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BEST PRACTICE GUIDELINE FOR THE CFD SIMULATION OF FLOWS IN THE URBAN ENVIRONMENT

Jörg Franke, Antti Hellsten, Heinke Schlünzen, Bertrand Carissimo

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**BEST PRACTICE GUIDELINE
FOR THE CFD SIMULATION OF FLOWS
IN THE URBAN ENVIRONMENT**

Edited by:

Jörg Franke, Antti Hellsten, Heinke Schlünzen, Bertrand Carissimo

COST Action 732

**QUALITY ASSURANCE AND IMPROVEMENT OF
MICROSCALE METEOROLOGICAL MODELS**

1 May 2007

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1 Background and Context

The main objective of the COST Action 732 is the improvement and quality assurance of microscale obstacle-accommodating meteorological models and their application to the prediction of flow and transport processes in urban or industrial environments (Schatzmann and Britter, 2005). The name microscale obstacle-accommodating meteorological models is used to discern them from cloud resolving models which are microscale meteorological models as well. Subsequently the short term CFD-code is often used as a synonym for the lengthy name ‘microscale obstacle-accommodating meteorological model’.

The quality assurance of the application is closely related to the users' knowledge of the models. Actually, numerical simulation is mainly a knowledge based activity as has been stated by Hutton (2005) and Coirier (2005). While both refer to CFD codes, their statement is also valid for non-CFD codes. The knowledge is, in general, most effectively transferred by the formulation of a best practice guideline (BPG) for the intended application, which is the prediction of dispersion in urban areas at neighbourhood and street scale (Hanna & Britter, 2003) within this COST Action. However, even for this well-defined application the formulation of BPGs faces the problem of giving general advice for specific problems that may vary substantially although belonging to the same field. The most up to date and complete BPG for industrial CFD from ERCOFTAC (Casey & Wintergerste, 2000) also acknowledges this problem with the introductory statement that it offers “roughly those 20% of the most important general rules of advice that cover roughly 80% of the problems likely to be encountered”. The following BPG is therefore also not exhaustive but tries to cover as many aspects of the proper usage of CFD for the prediction of urban flows as possible. Non-CFD codes are not addressed in this document.

The BPG is based on published guidelines and recommendations that are introduced in section 5.1. These works mainly deal with the prediction of the statistically steady mean flow and turbulence in the built environment for situations with neutral stratification. The BPG is therefore mainly focusing on statistically steady RANS simulations of the flow and turbulence for situations with neutral stratification. However, users of other models like unsteady RANS (URANS) and LES models should consider the same suggestions. More, but still not comprehensive, information for URANS and LES applications is given in the corresponding paragraphs. The guidelines presented here can be used directly within the COST action 732 which concentrates on the flow field in urban areas and the dispersion of a passive scalar, with similar density as the background fluid and where thermodynamic or chemical processes will not be taken into account. For this COST action an extension of the section on unsteady flow simulations, especially Large Eddy Simulation, will be one of the main targets as these methods will play an increasingly important role in the near future.

Dispersion modelling is also not addressed at this stage because specific guidelines or recommendations on this topic are not yet available from the literature. Guidance will be extracted in the course of the COST Action from the results of the simulations used for the validation of the numerical models. As CFD and non-CFD codes will be validated, BPG for non-CFD codes will also be available at the end of the action.

2 Introduction

This document provides best practice guidelines for undertaking simulations that are used to evaluate microscale obstacle-accommodating meteorological models. First the different sources of errors and uncertainties that are known to occur in numerical simulation results are listed and defined. The sources of error that can be controlled and quantified by the user are then discussed in detail and best practice guidelines for their reduction and quantification are given. These best practice guidelines are based on available guidelines as far as possible. For topics that have not yet been covered by existing guidelines further needs for research within this COST action are indicated.

For the evaluation of CFD codes it is necessary that all the errors and uncertainties that cause the results of a simulation to deviate from the true or exact values are identified and treated separately if possible. Several classifications of these well-known errors and uncertainties exist. The most general discrimination divides them into two broad categories (Coleman & Stern, 1997)

- Errors and uncertainties in modelling the physics
- Numerical errors and uncertainties

The errors and uncertainties in modelling the physics arise from the assumptions and approximations made in the mathematical description of the physical process

- simplification of physical complexity
- usage of previous experimental data
- geometric boundary conditions
- physical boundary conditions
- initialisation

Numerical errors and uncertainties result from the numerical solution of the mathematical model. The sources for the numerical errors and uncertainties are

- computer programming
- computer round-off
- spatial discretisation
- temporal discretisation
- iterative convergence

When performing validation simulations it is mandatory to quantify and reduce the different errors and uncertainties originating from these sources. The following sections 3 and 4 therefore first provide a definition of the error or uncertainty. Finally section 5 provides best practice advice on how to avoid errors and where this is not possible how to estimate and reduce errors and uncertainties in the numerical solutions. These best practice guidelines are meant to avoid or at least reduce what is known as user errors. User errors originate from the incorrect use of CFD and related codes due to either a lack of experience or a lack of resources. In the course of a simulation the user may make mistakes or unwise choices, which then manifest themselves as one, or more, of the above mentioned errors. In addition, the user should be aware of the uncertainties that exist in the simulation of flow and dispersion in the urban or industrial environment.

In the appendices there are examples of common practice from two participating institutions of this COST 732 action together with best practice advice for the use of the flow solver MISKAM (Eichhorn, 2004).

3 Modelling errors and uncertainties

3.1 Simplification of physical complexity

In general, it is necessary to use a simplified mathematical model of reality to render a simulation feasible. The most prominent example is the use of turbulence closure models. The Navier-Stokes equations are normally used to model the flow in the atmospheric boundary layer. However, their direct solution to describe the turbulent flow is prohibitively expensive in the area of urban flow problems. What is known as Direct Numerical Simulation is at present restricted to flows with low Reynolds numbers in relatively simple geometries because of the very large range of scales that have to be resolved. The physical complexity of turbulent flows is reduced by using the averaged Navier-Stokes equations where averaging is performed in space for Large Eddy Simulations and in time for the Reynolds-Averaged approach. The solution of these averaged equations however requires turbulence closure models that describe the influence of the unresolved scales on the resolved flow field. These approximate models then introduce errors and uncertainties to the results of the numerical solution. The same is true when introducing approximations to the continuity equation (e.g. the anelastic approximation, non-divergent flows).

When the atmosphere is not neutrally stratified, prognostic equations have to be solved for the temperature and, if humidity effects are of relevance e.g. for chemical reactions, for humidity. Furthermore, prognostic equations have to be solved for liquid water and solid water components, if liquid water effects (e.g. chemical reactions) or solid water effects (e.g. fog formation, snow drift) are relevant. The effect of temperature, humidity and other compounds in the air on air density needs to be considered in the model by either solving the full continuity equation or by employing the Boussinesq approximation.

Generally, the equations are solved on the rotating Earth, resulting in a change of wind direction with height owing to the Coriolis force. This is included in most meteorological microscale obstacle-accommodating models. The effect of the Coriolis force is, however, of little relevance in microscale domains and it thus may be neglected. The main influence of the Coriolis force needs however to be included in the model by properly selecting the incoming flow profile (VDI, 2005).

The different approaches for simplifying the physical complexity are introduced and briefly discussed in section 5.3.

3.2 Usage of previous data

This point mainly refers to adjustable parameters used within the model that were specified using data from earlier experiments. The equations of state, the kind of dependence of viscosities and diffusivities on the thermodynamic variables and the data for chemical kinetics are examples of such data that have some inherent uncertainty.

3.3 Physical boundary conditions

The computational domain normally contains only a part of the urban or industrial area. Therefore the choice of the position of the boundaries of the computational domain influences the results. This influence definitely adds to the uncertainty of the simulation results but can also lead to errors if the choice is inadequate.

The influence of the external surroundings on the flow and dispersion within the computational domain is taken into account with the prescription of the behaviour of the flow variables at the boundaries. For the boundaries through which the flow enters the computational domain complete information on all flow variables is necessary. Many experiments do not provide this information. Thus the necessary approximation of some or all flow variables at the inflow boundaries adds to the uncertainty of the numerical results. This is also the case for the choice of the boundary conditions at solid walls. Here especially the prescribed roughness and the chosen wall functions are important. For boundary layer flows the roughness at the ground has to be chosen in accordance with the prescribed inflow profile of the velocity.

Recommendations on the prescription of physical boundary conditions are given in section 5.6.

3.4 Geometric boundary conditions

Defining the computational domain in which the flow and dispersion field shall be computed requires knowledge of the geometrical details of the urban or industrial environment. This information is often not available with sufficient accuracy. The missing information therefore adds to the uncertainty of the simulation results, as the simulated geometry and the experimental geometry do not have to be the same.

Another source of error and uncertainty within this context is the simplification of the geometrical complexity present in the experiment. To reduce the computational costs geometric details are often omitted. How to rationalise this omission is described in section 5.4 together with recommendations on the size of the built environment that should be taken into account.

4 Numerical errors and uncertainties

4.1 Computer programming

This point pertains to CFD codes in general and therefore to the code developers' area of responsibility. Computer programming or software errors are mistakes that exist in the computerised model. Errors that have been made while programming the conceptual model can be detected and removed with the aid of code verification as described in Appendix A.2 and briefly in the Background and Justification Document of COST action 732 (COST732, 2007). Other errors can originate from the use of the code on different platforms (hardware, operating systems, compilers, run-time libraries). These errors are treated within the realm of software quality engineering (Oberkampf et al., 2004). Both kinds of errors do not fall into the responsibility of the code users.

4.2 Computer round-off

Computer round-off errors result from the finite representation of numbers by the computer. Single precision numbers are stored in 32 bits and, for example, have a relative precision of 6-7 decimal places in FORTRAN 95. Double precision numbers use 64 bits of storage and have a relative precision of 14-15 decimal places in FORTRAN 95. Commercial CFD codes are normally available as single and as double precision. Executable, microscale obstacle-accommodating meteorology models generally use double precision.

4.3 Spatial and temporal discretisation

The spatial and temporal discretisations are probably the most crucial sources of numerical error (Casey & Wintergerste, 2000). These errors describe the difference between the exact solution of the basic system of partial differential equations and the numerical solution obtained with finite discretisation in space and time. In theory, the analytical solution is approached with refinement of the discretisation (increased resolution) when the discretisation scheme is consistent. However mesoscale model studies have shown that an increased resolution does not necessarily improve the model results (Belair et al., 1998). The reasons for this are not fully clear, but shortcomings in the parameterisations applied are one very probable reason (Schlünzen & Katzfey, 2003). The model formulation of microscale obstacle-accommodating meteorological models, similar to mesoscale models, must be dependent on the model resolution. For example, sub-grid-scale turbulence parameterisations need to describe only that part of the energy spectrum which is sub-grid scale. In fact, the RANS parameterisations do not correctly include a scale dependence, since they are based on time averages and do not include changes resulting from increases in resolution. Therefore, meteorological RANS and URANS models do not fulfil the theoretical requirement of consistent schemes, if the sub-grid-scale parameterisations used are not adjusted.

