easier comparison.

![Graph showing values of $L^2$ norm for $C^*$ normalized passive scalar concentration as a function of cell number (triangle – tetrahedral, pentagon – polyhedral, square – Cartesian hexahedral, rotated square – body fitted hexahedral, recall Figure 4.6 for symbols)](image)

Figure 6.2: Values of $L^2$ norm for $C^*$ normalized passive scalar concentration as a function of cell number (triangle – tetrahedral, pentagon – polyhedral, square – Cartesian hexahedral, rotated square – body fitted hexahedral, recall Figure 4.6 for symbols)

Results for the two metrics are shown in Figure 6.2 for $L^2$ and Figure 6.3 for $FAC^2$. What is straightforward at first look is that all the expected properties which were found for the flow field are not valid anymore for the dispersion results. No improvement can be observed with mesh refinement except for the tetrahedral mesh and the tetra meshes show no better results, neither the second order differencing scheme results. As this test case has no modelling results in the literature yet, it is not possible to compare the values to other models. However we can consider the $L^2$ norm as an averaged normalized error, and we see that almost all of the models have an error between 20 – 35%. The high $FAC^2$ values in Figure 6.3 show the same, almost all of them being above 70% (Remember that the graph shows $1 - FAC^2$).

In the following parts the concentration field will be investigated in more detail to find out the cause of this behaviour. To understand better the single transport equation for a passive scalar must be recalled from Equation 3.9. It contains the mean velocity field which was found to be modelled quite well but some important deficiencies were found in the urban canopy, exactly where there are the concentration measurement points. The diffusion is governed by the turbulence field which were shown to have rather big differences from the measured values already and the gradient diffusion hypothesis is used for the turbulent diffusion fluxes, see Equation 3.11 which has a single and often questionable closure constant, the turbulent Schmidt number.
6.1.3 Effects of the flow field: on the convective flux

The dispersion measurements were carried out at a height of 7.5 m in full scale while flow field measurements were done only at 2 and 9 m. The results of the last are compared here together with the dispersion results in Figure 6.4. Flow field results of the finest body fitted hexahedral mesh were used for the figure.

With the limited points where the flow and dispersion measurements are close to each other it cannot be justified that deficiencies are caused by the flow field. The most problematic dispersion points, which are in the first lateral street canyon, apparently underestimating the spread of the plume in lateral direction, have no flow field measurement data.

To have a view on the flow field in the street canyons however in Figure 6.5 three streamlines in the street canyons are shown together with the dispersion contour of simulations and points for experiments. As graphical visualization of all the cell values—what is necessary for the streamline calculation—is very demanding, the results of the coarsest body fitted hexahedral mesh were used for the figure.

The greatest underestimation of the spread of the plume by the simulation is in the first streamwise canyon where the intensive vortex circulation can be observed. This vortex in the simulation is rotating perpendicular to the length of the canyon, possibly blocking the lateral movement of the plume. This can cause a difference if in the experiments the vortex is less intensive. Unfortunately this guess cannot be justified without more experimental results.

Gousseau et al. 2011 have shown that convective and turbulent fluxes are of the same order of magnitude in vertical direction. They say that turbulence even dominates convection, except on the centerline of the plume. This also underpins the necessity of more flow field measurement results. As long as the
Results and discussion: passive scalar dispersion calculation

Figure 6.4: Possible effects of flow field on dispersion: 9m flow vectors (black - experiment, red - simulation), 7.5m dispersion results (square - experiment, contour - simulation) dash-dot line and numbers: location of profiles

Figure 6.5: Streamlines in street-canyons and 7.5m dispersion results (sphere - experiment, contour - simulation)

convective and turbulent fluxes are in the same order of magnitude, it is difficult to see the effect of the flow field on the results. This is shown in Figure 6.6 where dispersion $L^2$ norm results are plotted as a
function of flow $L^2$ results. We could expect to have better dispersion results for better flow field, but this is not the case, showing that some of the errors in the flow field cancel out probably errors in the dispersion model.

![Graph showing dispersion metrics as a function of flow field metrics - $L^2$](image)

**Figure 6.6:** Dispersion metrics as a function of flow field metrics - $L^2$

In Figure 6.8 the underestimation of the lateral spread of the plume in the street canyons is also visible. This is not a general behaviour however, rather a property of the experimental dataset. As a counterpart of this behaviour an overestimation can also be observed. The location of the overestimation is the top of the vertical profiles, see Figure 6.9, while underestimation happens at the edge of horizontal profiles, and can be a results of the deficiency of the turbulent scalar flux closure not to model properly the dispersion of a Gaussian plume, see Gorlé et al. 2008 and other related deficiencies Tominaga and Stathopoulos 2007.

To maintain mass conservation this underestimation must be balanced, but probably no measurement points are located at those points where overestimation occurs. Also the $c_*$ values investigated differ several orders of magnitude, so this underestimation of small values can be balanced with small overestimation in higher $c_*$ regions. In Figure 6.7 this can be investigated with all the higher experimental results available, slices showing the shape of the plume.

At the slice closest to the source in Figure 6.7 the plume looks rather thin and seems to spread to a higher $z$ value than in case of the measurement, the green contour containing the blue sphere. But this limited location is not enough to draw strong conclusions, more measurement results would be necessary for these cross sections. It is also important to remember that the scale is logarithmic, so to balance the underestimation in the edge of the plume for mass conservation, not so strong overestimation is necessary.

The gradient diffusion hypothesis used here was criticized in Dezso-Weidinger et al. 2003. They carried out simultaneous measurements of the flow field and concentration field to evaluate the turbulent scalar fluxes, and in the urban canopy sometimes they had opposite direction of fluxes than the concentration gradient. In this experiment where flow field and dispersion measurements are not simultaneous and are not carried out at the same locations, no direct conclusions can be gained about the scalar fluxes for model development. Nonetheless a more elaborate anisotropic model will be used in Section 6.2.

Another important thing to remember here is that although the boundary conditions in the experiments are stationary in the averaged values, the flow is essentially time dependent, with vortex shedding.
around the bluff bodies which change the location of the vortices. Hertwig et al. 2012 have shown that close to street intersections several locations have bi-modal velocity distributions evaluated from the time series of the results. This means that in the experiment the pollutant is directed to one street or to the other varying in time, which is not reproducible with my steady model.

As no further conclusion can be drawn from the effect of the flow field, in the following the effects of the numerical discretization are investigated in more detail.

6.1.4 Effects of grid type and resolution sensitivity: on uncertainty due to numerical discretization

The results of the four different mesh types are shown in Figure 6.8 as scatter plot and 6.9 as profiles. The location of the profiles was shown in Figure 4.4 and 6.4.

With the change of the mesh type the problem stated before does not diminish. This was already concluded from the simple metric comparison in Figure 6.2 and 6.3. The tetrahedral meshes, which performed the best for the flow field simulation due to the lowest numerical discretization uncertainty as was shown in Chapter 5, show no remarkable difference from the other types.

The same can be said about mesh refinement, no significant difference can be seen, although one would expect an improvement with refining the spatial discretization. This must be a consequence of the cancelling out of the numerical and the modelling errors, which makes the evaluation difficult.

Profiles for mesh refinement are very similar to the ones comparing the mesh type, so they are not shown here separately, but are added to Appendix B. For easier reading the different mesh type profiles are separated. For the tetrahedral mesh scatter plot can be found in Figure B.1, the profiles in Figure B.2. For polyhedral in Figure B.3 and B.4, for the body fitted hexahedral in B.5 and B.6.

With the four methods of numerical discretization uncertainty estimation explained in Section 3.3 and used in Section 5.3, I checked the ratio of numerical uncertainty and the difference between experimental and numerical results to make sure that differences are not only due to the numerical discretization error. More detail on this can be found in Section 6.4. In case of several points the difference between experimental and simulation results is greater than the validation uncertainty, so also modelling error can be justified, as expected. This underpins the following investigations on the most important model parameter, $Sc_T$. 