With regard to the space discretisation, it is not only the degree of resolution that is important but also the distribution of the grid points. Therefore the mesh used to discretise the space is of great importance for the accuracy of the results. Recommendations for the meshes are given in section 5.7.

Another important aspect is the approximation of the spatial and temporal variation of the flow variables. This is normally done by a polynomial representation of the variation, which then serves to define the order of a numerical approximation with regard to the truncation error of a Taylor series expansion. Recommendations on proper methods for the spatial and temporal approximations are provided in section 5.8.

4.4 Iterative convergence

The non-linear algebraic system that results from the discretisation of the basic system of partial differential equations is either entirely or partly solved with an iterative method or by time integration towards a steady state. If the iteration or time integration is stopped too early then the iterative convergence error is the difference between this intermediate solution and the exact solution of the algebraic system of equations. Judgement of the iterative convergence is normally based on the residuals, which indicate how far the present solution is away from the exact solution within

each cell. The monitoring of the residuals is based on scaled norms of the residual vector for each conservation equation.

In addition to the residual, the physical target values are normally monitored with the iteration number or with time. Convergence can then also be checked by requiring that these values become constant with the iteration number or with time. Recommendations on iterative convergence are summarised in section 5.10.

5 Best Practice Guideline

5.1 Review of existing guidelines

As stated in section 1 best practice guidelines provide procedures for the model user so as to estimate and reduce errors and uncertainties in the results of a numerical simulation. There are several initiatives to establish best practice guidelines in the field of flow simulation for the built environment. For industrial CFD in general the ERCOFTAC Best Practice Guidelines exist (Casey & Wintergerste, 2000) and these provide valuable information on general topics of CFD that are also relevant for the intended applications of this COST action. However, topics particular to atmospheric boundary layer flows have been deliberately omitted. The ERCOFTAC guidelines also focus on the industrial end user of CFD codes and not on the evaluation and validation of CFD codes. Best practice guidelines based on the ERCOFTAC guidelines modified and extended specifically for CFD code validation, have been presented by Menter et al. (2002) within the EC project “Evaluation of Computational Fluid Dynamic Methods for Reactor Safety Analysis (ECORA)”.

Best practice guidelines on CFD for wind engineering problems have been also published by the Thematic Network for Quality and Trust in the Industrial Application of CFD (QNET-CFD, <http://www.qnet-cfd.net>). Within that network the Thematic Area on Civil Construction and HVAC (Heating, Ventilating and Air-Conditioning) and the Thematic Area on the Environment present amongst other things best practice advice for the simulation of flow with and without dispersion (Scaperdas & Gilham, 2004; Bartzis et al., 2004).

Besides these European activities the Architectural Institute of Japan has a cooperative project for CFD prediction of the wind environment. In this project a detailed comparison of numerical methods for the simulation of the flow around single high-rise buildings and an idealised urban geometry is made, as well as a first comparison of numerical methods when applied to a real urban area (Mochida et al., 2002; Tominaga et al., 2004; Yoshie et al., 2005). The specific purpose of the comparison is the analysis of the predictive capability of CFD for pedestrian wind comfort in the built environment.

For the same application a working group of the COST action C14 “Impact of Wind and Storms on City Life and Built Environment” has compiled recommendations for conducting a CFD simulation from a literature review (Franke et al., 2004). This compilation also contains a section on the validation requirements for CFD codes.

Pankus (2000) suggests, and applies, test cases to evaluate obstacle-accommodating microscale obstacle-accommodating meteorology models. The guideline of the VDI (the German Association of Engineers) concentrates on evaluation and validation of these models for flow around buildings and obstacles (VDI, 2005). It contains a few

general recommendations for the set-up of the numerical model, the grid to be selected and includes several test cases, the corresponding comparison data sets and evaluation measures.

Thus there are several existing guidelines available, at least for the computation of the flow in the urban and industrial environment with the statistically steady RANS equations for neutrally stratified flow fields. The best practice guidelines presented in the following are based on the works cited above and therefore are mainly intended for the solution of the RANS equations for neutrally stratified flow fields with limited attention paid to the dispersion modelling. Only general guidelines are extracted as most parameters depend to a large extent on the details of the application problem. Because the possible validation test cases have just been selected it is impossible to present more specific guidelines. For non-neutrally stratified flow, for example, additional guidelines are necessary.

The guidelines are structured according to the general steps of conducting a numerical simulation (Casey & Wintergerste, 2000; Franke et al., 2004; Menter et al., 2002).

- Choice of target variables
- Choice of approximate equations describing the physics of the flow
- Choice of geometrical representation of the obstacles
- Choice of computational domain
- Choice of boundary conditions
- Choice of initial conditions
- Choice of computational grid
- Choice of time step size
- Choice of numerical approximations
- Choice of iterative convergence criteria

As this structure might indicate a single sequential way to conduct a numerical simulation, it should be stressed at this point that there is interdependence among these steps. In general, the numerical simulation requires iteration within these steps. Therefore this guideline is specific about the initial parameter choice and recommends the proper way of identifying the sensitivity of the numerical simulation results for the target values on the corresponding parameters like boundary conditions, turbulence closure models or grid resolution. The recommended strategies refer to ideal situations which might not be encountered in all simulations due to resource limitations or failure of the strategies in principle. It should be however always tried to estimate the errors and uncertainties in the results.

5.2 Choice of target variables

As proposed by Schlünzen (1997) and Menter et al. (2002) the first step should be the definition of the target variables. These should include the variables that are representative of the goals of the simulation and those that can be compared with the corresponding experiments. Further criteria are (Menter et al., 2002):

- Sensitivity to numerical treatment and resolution

- Computation with existing post-processing tools
- Computation inside the solver and ideally display during run-time

The first point is important as the target variables should be indicative of the numerical errors and uncertainties. The last two points simplify the definition and the monitoring of the variables which is especially important for the judgement of iterative convergence.

5.3 Choice of approximate equations describing the physics of the flow

The choice of the basic equations has the largest impact on the modelling errors and uncertainties. First it has to be decided whether the application requires an unsteady or a steady treatment. As the atmospheric boundary layer flow is turbulent, an unsteady treatment is required in principle. The turbulent flow within urban or industrial environments is in general modelled by the Navier-Stokes equations. Temperature and humidity equations as well as equations for liquid and solid water compounds need to be considered if relevant for the simulations (e.g. non-neutral atmospheric stratification, small wind speeds and large temperature gradients). However, in many cases, approximations may be used that still ensure reliable model results.

When pollution dispersion is taken into account, then one or more additional transport equations for the pollutant(s) have to be solved. Depending on the state of the pollutants (gaseous, liquid, solid) further physical complexities like chemical reactions, break-up, coalescence, evaporation and particle-particle interaction may have to be modelled. Neglecting liquid and solid pollutants one still has to decide whether the gaseous pollutant affects the flow field through a substantial change in density.

For simulating flow within the obstacle layer the full compressible equations do not have to be solved but simplifications may be used (VDI, 2005). These include the anelastic approximation jointly used together with the Boussinesq approximation (Wippermann, 1981). If only the lowest 200 m of the atmosphere are investigated, the assumption of non-divergent flow fields and constant density might be used without losing accuracy in the model results. If temperature heterogeneities or concentrations of pollutants with densities different from air are to be included, the Boussinesq approximation has to be applied and, in addition, prognostic equations for the potential temperature and the concentration need to be solved, together with the full continuity equation or the anelastic approximation of the continuity equation.

The effect of changes in wind direction with height is to be included in the model by properly selecting the incoming flow profile (VDI, 2005). In addition, the model may have to consider the Coriolis force explicitly.

Even in the simplest case in which the density can be treated as a constant which is normally done in the context of flows in urban areas (Castro, 2003), the continuity, momentum and gaseous pollutant transport equations cannot directly be used to compute the flow and dispersion due to the turbulent nature of the flow. The direct solution of these equations would require the resolution of all the spatial and temporal scales which is impossible in the foreseeable future due to insufficient computational resources. Thus the system of equations has to be simplified to render it numerically solvable. This is accomplished by averaging the basic equations to filter out the many scales of the turbulent flow and selecting a turbulent closure to model these filtered out scales.

5.3.1 *Steady RANS*

A common average is the (infinite) time average leading to a statistically steady description of the turbulent flow. While this averaging is very effective as it eliminates the time dimension it is questionable whether the resulting equations are still a useful model of the inherently unsteady meteorology. However, for a comparison with wind tunnel experiments, these so called Reynolds Averaged Navier-Stokes (RANS) equations are an adequate representation of the wind tunnel's reality as the time averaged approach flow conditions of the tunnel do not change.

The influence of the removed scales on the mean flow field has to be modelled. In the momentum equation the averaged scales appear as the Reynolds stress tensor and in the scalar equation as the vector of turbulent transport. For the Reynolds stress tensor two main modelling approaches are generally employed. In the first approach, the eddy viscosity hypothesis (1st order closure) is used that relates the turbulent stresses to the velocity gradients of the mean flow. Depending on whether this dependence is linear, as with molecular stresses, or non-linear, leads to linear and non-linear eddy viscosity models. With these models the modelling effort is reduced to the specification of the eddy or turbulent viscosity (exchange coefficient for momentum) in terms of the local turbulence in the flow. Spalart & Allmaras (1992) developed a turbulence model based on a transport equation for the turbulent viscosity. The most common models relate the eddy viscosity to two scalars which are representative of the turbulence in the flow. This is normally the turbulent kinetic energy and its dissipation or specific dissipation or a turbulent length scale. If for each of these two scalars an additional transport equation is solved in which further modelling assumptions are incorporated, one talks of two equation modelling. In one-equation models only one additional transport equation with further approximations is solved (usually for the turbulent kinetic energy) and the length scale is determined from algebraic relations.

The second modelling approach for the Reynolds stress tensor is known as Reynolds Stress Modelling (RSM) or, more accurately, as Second Moment Closure (SMC), known also as second order closure. Within this approach, additional transport equations are solved for each of the Reynolds stresses and the dissipation of the turbulent kinetic energy. The modelling need is shifted towards the higher moments appearing in these transport equations.

For both modelling approaches a separate treatment for the turbulence close to the wall is necessary. Normally the wall function approach for rough walls is used which is further discussed in section 5.6.

Concerning the performance of the various turbulence models available within the two basic modelling approaches no definite statement is possible. The performance is highly application-dependent and depends also on the mesh resolution. A literature review of the application of many different turbulence models for the flow around single and multiple obstacles can be found in Franke et al. (2004). Further comparisons can be found e.g. in Yoshie et al. (2005) and in Franke & Frank (2005). All of them are restricted to the mean flow and turbulence.

Like the Reynolds stresses the turbulent transport of scalars (e.g. temperature, concentrations) has to be modelled. Nearly exclusively first order closure models are used for that purpose. They are based on the Reynolds analogy between turbulent momentum and scalar transfer. Within these models the turbulent flux is proportional

to the gradient of the mean scalar. The exchange coefficient for scalars is computed from the eddy viscosity (exchange coefficient for momentum) and the turbulent Schmidt number (relation of turbulent exchange coefficient for momentum and for heat).

As for the Reynolds stresses, SMC is also possible for the turbulent scalar transport. For the temperature as scalar several SMC models exist that solve four additional scalar equations, three for the components of the turbulent heat flux vector and one for the dissipation of the temperature fluctuations. But there seem to be no applications of these models for pollution dispersion within the urban or industrial environment.

No best practice advice for the choice of the turbulence models is given here. Rather a validation strategy is proposed to evaluate the performance of the different turbulence models. The validation test cases should be computed with several different turbulence models for the Reynolds stresses. The results should be compared with available measurements of the velocities and the Reynolds stresses. In the absence of reliable measurement data, no direct validation can be made. In such situations, it is recommended to look for simpler test cases with reliable reference data (Oberkampf et al., 2004). The test cases to be chosen must include the critical basic features of the actual problem of interest. There are usually several critical basic features present in complex urban-scale problems. On the other hand, a good validation test case ideally involves only one isolated critical feature. Therefore, the models should be validated for several different test cases. A key question here is: how to identify the critical features of a given problem? Again, it is difficult to give any general advice. The identification of the critical features requires experience and understanding about the flow of interest and about the turbulence modelling, the specific weaknesses of different modelling approaches and individual models.

After validating the turbulence models for the Reynolds stresses, different models for the turbulent scalar transport should be tested, including SMC models. If the pollutant can be treated as a passive scalar, the simulation of the dispersion can be done as post-processing. This is the most efficient way to test several turbulent flux models with a given flow and Reynolds stress distribution. By independently comparing the computed flow and Reynolds stresses with experiments and the computed mean scalar distribution with experiments it is possible to detect whether differences between simulation and experiment are mainly due to the inadequate prediction of the flow or the inadequate prediction of the scalar field. From these comparisons suggestions for improved modelling can be derived.

5.3.2 Unsteady RANS (URANS)

The turbulence models described above within the statistically steady RANS approach are also used for what is known as Unsteady RANS (URANS). The basic equations of URANS are formally derived by applying ensemble averaging. Only with ensemble averaging the resulting equations comply with the steady RANS equations now containing the partial time derivatives. This is not the case when time averaging is performed over finite time intervals, either with or without a moving average (Gryning & Batchvarova, 2005; Aldama, 1990). Besides these theoretical subtleties URANS depends strongly on the turbulence models that are used with it. In general, two-equation models are used which produce less eddy viscosity than the standard k- ϵ model (Launder & Spalding, 1972). As the approach also requires a high spatial

resolution it is recommended to directly use Detached or Large Eddy Simulations which are briefly introduced next.

URANS however also allows for simulating temporal changes in the flow field caused, for example, by different surface temperatures (Kim & Baik, 1999; Louka et al., 2002; Bohnenstengel et al., 2004; Tsai et al., 2005).

5.3.3 *Large Eddy Simulation (LES) and hybrid RANS-LES approaches*

The LES approach is based on the spatially filtered Navier-Stokes equations where the filtering is performed over a small volume related to, but not necessarily equal to, the local grid size. The influence of the unresolved spatial scales then has to be modelled with what is known as a sub-filter model in LES. The hybrid RANS-LES approach uses the URANS approach near walls and LES elsewhere. This is because near walls even the largest turbulent eddies are very small if the Reynolds number is not small. This fact renders pure LES of high Reynolds number wall-bounded flows difficult or impossible.

The concept of Detached Eddy Simulation (DES) proposed by Spalart et al. (1997) is perhaps the most widely known hybrid modelling strategy. DES uses the one-equation turbulence model of Spalart & Allmaras (1992) which uses the minimum of a measure of the local wall distance and the local cell size as characteristic length scales for the unresolved scales. Near walls it may also be used with the wall-function approach in urban applications, although it is originally designed to be solved down to the wall. The same is done in the sub-filter models of LES which normally do not resolve the boundary layer at the obstacles in urban applications. The hybrid methods, such as DES, can be seen as more advanced alternatives to the LES-wall-function technique. However, one should remember that matching URANS and LES is not free of problems. URANS and LES are fundamentally different approaches; hence there is no strict justification for such matching. The matching is always approximate and gives an additional contribution to the modelling error.

For the sub-filter stresses away from the walls algebraic relations are mostly used. However one- and two-equation models also exist. Another option is to entirely neglect the modelling of the sub-filter stresses in the basic equations and use the built-in dissipation of advanced numerical approximations for the convective terms. This approach is known as MILES (Monotonically Integrated Large Eddy Simulation) and has been successfully applied to many flow problems (e.g. Grinstein & Fureby, 2004), including urban dispersion (Patnaik & Boris, 2005). Both LES and hybrid approaches may lead to similar results when solved on the same mesh with the same time step size, as was shown by Breuer et al. (2003) for LES and DES.

Both methods perform in general better than RANS and URANS methods (see Franke et al., 2004 for a brief review). The reason is that a large part of the unsteady turbulent motion is resolved and only the small scales are modelled. Furthermore, LES and hybrid methods provide much more information about the flow field and the dispersion process than the RANS approach which directly gives only the mean field and provides only statistical estimates for the turbulent transport. This may be an important point in urban dispersion problems in, for example, street canyons where fluctuations may dominate the flow field over a possibly weak mean field. Due to the unsteady simulation, these approaches allow also for the prediction of instantaneous maximum and minimum concentrations. They need, however, substantially greater computing times than RANS. Additionally, they require time and space resolved data

as boundary conditions to properly simulate the inflow. This means that highly resolved experimental data is needed to provide the input conditions. Such data is rarely available in practice, and therefore the above requirement may be extremely difficult to satisfy.

5.4 Choice of the geometrical representation of obstacles etc.

Normally the distribution of buildings has the greatest impact on wind flow patterns. Secondary influence factors in the urban area include vegetation, orography and surface characteristics (e.g. roads, grass, sand). The level of detail required for individual buildings is dependent on their distance from the central area of interest. Buildings further away may normally be represented as simple blocks.

The central area of interest should be reproduced with as much detail as possible. This naturally increases the number of cells that are necessary to resolve the details. The available resources therefore limit the details which can be reproduced. To assess the influence of the omission of details simulations can be made with and without inclusion of details in a small region around the central area. The comparison of the respective results then shows the influence of the details.

If the exact geometry of the buildings or vegetation, orography and surface characteristics are not known, the sensitivity of the results on the geometry has to be tested. As for all other uncertain parameters, at least two settings should be examined (Menter et al., 2002; VDI, 2005).

5.5 Choice of the computational domain

The size of the entire computational domain in the vertical, lateral and flow directions depends on the area that shall be represented and on the boundary conditions that will be used. For LES one additional requirement on the overall size of the computational domain is that it is large enough to contain also the largest, energetically relevant flow structures.

The extent of the built area (e.g. buildings, structures or topography) that is represented in the computational domain depends on the influence of the features on the region of interest. An experience from wind tunnel simulations is that a building with height H_n may have a minimal influence if its distance from the region of interest is greater than $6-10H_n$. Thus as a minimum requirement a building of height H_n should be represented if its distance from the region of interest is less than $6H_n$. In case of uncertainty about the influence of distant features on the flow and dispersion in the area of interest it is recommended to perform simulations with and without the features, i.e. larger and smaller built areas. All recommendations presented in the following sections depend on the boundary conditions which are generally applied. These boundary conditions are presented in section 5.6. Furthermore a computational domain of cuboid shape is presumed.

5.5.1 Vertical extension of the domain

For single buildings the top of the computational domain should be at least $5H$ above the roof of the building, where H is the building height (Hall, 1997; Cowan et al., 1997; Scaperdas & Gilham, 2004). In contrast to this proposal, VDI (2005) suggests a blockage dependent distance between the computational domain's top and the building, where the blockage is defined as the ratio of the projected area of the building in flow direction to the free cross section of the computational domain. For a

small blockage, $4H$ is suggested, and $10H$ for a large blockage. Based on the guidance for wind tunnel modelling (VDI, 2000) the maximum blockage is suggested to be below 10% (VDI, 2005). In the CFD community a smaller maximum blockage of 3% is normally recommended, based on the results of Baetke et al. (1990) for the flow over a wall mounted cube.

The large distances given above are necessary to prevent an artificial acceleration of the flow over the building, as most boundary conditions applied at the top of the computational domain do not allow fluid to leave the domain. For urban areas with multiple buildings the top of the computational domain should be $5H_{\max}$ away from the tallest building with height H_{\max} .

If the simulations are to be compared with boundary layer wind tunnel measurements, then it is recommended to use the cross section of the wind tunnel's test section for the computational domain, i.e. the computational domain should have the same height as the boundary layer wind tunnel. In this way the computational model accurately replicates the geometry of the wind-tunnel test section. If the height of the wind tunnel is much larger than $6H_{\max}$, then a lower height of the computational domain can be tested.

5.5.2 Lateral extension of the domain

After having chosen the height of the computational domain the lateral extension of the domain can be determined by the required blockage. For a single building of height H with quadratic projected area in the flow direction and a domain height of $6H$ the requirement of 3% blockage leads to a distance of approximately $2.3H$ between the building's sidewalls and the lateral boundaries of the computational domain. The published recommendations for this distance are however much larger. Hall (1997), Cowan et al. (1997), Scaperdas & Gilham, (2004) and Bartzis et al. (2004) all recommend using $5H$, leading to a blockage of only 1.5%.

For buildings with an extension in the lateral direction much larger than the height, the blockage should also be below the maximum allowed value. In that case the ratio of the lateral extension of the computational domain to its height should be similar to the corresponding ratio for the building (Blocken et al., 2004).

Again, if the simulations are to be compared with boundary layer wind tunnel measurements, then it is recommended to use the cross section of the wind tunnel's test section for the computational domain, i.e. the computational domain should have the same lateral extent as the boundary layer wind tunnel. If the distance of the lateral walls of the wind tunnel from the built area is much larger than $5H_{\max}$, then a smaller extent of the computational domain can be tested.