Figure 6.7: Cross sections at profile locations with dispersion results (sphere - experiment, contour - simulation)
Results and discussion: passive scalar dispersion calculation

6.1.5 Effect of $Sc_t$ number: on turbulent scalar flux

The scatter plot and profiles already familiar from previous comparisons are shown in Figure 6.10 and 6.11 to see clearly the effect of the closure constant, the turbulent Schmidt number ($Sc_t$) on the results.

Putting a small value like $Sc_t = 0.1$ enhances turbulent diffusion very much so the lateral profiles become more flat and pollutant is spread out of the main streamwise street canyon. On the contrary, the bigger value like $Sc_t = 1$ reduces diffusion and more pollutant remains in the streamwise street canyon. It is obvious from Figure 6.11 that in some locations one effect increases matching with the experiments while in other locations the contrary.

The default value in Fluent e.g. is $Sc_t = 0.7$ (see Ansys 2009) but Tominaga and Statopoulos 2007 argues that that is defined for Fluid Mechanics academic test cases and not urban problems and Gorlé et al. 2008 also shows a lower optimal value for a test case of dispersion around a cube.

As for this case just looking at the profiles it is difficult to define an optimal value the already used $L^2$ and $FAC^2$ metrics are taken again to have a statistical view on the situation. In Figure 6.12 those metrics are shown as a function of $Sc_t$ for source S2. Simulations were run on the coarsest body fitted hexahedral mesh for $0.1 < Sc_t < 1$ with a resolution of 0.1, with second order discretization to reduce numerical diffusion which may change the picture. The originally defined 0.7 value remains valid for this test case.

One reason for this can be that Gorlé et al. 2008 and Tominaga and Statopoulos 2007 focus on test cases around a single building, with detailed measurements in the wake of the building and the rooftop recirculation. The test case used here has a better represented measurement point distribution in the urban canopy, with buildings surrounding each other, which is a more realistic situation. Also in those cases the emission from from a point close to the single building, while the source S2 is in an open square.

To see the effect of $Sc_t$ on the lateral diffusion, a slice of the simulation is shown at the height $z = 7.5m$ in full scale in Figure 6.13, where the dispersion measurement are available. Results for $Sc_t = 0.4$ and $Sc_t = 0.7$ are shown, and it can clearly be seen that for 0.4 the plume is more spread in the lateral direction, while it is shorter, see the orange region in the core of the plume. At first sight
72 Results and discussion: passive scalar dispersion calculation

![Graph of results from different mesh type simulations.](image)

Figure 6.9: Profiles of the results from different mesh type simulations, results shown here are from the coarsest meshes, upwind convective discretization. Note that $c_*$ scales are logarithmic except for the streamwise profile.

This would favour the $Sc_t = 0.4$ solution, that is why it is important to use metrics for comparison, as graphical comparison can be misleading.

A similar effect can be observed in Figure 6.14 where the two other direction cross sections can be seen. For these no measurement results are available. The cell centre results are plotted, that is the reason for the dotted appearance. For a contour plot triangulation would be necessary, but that uses an interpolation which gives results also inside buildings so that is avoided. In this figure it can also be observed that the change of $Sc_t$ has the same result on both lateral and vertical diffusion, growing or reducing the plume equally. This is the isotropic behaviour which is criticized by Gorlé et al. 2008 for example, that there is no directional preference in the dispersion model.

### 6.1.6 Sensitivity to source location

So far only results of the source S2, the one located in the open square, were investigated. Usually in the literature no special attention was payed to the sensitivity to the source location, mostly because usual test cases contain only one source. But in the Michelstadt experiment several source locations were measured, which makes it possible to investigate this effect as well.

The same procedure is carried out for the other two sources. For source S4, the source in a street canyon, the $Sc_t$ optimization results can be found in Figure 6.15, while the same horizontal cross section in Figure 6.16, the other two in Figure 6.17.
Results and discussion: passive scalar dispersion calculation

Figure 6.10: Scatter plot

Figure 6.11: Profiles
Interestingly, here the opposite can be observed about the convected plume, the measured plume is convected more than the simulated. Note the pink squares in the orange region as opposed to the green squares in the orange region in Figure 6.13. For the lateral dispersion it can be seen that in the right direction the plume is not spread enough, while for the left, it is more spread for the simulations. This cannot be corrected by the $Sc_t$ number changes, but can be due to the error in the underlying flow field. For this source we have flow field measurements quite close to its location, the resulting vectors are also plotted in Figure 6.16. It can be seen that in the region of the first lateral street canyon after the source, the mean velocity vectors of the measurements and the simulation already differ, which can cause the difference in the convected plume. For the optimal $Sc_t$ for this source location, not only we can observe that 0.7 is not the best value anymore, but also we find a contradiction in the behaviour of the metrics. The results were double checked as it looks like a plotting error. No best choice can be given for $Sc_t$ in this case, and the metrics are in general higher, showing that this source location is more difficult to
Results and discussion: passive scalar dispersion calculation

Figure 6.14: Cross section for $Sc_t = 0.4$ and $Sc_t = 0.7$ for source S2

Figure 6.15: Metrics as a function of $Sc_t$ for source S4

model. If we again consider the $L2$ norm as an averaged normalized error, it is found that this source can be modelled with an error reaching from 70% to even 100%.

The last investigated source location is source S5, in a street intersection, its results are shown in Figure 6.18 for the $Sc_t$ optimization, Figure 6.19 for the horizontal plane and Figure 6.20 for the other cross sections. The size of the convected plume seems to be better predicted here by the simulation, but the lateral spread is problematic, just as in the case of S4. This behaviour can be expected as this source is exactly in the lateral street canyon where already the flow field modelling is difficult. For the optimal $Sc_t$ value in this case, 0.5, can be chosen by both metrics, but it can also be observed here that metrics are higher than for S2, showing that the source location is also more difficult than the open square, as could be expected. Results with around 80% normalized error are encountered.

Seeing the results of both 3 sources, it can be argued that even in the same geometry and flow field no general $Sc_t$ can be suggested, which calls for a method to define it as a local function of the flow field, or
to use a more elaborate model for the turbulent scalar flux than the simple gradient diffusion hypothesis. However it is interesting to note that while for source S2 the normalized error was changing between 30-90%, showing a large effect of a 60% range difference caused by the $Sc_t$ change, in case of S4 and S5 this range is only 30% and 10%, respectively. This results suggests the use of $Sc_t = 0.7$ in a general urban geometry, as if the source is inside the urban canopy, the result depends less on the choice, and no universal optimum can be given.

For sources that are in difficult locations, like street canyons or street intersections, already the modelling of the underlying flow-field is difficult for a steady state RANS model, however that is an often used approach due to the large computational resource needed for the time dependent modelling. In this case we have to be aware that the dispersion modelling results can be misleading due to the errors in the flow-field.

### 6.1.7 Discussion

We have seen that for the passive scalar dispersion the results are showing less the general requirement of improvement with grid refinement, and in general the statistical metric results have a large scatter due to the effects of several factors: the error in the underlying flow field, the numerical discretization, the dispersion model. For the most often used gradient diffusion hypothesis the turbulent Schmidt number is...
Results and discussion: passive scalar dispersion calculation

Figure 6.18: Metrics as a function of $Sc_t$ for source S5

Figure 6.19: Cross section for $Sc_t = 0.4$ and $Sc_t = 0.7$ for source S5

the most important model parameter, for which no clear optimal value could be found.

The following thesis statement is suggested from this Section:

**Thesis statement 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
Results and discussion: passive scalar dispersion calculation

Figure 6.20: Cross section for $Sc_t = 0.4$ and $Sc_t = 0.7$ for source S5

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.