For urban areas with multiple buildings the lateral boundaries of the computational domain can be placed closer than $5H_{\max}$ to that part of the built area (e.g. buildings, structures or topography) which surrounds the region of interest. As the influence of the lateral boundaries on the flow and dispersion in the region of interest is highly case-dependent, it is recommended to test at least two different distances from the built area.

5.5.3 Extension of the domain in flow direction

Concerning the longitudinal extension of the domain the region in front of (approach flow) and the region behind (wake) the built area have to be discerned. For a single

building a distance of again $5H$ between the inflow boundary and the building is recommended if the approach flow profiles are well known (Hall, 1997; Cowan et al., 1997; Scaperdas & Gilham, 2004). Bartzis et al. (2004) even recommend $8H$. If the approach flow profiles are not available, then an even larger distance should be used to allow for a realistic flow establishment (Bartzis et al., 2004).

Contrary to the recommendation of $5H$, VDI (2005) suggests blockage and building type dependent distances. If a single building with little blockage is considered, the inflow is suggested to be $2H$ from the building. When the flow is blocked to a larger extent (e.g. 10%), a distance of $8H$ is recommended.

The region behind the built area is terminated by the outflow boundary. In the case of a single building this boundary should be positioned at least $15H$ behind the building to allow for flow re-development behind the wake region, as fully developed flow is normally used as a boundary condition in steady RANS calculations (Cowan et al., 1997; Scaperdas & Gilham, 2004; Bartzis et al., 2004).

For urban areas with multiple buildings a smaller distance between the outflow boundary and the built area surrounding the region of interest can be used. The distance depends on the type of boundary condition used at the outflow. For steady RANS simulations, open boundary conditions (either a constant pressure or so called outflow condition, see section 5.6.5) are normally applied with commercial codes. These boundary conditions in principle allow fluid to enter through the outflow boundary. Flow entering the domain through the outflow boundary should be avoided (Casey & Wintergerste, 2000) as this can negatively impact on the convergence of the solution or even allow no converged solution to be reached at all.

5.6 Choice of boundary conditions

The boundary conditions represent the influence of the surroundings that have been cut off by the computational domain. As they determine to a large extent the solution inside the computational domain, their proper choice is very important. Often, however, these boundary conditions are not fully known. Therefore the boundaries of the computational domain should be far enough away from the region of interest to not contaminate the solution there with the approximate boundary conditions.

5.6.1 Inflow boundary conditions

At the inflow an equilibrium boundary layer is usually prescribed, at a distance of at least $5H_{\max}$, see section 5.5.3. The mean velocity profile is usually obtained from the logarithmic profile corresponding to the upwind terrain via the roughness length z_0 or from the profiles of the wind tunnel simulations. Available information from nearby meteorological stations is used to determine the wind speed at the reference height.

For steady RANS simulations, the mean velocity profile and information about the turbulence quantities is required. Their profiles can be obtained from the assumption of an equilibrium boundary layer. The general derivation of these profiles and the resulting formulae for the standard $k-\varepsilon$ model are described by Richards & Hoxey (1993). The same coefficients that are used in the turbulence model should be used in the analytical formulation of the boundary conditions. If wind tunnel data for the turbulent kinetic energy are available, they should be used. If in addition the Reynolds stresses are measured, the turbulent dissipation can be calculated with the assumption of a local equilibrium, i.e. the production and dissipation rates of the kinetic energy of turbulence are equal to each other, $P=\varepsilon$.

In case of a homogeneous equilibrium boundary layer flow, the prescribed profiles should not change until the built area is reached. Before simulating the flow over obstacles therefore an analysis should be carried out to ascertain whether the chosen grid and boundary conditions are consistent and there is no substantial change in the specified inflow boundary profiles. Whether this requirement is fulfilled depends crucially on the roughness of the bottom wall (see section 5.6.2) and on the boundary condition at the top boundary of the computational domain (see section 5.6.3).

One method to generate inflow profiles which will not change within the computational domain in front of the built area is to first perform a simulation in the empty domain with the same grid and periodic boundary conditions to obtain constant profiles that match the velocity measurements at the meteorological station (Wright & Easom, 1999). Meteorology models normally use a 1D version of the same model for calculating an inflow profile that is consistent with the 3D model. By doing this horizontal homogeneity is assumed. Another possibility is to explicitly model the roughness blocks that are used in a corresponding wind tunnel study using only smooth wall boundary conditions. This has been done e.g. by Miles & Westbury (2003) and leads to a significant improvement of the computed results compared to the results obtained with an approach flow over a smooth flat wall.

For LES and other unsteady simulation approaches, time dependent boundary conditions are required at the inflow. Artificial stochastic inflow data generation methods based on statistical description of turbulence have been proposed and evaluated for LES (Kondo et al., 1998; Kempf et al., 2005; Majander, 2006). Other possibilities are the usage of a fetch comparable to the ones used in wind tunnels (e.g. Nakayama et al., 2005) or periodic simulations over roughness elements as proposed by Nozawa & Tamura (2002).

5.6.2 Wall boundary conditions

At solid walls the no-slip boundary condition is used for the velocities. For the shear stress at smooth walls, two different approaches are available for RANS simulations and LES. The so called low-Reynolds number approach resolves the viscous sublayer and computes the wall shear stress from the local velocity gradient normal to the wall. The equations for the turbulence quantities contain damping functions to reduce the influence of turbulence in this region dominated by molecular viscosity. The low-Reynolds number approach requires a very fine mesh resolution in wall-normal direction. The first computational node should be positioned at a non-dimensional wall distance of $z^+ = zu_\tau/\nu \approx 1$, where z is the distance normal to the wall, $u_\tau = (\tau_w/\rho)^{1/2}$ is the shear velocity, computed from the time averaged wall shear stress τ_w , and ν the kinematic viscosity.

To reduce the number of grid points in the wall-normal direction and therefore the computational costs, wall functions are applied as an alternative approach to compute the wall shear stress. With the wall function approach, the wall shear stress is computed from the assumption of a logarithmic velocity profile between the wall and the first computational node in the wall-normal direction. For the logarithmic profile to be valid, the first computational node should be placed at a non-dimensional wall distance of z^+ between 30 and 500 for smooth walls. Also for wall function modelling the turbulence quantities have to be modified at the first computational node off the wall. They are usually calculated assuming an equilibrium boundary layer, consistent with the logarithmic velocity profile. This modelling is known to be invalid in regions

of flow separation, of reattachment and of strong pressure gradients (e.g. Hanjalić, 1999). Also the transition from laminar to turbulent boundary layers cannot be predicted with the standard wall functions. The effect of wall functions on the solution away from the wall is however regarded as small in the built environment (Castro, 2003).

In addition to smooth walls, rough walls are encountered in urban areas. For these, the wall function approach is also used. In meteorological codes, the roughness is included by the hydrodynamic roughness length z_0 . The corresponding modifications of the turbulence quantities at the first computational node off the wall are again derived assuming an equilibrium boundary layer flow (Richards & Hoxey, 1993).

In most commercial general purpose CFD codes, the roughness of a wall is implemented for sand-roughened surfaces with a corresponding roughness height k_s . For a fully rough surface the roughness length z_0 and the roughness height k_s are analytically related via $k_s = z_0 \exp(\kappa B)$, where κ is the von Karman constant ($\kappa \approx 0.4$) and $B \approx 8.5$ is the constant in the logarithmic velocity profile for rough surfaces. For these values the relation is $k_s \approx 30 z_0$, showing that the roughness height is one order larger than the roughness length. This often leads to very large computational cells, i.e. a bad resolution, at the rough wall since the first calculation node off the wall must be placed at least k_s away from the wall. As Blocken et al. (2006) have shown for two commercial CFD codes, the use of a smaller k_s value than the one corresponding to the inlet profiles allows for a better horizontal resolution near the wall but leads to substantial streamwise changes of the inflow profiles even in the case of a laterally and horizontally homogeneous roughness in a domain without obstacles.

Even when placing the first wall-normal computational node at a position which is larger than the k_s corresponding to the inflow profiles, commercial CFD codes generate more or less substantial horizontal changes of these profiles in an empty domain with homogeneous roughness. Hargreaves & Wright (2006) have recently shown that this is due to the specific implementation of the wall function approach in commercial CFD codes. Before simulating the flow over obstacles therefore an analysis should be carried out to ascertain whether the chosen grid and boundary conditions are consistent with the inflow profiles and whether there is no substantial horizontal change in these profiles.

In addition positions where a solution is sought should in general not be placed in the immediate neighbourhood of a wall, due to the wall function modelling of the flow at the wall. The VDI guideline (VDI, 2005) recommends placing at least two nodes between a wall and the position of interest, if the results are to be used for dispersion studies.

As with RANS models described above wall functions can also be applied in LES for flows over rough walls (Mason & Callen, 1986). An alternative is the distributed roughness approach which models the roughness elements with a porous region with prescribed losses for the resolved momentum equations (e.g. Nakayama et al., 2005). For smooth walls either the wall function approach or the resolution of the viscous sublayer with damping of the subgrid scales is used, see Sagaut (2001) for an overview.

5.6.3 Top boundary conditions

The choice of the top boundary condition is very important for sustaining equilibrium

boundary layer profiles. These are normally derived under the assumption of a constant shear stress over the boundary layer (Richards & Hoxey, 1993; Hargreaves & Wright, 2006). Therefore the prescription of a constant shear stress at the top, corresponding to the inflow profiles, is recommended to prevent a horizontal change from the inflow profiles. Another option is to prescribe the values for the velocities and the turbulence quantities of the inflow profile at the height of the top boundary over the entire top boundary (Blocken et al., 2006).

In microscale obstacle-accommodating meteorology models a free slip condition at a rigid lid is sometimes used. Symmetry boundary conditions that enforce a parallel flow by forcing the velocity component normal to the boundary to vanish also prescribe zero normal derivatives for all other flow variables and therefore lead to a change from the inflow boundary profiles (which can have a non zero gradient at the height of the top of the domain). This condition is therefore an approximation and should be used only if the domain top is outside the boundary layer. The same will happen if the top boundary is handled as an outflow boundary, allowing a normal velocity component at this boundary. In this case however, the natural outflow, which is due to the increasing displacement of the fluid even in a boundary layer flow without obstacles, is taken into account.

Finally, if the computations are to be compared with wind tunnel measurements obtained within a closed test section, then the top boundary located at the position of the wind tunnel's top wall should be treated as a solid wall. However it should be noted that most boundary layer wind tunnels use a spatially adjustable roof.

5.6.4 Lateral boundary conditions

In commercial CFD codes symmetry boundary conditions are frequently used at the lateral boundaries when the approach flow direction is parallel to them. In case different wind directions are to be simulated with the same computational domain, then the lateral boundaries become inflow and outflow boundaries with corresponding boundary conditions, see sections 5.6.1 and 5.6.5. As symmetry boundary conditions enforce a parallel flow by requiring a vanishing normal velocity component at the boundary, the boundary should be positioned far enough away from the built area of interest to not lead to an artificial acceleration of the flow in the region of interest (see section 5.5.2).

In microscale obstacle-accommodating meteorological models, open lateral radiation boundaries are frequently used at the lateral boundaries. With these, every horizontal boundary grid point can allow for inflow and outflow and this might also change in time (e.g. URANS applications). When using this boundary condition, the model domain can be smaller in the lateral direction (see section 5.5.2) and it can be sufficient to include only a few grid points between a building that is close to the boundaries and the boundary.

If the computations are to be compared with wind tunnel measurements obtained within a closed test section, the top and lateral boundaries should be treated as solid walls at least in those cases in which the wind tunnel domain is too small to provide measurements that are independent of the wind tunnel cross section.

5.6.5 Outflow boundary conditions

At the boundary behind the obstacles (where all or most of the fluid leaves the computational domain), open boundary conditions are used in commercial CFD and

microscale obstacle-accommodating meteorology models. The open boundary conditions in commercial CFD codes are either outflow or constant static pressure boundary conditions. With an outflow boundary condition the derivatives of all flow variables are forced to vanish, corresponding to a fully developed flow. Therefore this boundary should be ideally far enough away from the built area to not have any fluid entering into the computational domain through this boundary as already stated in section 5.5.3. This also holds for the use of a constant static pressure at the outflow boundary, where then only the derivatives of all other flow variables are forced to vanish.

With the radiation open boundary conditions used in microscale obstacle-accommodating meteorological models, the requirement of having no fluid entering through the outflow boundary can be relaxed.

For LES, convective outflow boundary conditions (e.g. Ferziger & Peric, 2002) should be used.

5.7 Choice of initial data

In RANS, URANS and LES models, a boundary and initial value problem has to be numerically solved. The larger the model domain or the smaller the wind speed, the more relevant the initial data become.

For RANS stationary solutions are searched, thus the iteration is stopped as soon as the solution is not changing any more or the solution converges (see section 5.11). In these cases mainly the boundary values influence the model solution and the impact of the initial data is small. Initialising with a flow field that is close to the final solution will reduce the computational efforts needed to reach stationary solutions.

For URANS and LES, the initial data determine the time dependent development in the beginning of the simulation. As a rule of thumb, the impact time can be estimated with a relation including the domain size and wind speed. During this initial period, the model results are very dependent on the initial data and should not be interpreted as solution which reflects the final flow.

Initial data and inflow data are very often used as one and the same. This is a good starting point for most models. However, if these initial data (and therefore the inflow profiles) do not correspond to the situation to be investigated (e.g. wrong wind direction) then a model result comparable to the situation to be modelled can not be expected. Since initial data are not known perfectly, but include uncertainties that result from measurement inaccuracy or a lack of representativeness of the measurement site, the initial input values are never perfectly known.

The initial data uncertainty should be reduced as much as possible by evaluating the reliability of the initial data and choosing only those initial data that have small uncertainties. However, quite often the number of input data is not even sufficient to know all variables that need to be initialised. There are rarely several data to choose from and the input data uncertainty is in general unknown. In all these (common) cases the uncertainty of the input data should be estimated e.g. from other experiments or from experience. Sensitivity studies in the uncertainty range of the initial data, e.g. for different inflow directions, allow to estimate the impact of initial data uncertainty on model results. This can be a very costly effort, and currently no method is established to determine which sensitivity studies are most worthwhile to perform to derive the information on the initial data influence on model results. The resulting

probability distribution for the model results can currently only be calculated when using a huge amount of computer resources. Therefore the current best practice advice is to keep initial data uncertainty as little as possible and keep in mind that the initial data influence the model results in unsteady simulations.

5.8 Choice of the computational grid

When referring to the computational grid one first has to define the discretisation method that shall be used for the basic equations. The following discussion is restricted to the closely related Finite Volume and Finite Difference methods with a strong bias towards the Finite Volume method as this is widely used in commercial CFD codes and microscale obstacle-accommodating meteorological models. For the Finite Element discretisation method different requirements exist for the quality of the computational grid (Casey & Wintergerste, 2000).

With the Finite Volume and Finite Difference methods the computational results depend crucially on the grid that is used to discretise the computational domain. The grid has to be designed in such a manner that it does not introduce errors that are too large. This means that the resolution of the grid should be fine enough to capture the important physical phenomena like shear layers and vortices with sufficient resolution. Also the quality of the grid should be high. Ideally the grid is equidistant. Therefore, grid stretching/compression should be small in regions of high gradients, to keep the truncation error small. The expansion ratio between two consecutive cells should be below 1.3 in these regions. Scaperdas and Gilham (2004), as well as Bartzis et al. (2004) even recommend a maximum of 1.2 for the expansion ratio. However, higher order numerical schemes might allow larger changes as the absolute value of the truncation error is smaller than with lower order schemes (Schroeder et al., 2006).

For LES, non-equidistant grids correspond to non-uniform filter widths. Their application to the basic equations leads to filtered equations that contain more unknown terms than the subgrid stresses. These result from the fact that filtering with a non-uniform filter width and a partial spatial derivation do not commute and are therefore called commutation errors. They describe the change in the definition of the resolved and subgrid flow variables that is due to the varying filter width. Ghosal & Moin (1995) have shown that the commutation error terms are second order in the filter width. When using numerical approximations of second order in the grid width, these commutation error terms are therefore normally neglected.

For the widely used Finite Volume methods another criterion for grid quality is the angle between the normal vector of a cell surface and the line connecting the midpoints of the neighbouring cells (Ferziger & Perić, 2002). Ideally these should be parallel. This also improves the accuracy of the schemes used in meteorological models that apply a surface fitting vertical coordinate by using a coordinate transformation.

With regard to the shape of the computational cells, hexahedra are preferable to tetrahedra, as the former are known to introduce smaller truncation errors and display better iterative convergence (Hirsch et al., 2002). On walls the grid lines should be perpendicular to the wall (Casey & Wintergerste, 2000; Menter et al., 2002). Therefore if a tetrahedral grid is to be used, prismatic cells should be used at the wall with tetrahedral cells away from the wall. For example Fothergill et al. (2002) found improved results for a prismatic/tetrahedral grid as compared to a purely tetrahedral grid.

It is impossible to make recommendations for the grid resolution in advance as this is highly problem-dependent. If simulations employ the logarithmic wall model, the position of the first computational node should, of course, be placed in the logarithmic region, corresponding to a non-dimensional wall distance of at least 30 (Casey & Wintergerste, 2000), see section 5.6.2. For the typically very rough walls this is automatically satisfied (Hargreaves & Wright, 2006).

In the area of interest, at least 10 cells per cube root of the building volume should be used and 10 cells per building separation to simulate flow fields. This must be understood as an initial minimum grid resolution. The necessary resolution then will have to be analysed by using grid refinement which is discussed in the following. However, the recommendation for the building separation also complies with the guidelines presented by Bartzis et al. (2004) for the simulation of the flow within an idealised 2D street canyon. For the vertical resolution of the canyon with width to height ratio of one they state that 10 cells are adequate. The same authors also give advice on the grid size for flow and dispersion over isolated hills and valleys. They recommend a careful grid design in the vicinity of the source location to adequately resolve the large gradients there.

Computations of flows in simplified geometries can be used to assess the necessary (initial) grid resolution, as has been done by Blocken et al. (2004). Their target application was the computation of the flow in passages within high rise buildings. To assess - amongst other things - the influence of the grid size on the computational results they conducted preliminary tests for a passage in a simplified building model for which experimental data are available (Blocken et al., 2003). The sufficient resolution obtained in this way was then used for the simulation of the complex building arrangement.

However, for validation simulations, a systematic grid convergence study using generalised Richardson extrapolation should be tried. This is straightforward for CFD codes using the RANS approach, which does not require grid-dependent parameterisations. For the Richardson extrapolation, at least solutions on three systematically refined/coarsened grids are necessary. From these simulation results, the error band (uncertainty) of the spatial discretisation error of the solution on the finest mesh can be estimated. The principle and the limitations of Richardson extrapolation as applicable to CFD codes using the RANS approach are described in the context of numerical error estimation in the Background and Justification Document of COST action 732 (COST732, 2007). Details on the method are provided in Appendix A.1.

For microscale obstacle-accommodating meteorological models the outcome of the Richardson extrapolation might not always be sufficient, since the parameterisations need to be adjusted to the resolution to ensure convergence. While for the Richardson extrapolation at least solutions on three systematically refined/coarsened grids are necessary, microscale obstacle-accommodating meteorological models should try at least two grids, and the results should be compared to check, for example, for the grid dependence of the parameterisation (Schlünzen, 1997). The two results should agree within allowed discrepancies (VDI, 2005).

For the assessment of the influence of the grid in LES, a similar problem to that with microscale obstacle-accommodating meteorological models exists. In the context of implicit LES, where the filter width is set approximately equal to the grid width (normally the cube root of the volume of the computational cell, see Sagaut, 2001),

grid refinement will lead to a DNS as the influence of the subgrid scale model is reduced with the reduction of the grid widths. A grid-independent implicit LES is therefore a DNS (Celik et al., 2005). This is not the case when a grid width independent filter width is used, as has been done by Geurts & Fröhlich (2002). With this approach they were able to discriminate between the modelling error resulting from the subgrid scale model and the numerical error from the spatial discretisation; the latter of course becoming smaller with increasing grid refinement. When using the implicit approach where filter width and grid width are approximately equal, the modelling and the spatial discretisation error can no longer be clearly separated. To assess the influence of the spatial discretisation error, Celik et al. (2005) have proposed an Index of Resolution Quality which is defined as the ratio of the resolved and the total turbulent kinetic energy. The unknown total kinetic energy is approximated with the aid of the Richardson extrapolation (see Appendix A.1), using two grids with different resolution. They further suggest that an Index of Resolution Quality of 75% to 85% is adequate for most engineering applications.

Klein (2005) also used the Richardson extrapolation to assess the quality of his implicit LES results. He however used solutions on three grids to estimate the numerical error in the solutions.

When a global systematic grid refinement is not possible due to resource limitations, then at least a local grid refinement should be used in the area of the main interest. Most commercial CFD codes offer the possibility to perform local refinement in the dependence of the local gradients or curvature of the flow variables. The choice of these indicator functions should depend on the target variables which shall be compared with experimental data.