Results were published in Rakai and Kristóf 2013, Rakai and Franke 2014b and Rakai et al. 2014a.
6.2 An attempt to go beyond the gradient diffusion hypothesis – anisotropic modelling

I have shown in the previous section that in a complex urban geometry the location of the source can have a significant effect on the results of the dispersion modelling, and the choice of the closure constant for the turbulent scalar flux, the turbulent Schmidt number becomes questionable, depending on the source location. This calls for a flow field dependent closure of the transport equation. Therefore a different model closure, namely an anisotropic model is investigated in this section. The recent investigations mentioned in Chapter 2 were carried out for simple geometries and no clear decision was made about their advantage over the isotropic model. Here their effect on the concentration field in this complex geometry is shown, with the three different source locations investigated before, S2 in the open square, S4 in the street canyon and S5 in a street intersection.

It is useful to recall Equation 3.12 which shows that in this model the velocity gradient tensor is also involved in the computation of the turbulent scalar flux, so there is an effect of the flow field. It is also important to note however, that just as $S_C$ is often criticized, this model contains two model constants which were not derived for special urban or atmospheric applications.

6.2.1 Source S2

During the simulations the first drawback of this more complicated model was observed when with the default settings used for the dispersion calculations convergence could only be obtained for the coarsest hexahedral meshes.

![Figure 6.21: Scatter plot of the anisotropic model test, coarsest body fitted hexahedral mesh results](image)

This already would exclude the use of this model for operational purposes which is in the focus of the current work. However the converged results are evaluated with the same scatter plot and profile plots in Figure 6.21 and 6.22 respectively. It is difficult to evaluate the results from these plots as there is no clear trend what is changing for the anisotropic model. It is interesting to note however that both the upwind
Results and discussion: passive scalar dispersion calculation

![Graph showing streamwise street-canyon with profiles and mesh results.](image)

Figure 6.22: Profiles of the anisotropic model test, coarsest body fitted hexahedral mesh results and 2nd order convective discretization scheme results are shown, and the effect of numerical diffusion can be observed. For the 1st lateral profile e.g. upwind results are closer to the measured values, as the plume is spread more due to numerical diffusion. So the effect is similar to reducing $Sc_t$ seen in Figure 6.11.

![Cross section for anisotropic and isotropic approach for source S2](image)

Figure 6.23: Cross section for anisotropic and isotropic approach for source S2

The horizontal cross section of the simulations is shown in Figure 6.23 compared to the isotropic...
Results and discussion: passive scalar dispersion calculation

... approach of $Sc_t = 0.7$. To find the differences between the two results, the details of the plume must be investigated. At first sight the two plots look identical, and only in a few areas can difference be spotted.

As no clear advantage can be observed on the plots the metrics are also compared. The $L^2$ metric seemed the more sensitive in Figure 6.12 so that is given here: 0.28 for the 1$^{st}$ order isotropic approach, 0.29 for the 2$^{nd}$ order, while for the anisotropic it is 0.24 and 0.23, respectively.

This shows statistically a small advantage, but before drawing further conclusions the remaining two source locations must also be investigated.

6.2.2 Source S4

The source in a street intersection was also modelled with the anisotropic approach. Results can be seen in a horizontal slice in Figure 6.24 compared here as well to the $Sc_t = 0.7$ isotropic result to remain consequent, however that is not the calculation with the bets statistical metrics.

No clear behaviour can be seen in these figures, but some change due to the change in the closure can be observed more easily on the left hand side of the plume.

![Figure 6.24: Cross section for anisotropic and isotropic approach for source S4](image)

The statistical metrics were calculated for this source as well. For the isotropic model with $Sc_t = 0.7$ the $L^2$ norm is 0.86, while one of the best results is obtained with $Sc_t = 0.4$, that is 0.73. The result of the anisotropic model closure for this source is 0.89, which is worse than any of the previous, so for this source location there is no point in using this closure, at least with this exact closure constants and in this form.

6.2.3 Source S5

The results of the last investigated source location, S5 in a street intersection are shown as well to the sake of completeness. The same horizontal plane can be seen in Figure 6.25.

Some differences can again be identified at the left hand side edge of the plume, but that does not help the objective comparision. The $L^2$ metric is compared again to underpin the conclusions. For the isotropic model with $Sc_t = 0.7$ the $L^2$ norm is 0.76, while one of the best results is obtained with $Sc_t = 0.6$, that is 0.75. The result of the anisotropic model closure for this source is 0.77. This is again worse than any of the previous, so the usage of the anisotropic closure in this form and with these model constants is strongly questionable for complex urban applications, and its use for operational purposes is not recommended.
6.2.4 Discussion

An anisotropic turbulent scalar flux closure was tested for the three available source locations to resolve the problem of the flow field dependent optimal turbulent Schmidt number. The closure of the turbulent scalar flux for this model contains the velocity gradient tensor, making it possible to consider the flow field in the diffusion parameter. The numerical stability of the model was found not to be sufficient for operational purposes.

From statistical point of view this model showed advantages only for a source in an open square like S2. For the other two source locations, the one in a street canyon and the one in a street intersection, the statistical metric results were found to be worse than for the isotropic closure.

There remains the possibility to investigate different anisotropic closures or tune the model constants for urban flows, but that is not in the scope of this thesis.

The following thesis statement is suggested from this Section:

**Thesis statement 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.

Results were published in Rakai and Kristóf 2011 and Rakai and Kristóf 2013.
6.3 Towards emergency response – short-term releases, alias puffs

So far only mean concentration results were compared for continuous releases, representing a stack emission or the pollution of a road with constant traffic. That method makes it possible to investigate the air quality in an urban area with the help of the model.

We now move to an even more demanding exercise for the RANS model, which is necessary to give answers for emergency response, and this is short-term release, i.e. puff modelling. In case of the short-term release modelling results are compared not only in space, but also in time, and a puff is characterized based on its dosage with parameters like arrival time or peak concentration to enable an objective comparison. See Figure 3.1 to recall puff parameter definitions.

Two meshes already shown were used for this exercise, the coarsest polyhedral (coarse from now on) and the finest body fitted hexahedral (fine from now on). See Table 4.1 for cell numbers and 4.2 for size of the volume source. They were chosen as they are the two extremities of the reasonable operational range. Even the coarsest polyhedral mesh gave acceptable results for the mean concentration. A general description of the difference of resolution in this exercise can be given by the average face size on Building 33 which has already been introduced in Figure 4.2. That building has a surface of 12000 $m^2$ in full scale, and the average face size on the coarse mesh is 5$m^2$, for the fine mesh 0.3$m^2$. Another useful measure is the size of the volume source compared to the size of the building. Building 33 has a volume of 59000$m^3$ in full scale, while the coarse volume source is 50$m^3$, the fine 0.18$m^3$. These sizes can be regarded as a general Central European city building size, as the test case was created with that in mind.

This investigation is motivated by 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” where I am a member of the modelling group.

Short-term release emissions are compared in the same three source locations which have already been introduced, source S2 in an open square, source S4 in a street canyon and source S5 in a street intersection. In the experiments around 200 puffs are necessary to have a statistically representative puff population, so measurements are available in fewer receptor points, as was shown in Figure 4.5.

6.3.1 Qualitative comparison

First a qualitative comparison is shown in Figure 6.26, where the calculated mean puffs are compared at each measured receptor location.

Calculations were carried out in the same flow field investigated in Chapter 5, with the same passive scalar dispersion solver as what was used for the continuous cases. The only difference is that for the puffs the volume source after 29 seconds was changed to zero. This is the same duration as what was used in the wind tunnel, which makes it possible to only scale the concentration values and not the time. For the time evolution used for qualitative comparison that is sufficient.

A simple grid sensitivity is shown with a very coarse and a very fine mesh. More elaborate studies would be necessary to make it possible to estimate uncertainty, but as puffs have not been modelled before in literature with the steady RANS approach, in the scope of this thesis only this preliminary analysis was carried out.

The mean puff comparison is shown in Figure 6.26. We can observe that for source S2, which is an easier source in an open square, the results of the two meshes are similar. However for the other two, difficult sources, the results of the finer mesh are clearly better. In case of the very coarse mesh, the calculated plume has probably a different direction, missing both receptor points in case of S4, and receptor point P9 in case of S5.