5.9 Choice of numerical approximations

To render the basic equations solvable on the computer, they have to be discretised and transformed into algebraic equations. The most important numerical approximation is the one used for the non-linear advective¹ terms in the basic equations (see e.g. Cowan et al., 1997; Menter et al., 2002).

For advection, first order methods like the upwind scheme should not be used for the final solution. They can and should be used for the initial iterations, but higher order approximations are advisable to be used for the final solution. Especially for pollution dispersion in urban areas, the use of first order approximations will lead to substantial numerical diffusion, if the CFL number (see section 5.10) is not close to one.

For time-dependent problems, second-order methods should also be chosen for the approximation of the time derivatives.

Although not directly a part of the numerical approximations, the question of reducing the round-off error is addressed here. A double precision solver should always be used. In case that a single precision solver is used it has to be demonstrated through a comparison with a double precision result that the results for the target variables are not strongly affected by the increased round-off errors.

¹ In engineering sciences advection is named convection (transport caused by the averaged flow field). Since convection is dedicated in Meteorology to describe a – mostly unresolved – vertical atmospheric movement forming in an unstable (convective) atmosphere, we use advection in this text.

5.10 Choice of the time step size

When performing unsteady simulations, the size of the time step is another important parameter for the accuracy of the results. If the relevant frequency range can be estimated, then the highest frequency should be resolved with at least 10 – 20 time steps per period (Menter et al., 2002). Another method to estimate the time step in advection dominated problems is the relation $\Delta t = \text{CFL} \Delta x_{\min} / U_{\max}$, where Δx_{\min} is the minimum grid width, U_{\max} is the maximum velocity and CFL is the Courant-Friedrichs-Lewy number. Choosing the minimum grid spacing and the maximum velocity makes this estimate conservative. In several models the time step is determined continuously as the minimum of all time steps calculated per grid point.

To assess the influence of the time step size on the results, a systematic reduction or increase of the time step should be made, and the simulation repeated. The two results can then be analysed with the Richardson extrapolation as described in Appendix A.1 and the Background and Justification Document of COST action 732 (COST732, 2007).

5.11 Choice of iterative convergence criteria

Most of the computer programs use iterative methods to solve the algebraic system of equations (e.g. the equation for the pressure). Starting from an initial guess the flow variables are recalculated in each of the iterations until the equations are solved up to a user-specified error. The termination criterion is usually based on the residuals of the corresponding equations. These residuals should tend towards zero. Scaling of the residuals is usually done with the residuals after the first iteration. The scaled residual then shows how much the initial error has dropped. In industrial applications typically a termination criterion of 0.001 is used, which is in general too high to have a converged solution. A reduction of the residuals of at least four orders of magnitude is recommended. For validation purposes of turbulence or other physical models much lower criteria should be used. If the residual is driven down to its theoretical value of machine accuracy (10^{-12} for double precision), there is no more iterative error present in the solution.

In addition to the residuals the target variables should also be recorded. If these variables are constant or oscillate around a constant value, then the solution can be regarded as converged. The same should be done for the integral balances of mass, momentum and energy. Based on the behaviour of the target variables and the integral balances it can be decided which termination criterion for the residuals is sufficient. A quasi-constant behaviour of these values can be expected if stationary solutions are sought (VDI, 2005). The values may change in correspondence to changes in boundary values or other source and sink terms for unsteady runs.

This procedure should also be followed when unsteady simulations are to be performed. Implicit time integration methods require iterations within the time steps so the above should be applied within each time step.

6 Conclusions

This best practice guideline is a collection of results from former initiatives in the field of CFD in general and for its application to urban flows. The guideline focuses on applications of the statistically steady RANS equations for situations with neutral

stratification without dispersion modelling. However, users of other models like unsteady RANS (URANS) and LES models should consider the same suggestions. Differences and some more – but not extensive – information for URANS and LES applications are given in the corresponding paragraphs. The guideline provides general advice that should be taken into account when performing the simulations for model validation within COST Action 732. From the results of these validation simulations specific guidelines for the validation test cases and refined general guidelines will be produced in the course of the action. These will include advice on pollution modelling within CFD codes and on the proper use of non-CFD codes.

In Appendix B.1 and B.2 specific procedures for the set up and conduction of CFD simulations are summarised from two institutions participating in the COST 732 action, namely the Laboratory of Heat Transfer and Environmental Engineering (LHTEE) at the Aristotle University Thessaloniki, Greece, and the Department of Fluid and Thermodynamics at the University of Siegen, Germany. In addition best practice advice for the software MISKAM is provided in Appendix B.3.

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APPENDIX

A Verification of CFD codes and numerical simulation results

In the context of quality assurance of CFD codes verification deals with the relationship between the conceptual and the computerised model (Oberkampf et al., 2004). The conceptual model comprises all the equations that are necessary to describe the physical system, including initial and boundary conditions. The implementation of these equations into an operational computer program is called the computerised model or CFD code. Verification therefore is purely mathematical. Contrary to that validation deals with physics and is based on the comparison of the results of a numerical simulation with experimental measurements. Validation is therefore concerned with the question whether the conceptual models together with the computerised model are an appropriate representation of reality while verification is concerned solely with the question whether the CFD code is an appropriate representation of the conceptual model. Or as Roache (1997) has formulated it succinctly, verification is used to check whether the equations are solved right and validation is used to check whether the right equations are solved.

There exist two kinds of verification. One is code verification which is used to demonstrate that the computerised model is consistent with the CFD code as stated above, i.e. that there are no programming errors or inconsistencies in the solution algorithm (Roy, 2005). This is normally done by the code developers. The other kind of verification is solution verification which is the estimation of the numerical error (Roache, 1997; Oberkampf et al., 2004; Roy, 2005) or uncertainty (Stern et al., 2001) of a specific simulation result and is to be done by the code user. Solution verification is also known as numerical error estimation (Oberkampf et al., 2004).

Both kinds of verification need to quantify the discretisation error which results from the fact that a system of partial differential is solved with finite discretisation in space and time. The most general method for estimating the discretisation error is the Richardson extrapolation (Richardson, 1910; Richardson, 1927) which is used in code verification and solution verification. Therefore the generalised Richardson extrapolation is introduced first and afterwards code and solution verification are discussed in general.

A.1. Generalised Richardson extrapolation

Richardson extrapolation is an a posteriori error estimator that is independent of the numerical method used to obtain the numerical solutions. It can be applied to the local flow variables as well as to derived integral quantities. The method can be used for the spatial discretisation as well as for the temporal discretisation. Here it will be introduced for the spatial discretisation.

If f_{ex} is the smooth exact solution and f_k the result of a numerical solution on the mesh indexed by k then these two can be related by a series expansion,

$$f_k = f_{ex} + g_p h_k^p + g_{p+1} h_k^{p+1} + g_{p+2} h_k^{p+2} + \dots \quad (1)$$

h_k is a (linear) measure of the grid width of mesh k , p is the order of accuracy and g are coefficients. When the solution on mesh k is in the asymptotic range then all terms of higher order than p can be neglected and p and g do not depend on h_k (Stern et al., 2001). The only unknowns that remain on the right hand side of (1) are then f_{ex} , g_p and

p . In the most general case (which is the one encountered in solution verification) none of these is known and three equations corresponding to solutions on three different meshes are necessary to estimate f_{ex} . If $k=1$ denotes the fine, $k=2$ the medium and $k=3$ the coarse grid, two grid refinement ratios can be introduced,

$$r_{21} = h_2/h_1, \quad r_{32} = h_3/h_2 \quad . \quad (2)$$

With these ratios the series expansions can be written as

$$\begin{aligned} f_1 &= f_{ex} + g_p h_1^p = f_{ex} + g_p h_1^p \\ f_2 &= f_{ex} + g_p h_2^p = f_{ex} + g_p (r_{21} h_1)^p \\ f_3 &= f_{ex} + g_p h_3^p = f_{ex} + g_p (r_{21} r_{32} h_1)^p \end{aligned} \quad . \quad (3)$$

The neglect of the higher-order terms in the series for the medium and coarse grid requires that these solutions are also in the asymptotic range. Another criterion for the applicability of the generalised Richardson extrapolation with solutions from three meshes is that the solution displays monotonic convergence (Stern et al., 2001). From the ratio of the solution changes, $R = (f_2 - f_1)/(f_3 - f_2)$, three different behaviours can be discerned.

- (i) $0 < R < 1$: monotonic convergence
- (ii) $R < 0$: oscillatory convergence
- (iii) $|R| > 1$: divergence

For divergence no error estimate can be obtained. Oscillatory convergence generally requires the use of more solutions than three to compute an error estimate. However, the main problem with oscillatory convergence in general is that it might manifest itself as (i) or (iii) (Coleman et al., 2001). Another problem is that R may become ill-conditioned when $(f_3 - f_2)$ approaches zero. Then the maxima and minima of the local solution should be analysed, possibly together with the ratio formed by the L_2 norms of the solution changes (Stern et al., 2001).

To calculate the solution changes it is necessary that all solutions are available at the same positions. In case of always doubling the number of cells in each coordinate direction ($r = r_{21} = r_{32} = 2$) without moving the nodes of the coarse grid this requirement is fulfilled. Otherwise interpolation from the fine and medium grid on the coarse grid is necessary (Cadafalch et al., 2002). The order of the method used for interpolation must be higher than the anticipated p to not contaminate the grid convergence study (Roache, 1998). If the generalised Richardson extrapolation is applied to integral values then no interpolation is necessary.