This shows that the puff modelling is more sensitive to the grid resolution, which is probably in correspondence with the size of the volume source or the resolution on the surface of the building. As
results are compared also in time, and only in a limited receptor points, if a puff misses a receptor, that is very significant.

### 6.3.2 Puff parameter comparison

To give a more quantitative comparison, mean dosage and peak time values are compared in Figure 6.27 for all receptor locations. It can be observed that for source S2 the results are even slightly better for the coarse mesh. Recall the position of the receptor points in Figure 4.5. The puffs at receptor point P7, which is in the streamwise street canyon, and P22, which is in the second right hand lateral street, are overpredicted, while at P19, in the first right hand side lateral street, there is an underprediction, probably because the flow does not turn enough into that direction in the simulations. The higher numerical diffusion of the coarse mesh can help to diffuse the plume more to that direction, thus improving results in a misleading way, giving a right answer for the wrong reason. For S4 and S5 the results of the finer mesh are clearly superior.

With finer mesh, with a resolution of 1 m² 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, which is considered good agreement for a comparison in both space and time.
6.3.3 Histograms of puff parameters

To give an even deeper insight into the puff modelling and its difficulties, histograms of the distributions of the measured results for approximately 200 puff measurements per receptor point are shown in Figure 6.28 together with the mean value of the measurements and the simulation values for one receptor point per each source. It can be seen that the distribution for the dosage is right-skewed, therefore the mean value does not correspond to the most probable value with the highest bar in the histogram. It is a difficult question to decide whether the results of the simulation should be compared to any other statistical value of the distribution, but I decided to compare the mean values, as the result of a RANS simulation is a Reynolds averaged value, so comparing to other than the average would add additional uncertainty to the comparison.

For the peak time distribution this question is not so difficult, as their distribution is less skewed. An interesting thing to note is that in case of the receptor point P5, the coarse mesh gives a value which is an outlier but was present in one of the puff measurements. As the flow-field in the wind tunnel is turbulent, the 200 puffs measured to give this distribution had different plume directions, and one of them could be similar to the one modelled by the coarse mesh. This does not justify the use of coarse meshes, but reminds to the large variability of the short-term release modelling, and that it is a very difficult task to model properly, also in the wind tunnel.

6.3.4 Discussion

The short-term release modelling with the steady approach was also investigated with a preliminary grid sensitivity analysis. It was found that this approach has a strong dependency on both the location of the source and the grid resolution, and still leaves a lot of open questions for this kind of modelling. For the relatively easy-to-model source in the open square the coarse mesh gave better results for the two investigated statistical puff parameters, the dosage and the peak time, giving a better answer for the wrong reason, possibly numerical diffusion. For the other two source locations the fine mesh had outstandingly better results for the compared mean statistical parameters.
Results and discussion: passive scalar dispersion calculation

Figure 6.28: Histograms of puff parameters from the experiment (courtesy of E. Berbekar)
The following thesis statement is suggested from this Section:

**Thesis statement 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, which is considered good agreement for a comparison in both space and time.

Results were published in Rakai et al. 2014a.

### 6.4 More on numerical uncertainties: one mesh estimators

The final investigation in the thesis is dealing with the continuous release again. Numerical discretization uncertainty estimation for the dispersion results was not shown in detail as that would just be a repetition of what was already seen for the flow field. But for the mean concentration, as it is only a scalar field, it is possible to use more simple estimator methods. Although Richardson extrapolation is the suggested and accepted method for numerical uncertainty estimation by ASME, the investigation of one-mesh estimators is encouraged for example by Roache 2009 for already verified codes.

In general numerical uncertainty estimation is not a widespread process, one of its reason being that it requires three different mesh densities. The application of one-mesh estimators therefore have the potential to make numerical uncertainty estimation more popular, but their behaviour have not yet been as thoroughly investigated as that of the standard method by ASME 2009.

A full statistically representative comparison on several simple test cases with analytical comparison is not in the scope of this thesis, but the behaviour of two one-mesh estimators, the residual and the moment error estimator introduced in Section 3.3.2 is investigated for the test case Michelstadt.

For source S2, error estimates of the one mesh estimators are compared to the uncertainty estimate calculated by the GCI Roy method in Section 6.4.1. A simple safety factor of 3 is used to convert the error estimates, as there is no literature available for a more suitable value.

For source S4 and S5 simulations were not carried out on three different mesh densities, so the application of one-mesh estimators is shown to give more detail on the simulation results as an example of how these estimators can be used in Section 6.4.2.

#### 6.4.1 Evaluation on source S2

First results of the uncertainty estimates by the GCI Roy method are shown in Figure 6.29. This shows the final goal of uncertainty estimation, plotting the results as error bars of the simulation results. In the scatter plot now there are both experimental and numerical error bars. Recall Figure 3.6 as a graphical explanation of the validation uncertainty, which appears in these kind of scatter plots as the length of a vector defined by the experimental and numerical uncertainty. With the help of this figure we have a visual interpretation of validated or non-validated points, and we see that there are several non validated points to justify the model development.

These non validated points are shown also in the horizontal plane of the urban canopy in Figure 6.30. No special patterns can be identified except for the first lateral street canyon, which has been proved to
Results and discussion: passive scalar dispersion calculation

be the most problematic in Section 6.1. No further conclusion were possible for this canyon, as no flow results are available in its vicinity. Changing the model constant, the turbulent Schmidt number could improve the results in this street canyon but made them worse elsewhere in the domain. For additional model development the black squares in Figure 6.30 have to be focused on.

To make this process less computationally demanding, one-mesh estimators are tempting. In Figure 6.31 results of two of these one-mesh estimators, the residual and the moment error estimator are compared to the estimated uncertainty of the GCI Roy method. Error estimates are multiplied by 3 as a simple safety factor.

Although in Figure 6.31 the uncertainty estimates are not matching perfectly, the trends and orders of magnitude are similar, especially for the moment error estimate. This suggests that with a more elaborate safety factor calculation the moment error estimator could be used for verified codes.

6.4.2 Application example on source S4 and S5

Finally the moment error estimates are plotted for the remaining two source locations, S4 in the street canyon in Figure 6.32 and S5 in the street intersection in Figure 6.33.

In both figures it is clear that the error bars of the experimental results and the simulation results are not overlapping in the profile plots on the left hand side. The location of the plots can be seen in Figure 6.24 and 6.25 for example marked with red lines. There is the lateral street at $X_F S = 0$, called cross street, a street with around 45° angle for both sources, and for S5 there is an additional at $Y_F S = 0$.

On the scatter plots the same can be found, results are far from the ideal line which would show exact matching. This essentially underpins what we have already seen and guessed, that the deviation from the experimental value is not caused by numerical discretization uncertainty, but by modelling error. The difficulty here is to find out in what ratio which modelling error takes place, namely differentiating the error of the underlying flow field which defines the convective fluxes, and the turbulence field with the simple gradient diffusion hypothesis closure which defines the turbulent scalar fluxes.

Here the aim was only to show that even a one-mesh estimator can give additional information to justify this kind of guesses, but it is not as accepted as the standard method. However, a one-mesh
Results and discussion: passive scalar dispersion calculation

Figure 6.30: Validated points in the 2m street canyon for the dispersion results

Figure 6.31: Comparison of the estimated uncertainty by GCI Roy to the error estimate methods
Figure 6.32: Estimated numerical error-3 with the moment method for source S4 see Figure 6.24 for profile locations.

Figure 6.33: Estimated numerical error-3 with the moment method for source S5 see Figure 6.25 for profile locations.
estimator is still more than no numerical discretization uncertainty estimation at all, what is often the case.

6.4.3 Discussion

In the final investigation of the thesis two one-mesh estimators were calculated and compared to the estimated uncertainty by the GCI Roy method for source S2. It was found that although no literature is available for their factor of safety to convert them to uncertainty estimators, using $FS = 3$ for the moment error estimator gives uncertainty estimates which have a similar trend than the standard method, although they give lower results. The moment error estimation method still needs thorough statistical investigation to suggest a more elaborate factor of safety for its usage, but it has a potential to make numerical discretization error and uncertainty estimation a more frequently used exercise for already verified codes. This helps the model development with clearly differentiating between numerical and modelling errors.

The following thesis statement is suggested from this Section:

**Thesis statement 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.

Results were published in Rakai and Franke 2014a.
Chapter 7

Conclusions

The main goal of the thesis was to evaluate the CFD flow and dispersion models from an operational point of view with proper solution verification and validation to differentiate between the deficiencies of the improper numerical resolution which is unavoidable for operational simulations and the deficiencies of the modelling approach.

I used a complex urban test case, Michelstadt, which has detailed flow and passive scalar dispersion measurements. The experiments were carried out in the Environmental Wind Tunnel Laboratory of the University of Hamburg and were at my disposal for the investigations. Well defined boundary conditions are available in the dataset thanks to the wind tunnel settings. Two components of the flow field as time series are included in the dataset, with dispersion time series from three different sources, and also short-term release measurements.

I carried out simulations for the flow field looking for the best available automatic meshing technique, and a thorough investigation of standard numerical discretization uncertainty estimating methods (Chapter 5). For the passive scalar dispersion I looked at different aspects which can cause error in the resulting scalar field, with an emphasis on the turbulent Schmidt number and anisotropic modelling and its sensitivity to source location. Additionally preliminary short-term release grid sensitivity and one-mesh error estimator performance was also shown (Chapter 6).

After it has been carried out I think the conclusion must be divided into two main part. An advice for operational modellers is given in Section 7.1. This is for people who would like to carry out simulations on a regular basis for wind comfort, air quality or emergency response purposes in a government or design office with the help of Computational Fluid Dynamics. Here clear instructions are given to reach a robust solution.

The other Section, 7.2, lists the thesis statements which I concluded from my PhD studies. They have more academic form, giving more information about possible model developments and their justification.

7.1 Advice for operational modelers

As a final note in the thesis a single model choice is given, based on the investigations and literature survey, which is the best for operational purposes in the opinion of the author. So the following instructions are designed for an environmental consulting or government office with low budget, one single strong PC and time constraints to finish a report on the environmental effects of a new construction.

As the open source code OpenFOAM® was found to be sufficient, and also its mesh generation tool, snappyHexMesh proved to be efficient, it is suggested to use that as the tool of the investigations to reduce licensing costs. The new versions of the code also include easily installable packages and built-in boundary conditions to model an atmospheric boundary layer inlet flow. See more details in Appendix A.
Inflow conditions are suggested to be based on Richards and Hoxey 1993 with the value corresponding fixed at the top of the domain. An .stl file of the investigated area must be generated, and a basic mesh must be built. For that the resolution of the street canyon can be based on the Best Practice Guideline Franke et al. 2007. The snappyHexMesh parameters must be set to allow maximum three stages of refinement. The maximum number of cells for a mesh to run on a PC can be estimated by Figure 5.4 as 1.5 times more than the RAM available in the computer. The body fitted hexahedral mesh of snappyHexMesh is suggested.

To reach convergence without instabilities it is recommended to run first with upwind discretization, than switch to 2nd order only for the momentum equation, and only finally run in full 2nd order convective discretization settings.

Dispersion is suggested to be calculated in a decoupled model, with a simple gradient diffusion hypothesis and $Sc_t = 0.7$ in an urban environment.

It is important to use the built in numerical error estimators of OpenFOAM®, the moment error estimator is suggested for the passive scalar results to have an idea of the numerical errors of the simulations.

### 7.2 Thesis statements

Investigations were carried out to evaluate the Computational Fluid Dynamics flow and dispersion models from an operational purpose point of view with proper solution verification and validation to differentiate between the deficiencies of the improper numerical resolution which is unavoidable for the operational simulations and the deficiencies of the modelling approach. The work can be both regarded as prognostic microscale obstacle resolving meteorological modelling and Computational Wind Engineering modelling. The following thesis statements were concluded:

**Thesis statement 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 simulations 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.

Results were shown in Section 5.2 and published in Rakai and Franke 2012b and Rakai et al. 2014b.

**Thesis statement 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.

---

1 For more details on OpenFOAM® specific settings see Appendix A
\[ VR = \frac{1}{N} \sum_{i=1}^{N} \delta_i \]
\[ \delta_i = \begin{cases} 
1 & D_i \leq U_{val} \\
0 & \text{for else} 
\end{cases} \]

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 \( k - \varepsilon \) to evaluate and compare the model performance including the numerical discretization uncertainty.

Results were shown in Section 5.3 and published in Rakai and Franke 2012a, Rakai and Franke 2013 and Rakai and Franke 2014a.

Thesis statement 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.

Results were shown in Section 6.1 and published in Rakai and Kristóf 2013, Rakai and Franke 2014b and Rakai et al. 2014a.

Thesis statement 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.

Results were shown in Section 6.2 and published in Rakai and Kristóf 2011 and Rakai and Kristóf 2013.

Thesis statement 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 $1m^2$ 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, which is considered good agreement for a comparison in both space and time.

Results were shown in Section 6.3 published in Rakai et al. 2014a.

**Thesis statement 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.

The results were shown in Section 6.4 and published in Rakai and Franke 2014a.
Chapter 8

Outlook

I was told once that a PhD thesis is never finished, it is always just stopped at a point in time to summarize what has been done and hopefully obtain the degree. This means the thesis is opening new directions which could not have been investigated thoroughly, some of which are listed here to motivate the reader to continue the research in urban Computational Fluid Dynamics.

- use scale resolving simulations and investigate numerical discretization uncertainty in time (inspired by Section 5.3)
- compare different turbulence model performances focusing on the regions where the deviation from the experiments was higher than the revealed uncertainties (inspired by Section 5.3)
- use finer resolution to see how the numerical discretization uncertainty can be further reduced
- use simultaneous flow field and dispersion measurements from Dezso-Weidinger et al. 2003 or Kukacka et al. 2012 to improve the turbulent scalar flux models (inspired by Section 6.1 and 6.2)
- carry out more detailed measurements for the Michelstadt case to be able to draw more conclusion on the simulation results, if possible with more measurements of the flow field and dispersion at the same locations (inspired by Section 6.1 and 6.2)
- carry out a full grid resolution sensitivity study for short-term release modelling, including timestep discretization error estimation (inspired by Section 6.3)
- elaborate analytical safety factors for one-mesh estimators and test their performance on the same test cases as the standard methods to increase their reliability and acceptability (inspired by Section 6.4)

Computational Wind Engineering and Microscale Obstacle Resolving Meteorology are an extensive field with a lot of unrevealed aspects, very active research community and high quality conferences, as a final sentence I encourage the reader to keep on investigating it.
Index

air quality forecasting, 1
anisotropic model, 11, 17, 80
Architectural Institute of Japan, 12
ASME VV standard, 7, 20, 27
Atmospheric Boundary Layer, 5, 35

Computational Wind Engineering, 1, 6
COST 732 Action, 12, 31, 35
COST C14 Action, 12
COST ES1006 Action, 11, 12, 31

evacuation response, 1
Ercoftac, 12, 37, 45
error classification, 6

gradient diffusion hypothesis, 17, 36, 71
Grid Convergence Index, 23

hit rate, 26, 43, 48

Large Eddy Simulation, 6, 11
linearUpwind, 20, 67

Method of Manufactured Solutions, 7, 20
microscale meteorology, 1, 6

non-orthogonality, 19, 44, 46
nonlinear turbulence models, 8
numerical error, 20, 23
numerical uncertainty, 20, 23, 56

operational models, 2, 44, 46
order of the discretization, 21, 55

passive scalar, 1, 10, 16, 36, 68

Richardson extrapolation, 21, 54

skewness, 19, 44
stagnation point anomaly, 8, 16
strong model concept, 27

turbulence modelling, 6, 15, 63

turbulent scalar flux, 17, 71
turbulent Schmidt number, 10, 17, 68, 73
turbulent viscosity, 16

URANS, 9

validation, 7, 20, 26
validation rate, 27, 59
validation uncertainty, 27, 59
VDI, 12, 49
verification, 7, 20
Own references

- A. Rakai and J. Franke (2014b). “Validation of two RANS solvers with flow data of the flat roof Michelstadt case”. In: Urban Climate 0, pp. –. DOI: http://dx.doi.org/10.1016/j.uclim.2013.11.003
- A. Rakai and J. Franke (2012b). “Validation of two RANS solvers with flow data of the flat roof Michel-Stadt case”. In: Proc. 8th International Conference on Air Quality – Science and Application, Athens, Greece
References


ERCOFTAC (2000). *Best Practice Guidelines*. Ed. by Casey, Michael and Wintergerste, Torsten. ERCOFTAC Special Interest Group on “Quality and Trust in Industrial CFD” (cit. on pp. 12, 16, 18, 37, 44).