Assuming that all solutions are available on the coarse grid and monotonic convergence according to (4), the order of accuracy can be calculated from (3) by solving the transcendental equation

$$p = \frac{\ln[(f_3 - f_2)/(f_2 - f_1)]}{\ln(r_{21})} - \frac{1}{\ln(r_{21})} [\ln(r_{32}^p - 1) - \ln(r_{21}^p - 1)] \quad (5)$$

with an iterative method. After elimination of g_p in (3) an estimate of the exact solution is obtained,

$$f_{ex} = f_1 + \frac{f_1 - f_2}{r_{21}^p - 1} \quad . \quad (6)$$

The second term on the right hand side of (6) defines a correction to the fine grid solution f_1 . This correction is only available at the positions of the variable on the coarse grid. To make the corrections available at every node or in every cell on the fine grid, interpolation is necessary (Roache, 1998). The error of the interpolation again has to be lower than the discretisation error. The (spatial) discretisation error DE_1 of the fine grid solution, i.e. the difference between the solution on the fine grid and the exact solution, follows from (6):

$$DE_1 = f_1 - f_{ex} = \frac{f_2 - f_1}{r_{21}^p - 1} \quad . \quad (7)$$

For the spatial discretisation errors on the medium and coarse grid the following relations are obtained:

$$\begin{aligned} DE_2 &= f_2 - f_{ex} = \frac{r_{21}^p (f_2 - f_1)}{r_{21}^p - 1} = r_{21}^p DE_1 \\ DE_3 &= f_3 - f_{ex} = \frac{r_{32}^p r_{21}^p (f_2 - f_1)}{r_{21}^p - 1} = (r_{32} r_{21})^p DE_1 \end{aligned} \quad . \quad (8)$$

With the aid of (8) it can be checked whether the three solutions are in the asymptotic range. In this case the following relation holds, where the first identity follows by definition:

$$DE_1 = \frac{DE_2}{r_{21}^p} = \frac{DE_3}{(r_{32} r_{21})^p} \quad . \quad (9)$$

The presented results are the most general form of the generalised Richardson extrapolation. They are simplified with a constant refinement ratio $r = r_{21} = r_{32}$. The order of the numerical solution can then be calculated explicitly from

$$p = \frac{\ln[(f_3 - f_2)/(f_2 - f_1)]}{\ln(r)} \quad . \quad (10)$$

The estimate (6) for the exact solution and the discretisation errors (7) and (8) are then:

$$f_{ex} = f_1 + \frac{f_1 - f_2}{r^p - 1} \quad , \quad (11)$$

$$DE_1 = f_1 - f_{ex} = \frac{f_2 - f_1}{r^p - 1} \quad , \quad (12)$$

$$\begin{aligned}
DE_2 &= f_2 - f_{ex} = \frac{r^p(f_2 - f_1)}{r^p - 1} = r^p DE_1 \\
DE_3 &= f_3 - f_{ex} = \frac{r^{2p}(f_2 - f_1)}{r^{2p} - 1} = r^{2p} DE_1
\end{aligned} \tag{13}$$

How the described Richardson extrapolation is used in code and in solution verification will be shown next. Here the main prerequisites which can also be viewed as disadvantages of the method are briefly restated.

- The applicability of the method requires smooth solutions. For solutions with discontinuities or singularities the effectiveness of the method is reduced (Roy, 2005).
- The method relies on having multiple solutions in the asymptotic range which can be very expensive.
- The method does not work with divergent changes in the solution, see (4). Oscillatory changes in the solution might not be detected.
- The method tends to amplify other sources of numerical errors like round-off and incomplete iterative convergence errors. Roy (2005) states that these two errors should be at least 100 times smaller than the discretisation error.

The advantages of the method are the following:

- As a post-processing tool it can be applied with every discretisation method (Finite Difference, Finite Volume and Finite Element).
- No intrusion into the code is necessary.
- The global error or estimates of this error can be calculated for every quantity.

A.2. Code verification

As stated in the beginning code verification is used to analyse whether the conceptual model is correctly implemented in the computerised model or CFD code. The correct implementation has to be demonstrated (Oberkampf et al., 2004).

If the numerical method is consistent then the basic partial differential equations are recovered from the discrete equations in case of vanishing grid and time step size. The rate at which the basic partial differential equations are approached is determined by the truncation error. E.g. if the smallest exponent of the grid width in the truncation error is 2 then the method is said to be of second order (accuracy) in space. Halving the grid size will therefore reduce the truncation error by a factor of 4 if the solution is already in the asymptotic range as defined above. The formal truncation error and thus the formal order of the computerised model can be found by using Taylor series expansion and subtracting the basic partial differential equations from the expanded discrete equations. Whether the formal order is observed in actual applications of the code is analysed with the aid of code verification by determining the observed order of accuracy. This is the most rigorous and therefore recommended acceptance test for code verification (Knupp & Salari, 2003).

The observed order of accuracy is determined with the aid of Richardson extrapolation as described above. Assuming that the exact solution to the partial

differential equations is known only solutions on two meshes are required, see (3). From these the observed order of accuracy p can be calculated.

$$p = \frac{\ln[(f_2 - f_{ex}) / (f_1 - f_{ex})]}{\ln(r_{21})} \quad (14)$$

From (14) the observed order of accuracy is defined at every node where both solutions are available. Assuming $r_{21} = 2$ which is the general but not necessary choice for code verification this requirement is fulfilled for the coarser mesh 2 without interpolation. For the verification of the code the computation of a global discretisation error suffices to calculate the observed order of accuracy. Roy (2005) describes the use of discrete L_∞ and L_2 norms, which are defined as

$$L_{\infty,k} = \max |f_{k,n} - f_{ex,n}|, \quad L_{2,k} = \left(\frac{\sum_{n=1}^N |f_{k,n} - f_{ex,n}|^2}{N} \right)^{1/2} \quad (15)$$

on every mesh k . Here n is the index of the nodes or cells of the mesh and N the total number of nodes or cells. From both or one of these norms the observed order of accuracy is calculated,

$$p = \frac{\ln(L_{k+1} / L_k)}{\ln(r)} \quad (16)$$

If the observed order and the formal order coincide code verification is achieved.

There are several possible reasons for the case that the observed and the formal order do not agree. The most important one is that there are programming errors. Indeed order of accuracy testing is an efficient tool to detect these mistakes. To that end the other possible sources of disagreement between the observed and formal order of accuracy should be eliminated. These sources mainly relate to the Richardson extrapolation and are solutions which are not smooth enough and round-off or incomplete iterative convergence errors. By assuring smooth solutions as well as negligible round-off and iterative convergence errors (at least 100 times smaller than the discretisation errors, see Roy (2005)), a failure of the order of accuracy test can be safely attributed to programming errors.

The method described above relies on the availability of exact solutions for the basic partial differential equations. Analytical solutions of the Navier-Stokes equations do only exist for simple problems or are obtained after substantial simplification of the basic equations. As an alternative for the use of analytical solutions to the Navier-Stokes equations the Method of Manufactured Solutions (MMS) is advocated as the best choice in code verification (Roache, 2002, Oberkampf et al., 2004, Roy, 2005). This method is based on the prescription of an analytical solution for all variables that are computed. These solutions do of course not fulfil the basic conservation equations but lead to additional source terms when inserted in the basic equations. Thus with MMS not the original system of equations is solved but a modified system of equations. However, the additional terms are known and can be implemented into the code in the exact analytical form. The corresponding initial and boundary conditions are also obtained from the prescribed analytical solutions. When the original code is

run with these extensions then results of the simulation must approach the prescribed analytical solutions at a rate with the formal order of accuracy when the grid or the time step are refined. The observed order test described above must therefore be applied to the solutions obtained with the modified equations. As the modification (hopefully) only introduces analytical, i.e. exact terms in the code, the untouched original part of the code is tested for programming errors.

Roy (2005) summarises code verification with MMS in the following six steps:

- Choice of the form of the governing equations.
- Choice of the form of the manufactured solutions.
- Derivation of the modified governing equations.
- Solution of the discrete form of the modified equations on multiple meshes.
- Evaluation of the global discretisation error (15) in the numerical solutions.
- Application of order of accuracy test to determine whether the observed order (16) matches the formal order.

He also formulates the following requirements of the manufactured solutions:

- The analytical functions and all their derivatives should be smooth (trigonometric and exponential functions recommended). Thus the observed order can be determined on relatively coarse meshes.
- The analytical functions are not allowed to lead to vanishing derivatives (also cross derivatives) in the governing equations.
- After insertion of the analytical functions all terms in the original equations should be of similar order.
- It must be certified that the analytical functions lead to realizable variable values only, e.g. the turbulent kinetic energy must be non negative.

The MMS for code verification is a powerful set of procedures to determine the correct implementation of the conceptual model in the code. It is independent of the basic discretisation method (Finite Difference, Finite Volume or Finite Element) and can deal with coupled sets of nonlinear partial differential equations. It can also be applied to other software than CFD codes. However, MMS depends on the possibility to implement arbitrary source terms as well as initial and boundary conditions into the code and is therefore code intrusive. While this is certainly no problem for code developers, mere code users may not be able to perform code verification. Another weakness of the method is its restriction to smooth solutions.

A.3. Solution verification (numerical error estimation)

As stated in the beginning, solution verification deals with the estimation of the numerical error or uncertainty of a given simulation result. It has been indicated previously that there exist several sources of the numerical error or uncertainty. This section deals only with the discretisation error. Numerical errors due to computer programming, round-off or incomplete iterative convergence are not addressed. Rather it is implied that these errors have been reduced to a negligible amount. The remaining numerical error can then be attributed to the finite resolution in space and time. The following methods for the estimation of this error can be applied to the

space discretisation and to the time discretisation. The presentation will however only describe the estimation of the spatial discretisation error.

Solution verification is also performed with the aid of the generalised Richardson extrapolation. As the exact solution to the partial differential equations is not known solution verification requires at least solutions on three systematically refined or coarsened meshes, i.e. the refinement or coarsening must be constant in the entire computational domain. Then the observed order of accuracy can be computed from (5) or (10) and the discretisation errors estimated from (7) and (8) or (12) and (13), respectively. Menter et al. (2002) propose to use the formal order of accuracy in the grid convergence study thereby reducing the necessary solutions to two. However, Stern et al. (2001) state that a two grid study does only provide information about the sensitivity of the solution to the space discretisation and not an error estimate.

The necessity to use solutions on three meshes makes the method expensive because all three solutions must be obtained on meshes which are fine enough for the solutions to be in the asymptotic range, which has to be analysed with (9). This requirement raises the question about the minimum refinement ratio r that should be used in the grid convergence study as it determines the required number of nodes or cells. For code verification it was stated that the ideal case is $r = 2$ corresponding to a doubling of cells in each coordinate direction. This increases the number of cells from the coarse to the fine grid by a factor of 64 and is therefore very demanding concerning the computational resources. Ferziger & Peric (2002) recommend at least an increase of 50% of the cells in each coordinate direction, corresponding to $r \approx 3.4$. Stern et al. (2001) state that for industrial applications $r = 2^{1/2}$ is an appropriate choice and Roache (1998) shows that even $r = 1.1$ is enough for simple meshes. The refinement or coarsening of the mesh is straightforward for structured meshes with hexahedral cells. The most efficient way is to start with the fine hexahedral mesh and then successively coarsen this mesh. For meshes with tetrahedral cells on the other hand it is easier to first generate the coarse mesh and then use refinement by sub-dividing every cell (Roy, 2005). On tetrahedral or unstructured meshes in general the refinement factor r can also be defined by (Roache, 1998)

$$r_{2l} = (N_1/N_2)^{1/D} \quad , \quad (17)$$

where N_k is the number of nodes or cells of the mesh and D the dimension of space.