References


Tominaga, Yoshihide et al. (2004). “Cross Comparison of CFD Results of Wind Environment at Pedestrian Level around a High-rise Building and within a Building Complex”. In: *Journal of Asian Architecture and Building Engineering* 3 (cit. on p. 1).
Yang, Yi. et al. (2007). “New inflow boundary conditions for modeling the neutral equilibrium atmospheric boundary layer in computational wind engineering”. In: *Journal of Wind Engineering and Industrial Aerodynamics* 97, pp. 88–95 (cit. on p. 12).
List of Figures
List of Figures

2.1 Location of the Atmospheric Boundary Layer in the troposphere by Stull 1988 .......... 6
2.2 Cross section contour plots of streamwise velocity and streamlines ......................... 9
2.3 Cross section contour plots of turbulent kinetic energy ................................. 10

3.1 Dosage based characterization of a puff (Harms et al. 2011) ......................... 18
3.2 Graphical representation of non-orthogonality ($\alpha$) and skewness ($\mu$) in a 2D nonconformal grid ................................................................. 19
3.3 Graphical explanation for calculating the order of grid convergence for Richardson extrapolation: change of solution with grid refinement/coarsening (left), computed observed order of grid convergence ($p$, right) .................................................. 22
3.4 Theoretical factor of safety ($FS$) of different methods based on the observed order of grid convergence ($p$) after Phillips and Roy 2011 ................................. 25
3.5 Inconsistency between face interpolation and the integration over a cell, the basis of residual error estimation method (from Jasak 1996) .............................. 26
3.6 The validation uncertainty with the strong model concept ($U_{input} = 0$) illustrated with two point-to-point comparisons extended to a validation uncertainty range ............ 28

4.1 Increasing complexity of wind tunnel models (photos from EWTL) ................ 32
4.2 Michelstadt computational domain with flow measurement points (triangles: vertical profiles, squares: horizontal planes, circles: street canyon planes), Building 33 and profile 29 and 62 highlighted ................................................................. 32
4.3 Source geometry in the wind-tunnel (from EWTL) ....................................... 33
4.4 Michelstadt with dispersion measurement points coloured differently for all used sources (2, 4 and 5), profile locations P7, P11 and P32 for source 2 highlighted .................. 34
4.5 Michelstadt with dispersion measurement points for puff measurements .......... 35
4.6 Coarsest surface meshes on Building 33, see location in Figure 4.2, note that the symbols in red will be used in the remainder of this work for plots to help to distinguish between mesh types ........................................................................................................ 37
4.7 Mesh sections in street canyon at ground level for the coarsest meshes ............... 38
4.8 Mesh cross sections at $y_{FS} = 0m$ .................................................................. 39

5.1 OpenFOAM® (OF) Fluent comparison for streamwise and lateral mean velocity at vertical profile 29 (see location in Figure 4.2), mesh codes are from Table 4.1 .................. 43
5.2 Different mesh quality metrics plotted as a function of cell number for the four different mesh types (recall labelling in Figure 4.6) .................................................... 44
5.3 Residual behaviour of a Cartesian mesh: first jump in residuals is caused by changing from full upwind to second order for only mean values, second jump by changing to full second order ............................................................. 46
5.4 Computational cost (memory usage - left and CPU time - right) of the simulations for the full upwind simulations, 4000 iterations ................................................................. 47
5.5 Sensitivity to discretization evaluated with the hit rate metric for four flow variables, streamwise and lateral mean velocities and their rms values (full upwind-11/mixed-21/full linearUpwind-22 results) ................................................................. 48
5.6 Sensitivity to discretization evaluated with the L2 metric for four flow variables, streamwise and lateral mean velocities and their rms values (full upwind-11/mixed-21/full linearUpwind-22) ................................................................. 49
5.7 Tetra (6.65 \cdot 10^6 cells) and hexa (8.0 \cdot 10^6 cells) mesh cross sections (diagonal lines are just visualization tool specific features in the hexa mesh), red horizontal lines indicate the height up to which high shear occurs ................................................................. 50
5.8 Profile 29 (recall location in Figure 4.2) of one tetra (6.65 \cdot 10^6) and hexa (8.0 \cdot 10^6) mesh (full second order discretization for the convective scheme), results for all measured flow variables ................................................................. 50
5.9 Observed difference between experiment and simulation, order of accuracy for all non-oscillatory points and used order by the method of Roy ................................................................. 54
5.10 Difference between experiment and simulation (|S - E|) and estimated absolute uncertainties of nondimensionalised velocity ................................................................. 55
5.11 Estimated numerical discretization uncertainties with the actual values in the 2m street canyon streamwise velocities ................................................................. 56
5.12 Non validated points in the 2m street canyon ................................................................. 59
5.13 The usage of the method for model development justification with tetrahedral mesh skew standard $k - \varepsilon$ closure, rke – realizable $k - \varepsilon$ closure ................................................................. 60
5.14 Vectors of the flow in the 2m street canyon, arrows: experiment – black hollow, simulation – gray full ................................................................. 61
6.1 Location of points where convergence was checked for the steady state passive scalar dispersion simulations for source 2 ................................................................. 65
6.2 Values of $L2$ norm for $C_s$ normalized passive scalar concentration as a function of cell number (triangle – tetrahedral, pentagon – polyhedral, square – Cartesian hexahedral, rotated square – body fitted hexahedral, recall Figure 4.6 for symbols) ................................................................. 66
6.3 Values of FAC2 metric for $C_s$ normalized passive scalar concentration as a function of cell number (triangle – tetrahedral, pentagon – polyhedral, square – Cartesian hexahedral, rotated square – body fitted hexahedral, recall Figure 4.6 for symbols) ................................................................. 67
6.4 Possible effects of flow field on dispersion: 9m flow vectors (black - experiment, red-simulation), 7.5m dispersion results (square - experiment, contour - simulation) dash-dot line and numbers: location of profiles) ................................................................. 68
6.5 Streamlines in street-canyons and 7.5m dispersion results (sphere - experiment, contour - simulation) ................................................................. 68
6.6 Dispersion metrics as a function of flow field metrics - $L2$ ................................................................. 69
6.7 Cross sections at profile locations with dispersion results (sphere - experiment, contour - simulation) ................................................................. 70
6.8 Scatter plot of the results from different mesh type simulations, results shown here are from the coarsest meshes, upwind convective discretization ................................................................. 71
6.9 Profiles of the results from different mesh type simulations, results shown here are from the coarsest meshes, upwind convective discretization. Note that $c_s$ scales are logarithmic except for the streamwise profile. ................................................................. 72
6.10 Scatter plot ................................................................. 73
6.11 Profiles ................................................................. 73
<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.12</td>
<td>Metrics as a function of ( Sc_t ) for source S2</td>
<td>74</td>
</tr>
<tr>
<td>6.13</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S2</td>
<td>74</td>
</tr>
<tr>
<td>6.14</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S2</td>
<td>75</td>
</tr>
<tr>
<td>6.15</td>
<td>Metrics as a function of ( Sc_t ) for source S4</td>
<td>75</td>
</tr>
<tr>
<td>6.16</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S4</td>
<td>76</td>
</tr>
<tr>
<td>6.17</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S4</td>
<td>76</td>
</tr>
<tr>
<td>6.18</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S5</td>
<td>77</td>
</tr>
<tr>
<td>6.19</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S5</td>
<td>77</td>
</tr>
<tr>
<td>6.20</td>
<td>Cross section for ( Sc_t = 0.4 ) and ( Sc_t = 0.7 ) for source S5</td>
<td>78</td>
</tr>
<tr>
<td>6.21</td>
<td>Scatter plot of the anisotropic model test, coarsest body fitted hexahedral mesh results</td>
<td>79</td>
</tr>
<tr>
<td>6.22</td>
<td>Profiles of the anisotropic model test, coarsest body fitted hexahedral mesh results</td>
<td>80</td>
</tr>
<tr>
<td>6.23</td>
<td>Cross section for anisotropic and isotropic approach for source S2</td>
<td>80</td>
</tr>
<tr>
<td>6.24</td>
<td>Cross section for anisotropic and isotropic approach for source S4</td>
<td>81</td>
</tr>
<tr>
<td>6.25</td>
<td>Cross section for anisotropic and isotropic approach for source S5</td>
<td>82</td>
</tr>
<tr>
<td>6.26</td>
<td>Comparison of mean puffs</td>
<td>84</td>
</tr>
<tr>
<td>6.27</td>
<td>Comparison puff parameters</td>
<td>85</td>
</tr>
<tr>
<td>6.28</td>
<td>Histograms of puff parameters from the experiment (courtesy of E. Berbekar)</td>
<td>86</td>
</tr>
<tr>
<td>6.29</td>
<td>Estimated numerical uncertainty with the GCI Roy method</td>
<td>88</td>
</tr>
<tr>
<td>6.30</td>
<td>Validated points in the 2m street canyon for the dispersion results</td>
<td>89</td>
</tr>
<tr>
<td>6.31</td>
<td>Comparison or the estimated uncertainty by GCI Roy to the error estimate methods</td>
<td>89</td>
</tr>
<tr>
<td>6.32</td>
<td>Estimated numerical error-3 with the moment method for source S4 see Figure 6.24 for profile locations</td>
<td>90</td>
</tr>
<tr>
<td>6.33</td>
<td>Estimated numerical error-3 with the moment method for source S5 see Figure 6.25 for profile locations</td>
<td>90</td>
</tr>
<tr>
<td>B.1</td>
<td>Scatter plot</td>
<td>126</td>
</tr>
<tr>
<td>B.2</td>
<td>Profiles</td>
<td>126</td>
</tr>
<tr>
<td>B.3</td>
<td>Scatter plot</td>
<td>127</td>
</tr>
<tr>
<td>B.4</td>
<td>Profiles</td>
<td>127</td>
</tr>
<tr>
<td>B.5</td>
<td>Scatter plot</td>
<td>128</td>
</tr>
<tr>
<td>B.6</td>
<td>Profiles</td>
<td>128</td>
</tr>
</tbody>
</table>
List of Tables

3.1 Choice of factor of safety (FS) and order of grid convergence (p) for the different methods to estimate numerical uncertainty from the estimated numerical error .......................... 24

4.1 Cell numbers (million cells) of the investigated meshes .................................................. 37

4.2 Size of the volume sources [m^3] for source S2 ................................................................. 37

5.1 Hit rates for OpenFOAM® / Fluent ......................................................................................... 42

5.2 Necessary iterations for convergence of the steady state flow field calculations (full upwind-11/mixed-21/full linearUpwind-22) ................................................................. 45

5.3 Summarizing the behaviour of the different meshing approaches ........................................ 52

5.4 Observed order of grid convergence with the global averaging method (p_{GA}) and grid convergence ratios of the investigated meshes, shown separately the ratio of theoretically correct orders (0.5 < p < 2) for streamwise and lateral mean velocity components .... 53

5.5 Grid convergence of mean velocity magnitude in the street canyons an example of evaluating integrated quantities, not point-to-point comparison values ........................................ 54

5.6 Different validation metrics (\|L2\| norm, hit rate HR and validation rates VR evaluated with the four numerical uncertainty estimation methods) compared for the streamwise and lateral velocity components for all mesh types .......................................................... 57

B.1 Hit rate metrics of results with second order discretization of the convective term for all measured variables of the flow field experiments ......................................................... 125
Appendix A

Practical issues with OpenFOAM®

This part of the thesis aims to give guidance on how to get to modelling an urban area with OpenFOAM® from the beginning. It is given as an appendix as it adds no scientific value, purely helps to overcome the difficulties of the steep learning curve of OpenFOAM® at the beginning.

It assumes basic knowledge of bash and OpenFOAM®, and most commands were used for OpenFOAM® 1.7.1 if not stated otherwise. Basic information can be found at:

- Official documentation: http://www.openfoam.org/docs/user/
- Community driven documentation: http://openfoamwiki.net/index.php/Main_Page
- Community driven development: http://www.extend-project.de/
- Basic course materials: http://www.tfd.chalmers.se/~hani/kurser/OS_CFD_2012/
- Community forum: http://www.cfd-online.com/Forums/openfoam-solving/

A.1 Mesh generation

To convert mesh from Fluent .msh or .cas file with scaling:

```
fluent3DMeshToFoam file.cas -scale 0.001 >convertLog&
```

To build the mesh with snappyHexMesh of OpenFOAM®, an .stl file of the geometry is necessary (MSgroundSnappy.stl in the example below). The most important part of the process is the surfaceFeatureExtract which will help later to have the mesh nicely snapped on edges, which exists only from 2.0. The example builds the mesh parallel on 4 cores and checks quality. First a blockMesh is needed from which snappyHexMesh will cut and refine around the geometry.

```
#!/bin/sh
# Source tutorial run functions
$WM_PROJECT_DIR/bin/tools/RunFunctions

cp system/blockMeshDict constant/polyMesh/
runApplication blockMesh
```
runApplication decomposePar
runApplication surfaceFeatureExtract --includedAngle 150 --writeObj
c  ontant/triSurface/MSgroundSnappy.stl michelstadt
runParallel snappyHexMesh 4
# tail --f log.snappyHexMesh
runApplication reconstructParMesh --latestTime
# tail --f log.reconstructParMesh
rm --rf constant/polyMesh/*
mv 2/polyMesh/* constant/polyMesh/
rm --rf 2
rm --rf constant/

For this this must be in snappyHexMeshDict (among the others of course):

snapControls
{
  nFeatureSnapIter 10;
}

A.2 Flow field calculation

A.2.1 Inlet BCs

For steady RANS calculations simpleFoam solver is used. To run on 16 cores and save results in a log file:

mpirun --hostfile hosts -np 16 simpleFoam -parallel >> log

From the boundary conditions the inflow is the most important. For the Richards and Hoxey 1993 inlet atmBoundaryLayerInletVelocity and atmBoundaryLayerInletEpsilon can be used which is an existing BC in OpenFOAM®.

To define a certain function as a profile, an additional application can be used, swak4foam which contains the groovyBC boundary condition which enables to define a function. (Documentation at wiki: http://openfoamwiki.net/index.php/Contrib/swak4Foam).

To define BC from measurements, TimeVaryingMappedFixedValue BC can be used.

A.2.2 Numerical and model settings

The system/fvScemes file contains the dicretization schemes for all equations. The schemes that were changed here for a full second order setup:

divSchemes
{
  default none;
  // div(phi,U) Gauss upwind:
Practical issues with OpenFOAM®

```cpp
5  div(phi,U) Gauss linearUpwindV cellLimited Gauss linear 1;
6 // div(phi,k) Gauss upwind;
7 div(phi,k) Gauss linearUpwind cellLimited Gauss linear 1;
8 // div(phi,epsilon) Gauss upwind;
9 div(phi,epsilon) Gauss linearUpwind cellLimited Gauss linear 1;
10 }
```

The system/fvSolution file contains linear equation solver settings, convergence limit can be
given for all equations separately and the relaxation factors are also set in that.
Boundary conditions are given in the 0/U etc variable files, the turbulence model can be changed in
constant/RASProperties.

A.2.3 Monitoring convergence

If the log file was saved, convergence of residuals can be monitored with gnuplot:

```bash
1 set logscale y
2 set title "Residuals"
3 set xlabel 'Residual'
4 set ylabel 'Iteration'
5 set terminal gif
6 set output 'residual.gif'
7 plot "< cat log | grep 'Solving for Ux' | cut -d ' ' -f9 | tr -d ',' title 'Ux' with lines lt rgb "forest-green" lw 2 pt 6, \
8 "< cat log | grep 'Solving for Uy' | cut -d ' ' -f9 | tr -d ',' title 'Uy' with lines lt rgb "blue" lw 2, \
9 "< cat log | grep 'Solving for Uz' | cut -d ' ' -f9 | tr -d ',' title 'Uz' with lines lt rgb "brown" lw 2, \
10 "< cat log | grep 'Solving for epsilon' | cut -d ' ' -f9 | tr -d ','," \n11 title 'epsilon' with lines lt rgb "gold" lw 2, \
12 "< cat log | grep 'Solving for omega' | cut -d ' ' -f9 | tr -d ','," \n13 title 'omega' with lines lt rgb "gold" lw 2, \
14 "< cat log | grep 'Solving for k' | cut -d ' ' -f9 | tr -d ','," \n15 title 'k' with lines lt rgb "dark-orange" lw 2, \
16 "< cat log | grep 'Solving for p' | cut -d ' ' -f9 | tr -d ','," \n17 title 'p' with lines lt rgb "violet" lw 2
```

Additionally integral variables or solution at certain points can be monitored adding to the end of a
controlDict file something like:

```cpp
1 functions
2 {
3    probes
4    {
5        type probes;
6        functionObjectLibs ("libsampling.so");
7        outputControl timeStep;
8        outputInterval 1;
9        probeLocations
10        (137.3 159.7 7.5)
11    );
12    fields
13    (}
```
This will print the value of \texttt{passiveC} at the point given at every timestep. This was used for monitoring convergence in dispersion calculations.

### A.3 Passive scalar dispersion calculation

There is no specific solver in OpenFOAM\textsuperscript{®} for turbulent dispersion calculations so a solver was written based on \texttt{scalarTransportFoam}.

```cpp
// define the basic equation without diffusion
dfScalarMatrix passiveCEqn(
    fvm::ddt(passiveC) + fvm::div(phi, passiveC);
)/ is there turbulent diffusion taken into consideration?
if (turbulentDiff > 0) // if this is turned on in the SIMPLE area of fvSolutions{
    Info<<"\nTurbulent diffusion turned on, turbulent Schmidt number SchT = 
éval(SchT)<<endl;
// add the isotropic Schmidt number based diffusivity part
passiveCEqn -= fvm::laplacian(nut/SchT, passiveC);
}
else{
    if (anisotropicDiff > 0) // if this is turned on in the SIMPLE area of fvSolutions{
        Info<<"\nAnisotropic diffusion coefficient tensor turned on"<<endl;
        scalar Cs1 = 0.134;
        scalar Cs2 = -0.032;
        volSymmTensorField Dtensor = ((Cs1 * (Foam::pow(k, 2)) / epsilon)*
            sphericalTensor::I) + (Cs2 * Foam::pow(k, 3) / Foam::pow(epsilon, 2)
            * symm(fvc::grad(U)));
        // add the tensor diffusivity part
        passiveCEqn -= fvm::laplacian(Dtensor, passiveC);
    }
    else{
        Info<<"\nTurbulent diffusion turned off"<<endl;
    }
}
// passiveCEqn.solve();
solve (passiveCEqn == passiveSource);
// solve (passiveCEqn);
```
The volume source term `passiveSource` is defined with the `setFields` utility of OpenFOAM®, where `setFieldDict` look like:

```
defaultFieldValues
{
  volScalarFieldValue passiveSource 0
};
regions
{
  nearestToCell
  {
    points ((-361.9 125.1 0));
    fieldValues
    {
      volScalarFieldValue passiveSource 10
    };
  }
};
```

The value 10 is given as it is easy to find in a text file. The volume of the source is necessary for the nondimensionalisation of the resulting concentration and it was done by looking up the same line number in a field which contained the cell volumes than the line number containing the `passiveSource` field.

This is a rather fast task even in huge fields with the `vi` editor:

```
vi passiveSource
:/10
vi cellVolume
:#line number
```

## A.4 One-mesh error estimation for the passive scalar

### A.4.1 Residual error estimate

```
{
  Info << "Reading passiveC" << endl;
  volScalarField passiveC(passiveCHeader, mesh);

  Info << "Reading U" << endl;
  volVectorField U(Uheader, mesh);

  #include "createPhi.H"

  errorEstimate<scalar> ee
  (
    resError::div(phi, passiveC)  
    - resError::laplacian(Dmolecular, passiveC)
  )
  ee.residual().write();
  volScalarField e = ee.error();
  e.write();
  mag(e).write();
}
```
A.4.2 Moment error estimate

```cpp
{ 
    Info << "Reading passiveC" << endl;
    volScalarField passiveC(passiveCHeader, mesh);
    Info << "Reading U" << endl;
    volVectorField U(Uheader, mesh);

dataInclude "createPhi.H"

    volVectorField gradpassiveC = fvc::grad(passiveC);
    volScalarField passiveCE = 0.5*sqr(passiveC);
    volScalarField L
    ( 
        IOobject
        ( 
            "L",
            mesh.time().timeName(),
            mesh,
            IOobject::NO_READ,
            IOobject::NO_WRITE
        ),
        mesh,
        dimensionedScalar("one", dimLength, 1.0)
    );

    L.internalField() = mesh.V() / fvc::surfaceSum(mesh.magSf())().internalField();

    // Divergence of the error in the passiveC squared
    volScalarField momError
    ( 
        IOobject
        ( 
            "momErrorL" + passiveC.name(),
            mesh.time().timeName(),
            mesh,
            IOobject::NO_READ,
            IOobject::NO_WRITE
        ),
        sqrt
        ( 
            2.0*mag
            ( 
                fv::gaussConvectionScheme<scalar>
                ( 
                    mesh,
                    phi,
                    tmp<surfaceInterpolationScheme<scalar>>
                )
            )
        )
    );
```
Practical issues with OpenFOAM®

A.5 Evaluation of the results

The paraView program suggested for OpenFOAM® is useful to have a look at the whole field or the mesh, but a more efficient for evaluation is to extract values at the interesting location and deal only with those files. It can be done with the sample utility. A typical sampleDict file:

```plaintext
setFormat raw;
surfaceFormat raw;
interpolationScheme cellPointFace:
fields
(passiveC);
sets
(allS2points
{
    type cloud;
    axis xyz;
    points (137.11 159.7 7.5);
});
surfaces
(surface
{
    type plane: // always triangulated
```
This enables to extract at the measurement points and also 2D surfaces for easier visualization of planes.

After this most of the post processing was done using gnuplot, GNU octave and Tecplot.
## Appendix B

### Additional figures and tables

<table>
<thead>
<tr>
<th>mesh</th>
<th>( U/U_{ref} )</th>
<th>( V/U_{ref} )</th>
<th>( U_{rms}/U_{ref} )</th>
<th>( V_{rms}/U_{ref} )</th>
<th>( uv/U_{ref}^2 )</th>
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<tr>
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<td>0.47359</td>
<td>0.60612</td>
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<tr>
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<tr>
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<tr>
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<tr>
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<td>0.48239</td>
</tr>
</tbody>
</table>

Table B.1: Hit rate metrics of results with second order discretization of the convective term for all measured variables of the flow field experiments
Additional figures and tables

Figure B.1: Scatter plot

Figure B.2: Profiles
Figure B.3: Scatter plot

Figure B.4: Profiles
Figure B.5: Scatter plot

Figure B.6: Profiles