With the use of $r \neq 2$ it has to be kept in mind that interpolation to the coarse grid is necessary and it has to be ensured that the interpolation error is smaller than the discretisation error to be analysed. The same interpolation problem arises if the correction to the fine grid solution is computed with the aid of equation (6) or (11). As the correction is only available on the coarse grid it has to be transferred back to the fine grid. Besides the interpolation another problem with the corrected solution is that it is in general no longer fulfilling the basic equations, e.g. mass conservation may not be fulfilled with the corrected fine grid solution. Therefore the most common approach with generalised Richardson extrapolation in grid convergence studies is to calculate the relative error or an error band. This is in general done for the solution on the fine grid.

For the fine grid the relative error is defined as

$$E'_l = \frac{f_l - f_{ex}}{f_{ex}} . \quad (18)$$

Roache (1998) has shown that this error can be approximated by

$$E_l = \frac{1}{r_{2l}^p - 1} \frac{f_2 - f_l}{f_l} = E'_l + O(h^{p+l}) . \quad (19)$$

Menter et al. (2002) suggest several practical error estimators based on (19):

- Field error

$$E_{l,f} = \frac{1}{r_{2l}^p - 1} \frac{|f_2 - f_l|}{range(f_l)} . \quad (20)$$

- Maximum error

$$E_{l,max} = \frac{1}{r_{2l}^p - 1} \frac{\max|f_2 - f_l|}{range(f_l)} . \quad (21)$$

- RMS error

$$E_{l,rms} = \frac{1}{r_{2l}^p - 1} \frac{rms(f_2 - f_l)}{range(f_l)} . \quad (22)$$

Here normalization of the discretisation error has been performed with the range of the solution on the fine grid, defined as $range(f_l) = \max(f_l) - \min(f_l)$, to exclude problems with vanishing f_l .

The field error (20) is defined at every node or cell of the coarse grid. From this error the average error in the entire computational domain can be formed. This average error is also needed for the computation of the RMS error (22), which again gives one value for the entire computational domain, like the maximum error (21).

The magnitude of the relative error (19),

$$|E_l| = \frac{1}{r_{2l}^p - 1} \left| \frac{f_2 - f_l}{f_l} \right| , \quad (23)$$

which is closely related to the field error (20), defines an error band around the solution on the fine grid, i.e. $f_l \pm |E_l|$. This definition of the error band however provides only 50% confidence that the true error falls within this error band (Roy, 2005). Therefore the error band (23) is in general multiplied by a factor of safety F_s to increase the confidence level of the estimate.

² Here the maximum of the absolute difference is used to ensure non negative $E_{l,max}$. Menter et al. (2002) do not use the absolute difference.

$$|E_{l,s}| = \frac{F_s}{r_{2l}^p - 1} \left| \frac{f_2 - f_1}{f_1} \right|. \quad (24)$$

Roache (1994) introduced this definition and called it Grid Convergence Index (GCI). For F_s he suggests two values depending on the number of meshes used and on the relation of the observed and formal order of accuracy:

- $F_s = 1.25$ if the order of accuracy is calculated from solutions on three meshes and this observed order matches the formal one.
- $F_s = 3$ if only two meshes are used, i.e. the observed order is assumed to match the formal one, or if three meshes are used but the observed and formal order do not match.

Stern et al. (2001) derived a variable factor of safety $F_{s,c}$ based on what they called correction factor C . Their introduction of the correction factor was based on the observation that the estimate for the discretisation error (7) has the correct form but that the observed order of accuracy is only poorly estimated with (5) or (10) unless the results on the three meshes are in the asymptotic range. The correction factor shall remedy this problem and account for the influence of the higher-order terms that have been neglected under the assumption that all solutions are in the asymptotic range. They propose two formulations for the correction factor, the simpler one of which is

$$C_l = \frac{r_{2l}^p - 1}{r_{2l}^q - 1}. \quad (25)$$

Here q is an improved estimate of the order of accuracy, normally the formal order of accuracy. The correction factor therefore measures the distance of the solutions from the asymptotic range. If all the solutions used lie within the asymptotic range then the observed order must match the formal order and $C_l = 1$. Their factor of safety then depends on the magnitude of C (Wilson, 2004),

$$F_{s,c} = \begin{cases} 9.6(I - C_l)^2 + 1.1 & |I - C_l| < 0.125 \\ 2|I - C_l| + 1 & |I - C_l| \geq 0.125 \end{cases}. \quad (26)$$

For $C_l = 1$ their factor of safety is $F_{s,c} = 1.1$ which is smaller than $F_s = 1.25$ from Roache (1994). Both factors are equal for $C_l = (0.875, 1.125)$. Between these two intersections $F_{s,c}$ is smaller than F_s and therefore less conservative. Outside the interval defined by the intersection points $F_{s,c}$ is larger and therefore more conservative if one does not already use $F_s = 3$. The choice of the appropriate factor of safety is a matter of an ongoing discussion. Especially the question which factor would provide a 95% confidence level (Roy, 2005).

B Examples of Common Practice

B.1. Practice of RANS CFD simulation at the AUTH LHTEE

The Laboratory of Heat Transfer and Environmental Engineering (LHTEE) at the Aristotle University Thessaloniki, Greece, makes use of the following CFD codes:

Commercial codes:

1. Grid generation software: ANSYS ICEM CFD (currently V5.1)
2. CFD code: TASCflow V 02.11.02 (Last version acquired)
ANSYS CFX 5.7.1

In house codes: MIMO (includes a grid generator)

Applications: All commercial codes have been used for many industrial applications mainly within the frame of EU sponsored projects (AEROHEX, PICADA, TRAPOS, ATREUS, SEC etc.). TASCflow has also been used in various inter-comparison exercises such as the one within the frame of the TRAPOS project. MIMO has also been evaluated and validated within the frame of TRAPOS and ATREUS. Furthermore, we have made quite a few comparisons with available wind tunnel data for different problems. Finally, all codes have been used in order to assess the sensitivity of results for environmental flows mainly around complex building structures and streets on:

- The roughness of walls (ground and building walls).
- Grid sensitivity analysis.
- Convergence criteria sensitivity analysis.

B.1.1. Problem definition

From our point of view proper definition and documentation of the following is essential:

- The aims and goals for the solution of the problem (what do we want to investigate?)
- The geometrical characteristics of the buildings and streets including their orientation. Some geometrical characteristics can influence the dispersion of traffic emitted pollution to a great extent. For example we have found that the existence of balconies within streets can result in considerably higher levels of concentrations in comparison with streets which possess the same general geometrical characteristics but their buildings have no balconies.
- The physical parameters that need to be taken into account on a problem specific basis (For example possible buoyancy forces from heat transfer effects?).

B.1.2. Specification of boundary conditions

A correct specification of the boundary conditions is quite important in the sense that a numerical model will only do what we tell it to do. With regards to the evaluation models some boundary conditions are quite important since they could lead to significant numerical errors.

a) Real cases:

1) Wind profile – roughness height:

In case there are available detailed meteorological measurements a wind profile from these measurements can be used as inflow boundary condition for numerical simulations (logarithmic exponent, reference height, directional vector etc). From the analysis of these approach flow boundary layer characteristics the roughness height for the ground inside the computational domain can be defined. However, since such detailed meteorological measurements are quite rare, the usual practice is to try and obtain some background meteorological measurements from a station as close to the geometry under investigation as possible. In this way, we can at least obtain some idea of the prominent wind directions and their intensity. Then we construct a wind profile based on some guidelines (VDI, ESDU etc) or by matching the approach flow profile up to a reference height where there is a real measurement.

2) Temperature related boundary conditions.

If we need to approximate heat transfer effects, in case there are detailed meteorological field measurements available, we can use them to obtain an ambient temperature profile. Otherwise we obtain the ambient temperature from background measurements from a station close by. Moreover, if measured building wall temperatures are available, we use them. In any other case, depending on the season of the year, the time of the day, the orientation of the geometry and the material of the wall building, we obtain a measure for the temperature (as realistic as possible that is) for the building walls by taking into account the amount of radiation that has been absorbed by the walls, up to the time of the day that the numerical simulation is supposed to approximate.

b) Wind tunnel defined cases.

When a study is undertaken in the frame of which comparison is made with wind tunnel measurements, all inflow boundary conditions are in accordance with the wind tunnel measurements.

B.1.3. Choice of the turbulence models

Both MIMO and the other two industrial codes have a variety of choices when turbulence models such as $k-\varepsilon$ models (including the standard $k-\varepsilon$, $k-\varepsilon$ by Kato and Launder and Renormalization group $k-\varepsilon$), $k-\omega$ (including $k-\omega$ SST) and other 2nd moment closure model (SSG) are applied. For most environmental flows in and around streets, buildings or array of buildings, we usually use the standard $k-\varepsilon$ model, since it has proven to be quite stable. However, the numerical errors that we have encountered (which result mainly from the use of the standard wall functions, and mainly lead to delayed separation and an overestimation of the length of separation

zones) have led us to investigate the use of other models. The choice of the turbulence model should, from our point of view, be problem specific.

B.1.4. Grid specification

From LHTEE's point of view, the definition of the appropriate grid is considered very important. MIMO and CFX TASCflow (now ANSYS) make use of structured hexa grid, while ANSYS CFX makes use primarily of unstructured grid (tetra) but it can also use structured one. In most cases of environmental flows (around buildings streets etc), we use MIMO and hence structured stretched grid.

The specification of the appropriate grid depends heavily on the choice of the turbulence model and the corresponding wall function (if a specific turbulence model makes use of wall functions). Furthermore, the resolution near the walls is dependant on the non-dimensional distance y^+ and the roughness of the wall itself. As a result, with respect to the resolution, there exist some restrictions for all models near the walls. Usually, we use an expansion ratio of no more than 1.4 and not less than 1.15, with a minimum cell size which corresponds (as closely as possible) to the y^+ requirements. Furthermore, the minimum cell size near the buildings and the ground has to be quite different. The reason is that for atmospheric flows by definition the ground should have a larger roughness height. Therefore, the minimum cell size at the ground is larger than the minimum cell size of the building walls. It is therefore not easy to obtain a rule for the definition of the appropriate grid.

It is for this reason, that we now perform simple grid sensitivity tests for every problem, prior to the initiation of the final computation as follows:

- 1) We perform a very simple and rough calculation for the possible y^+ requirements.
- 2) By knowing this requirements and bearing in mind the restrictions in the available computing power, we initially construct a more or less "lighter" grid and we perform an initial numerical simulation (using the geometry and boundary conditions specified in the previous tests).
- 3) We extract results at a specific location of interest, which is usually near the wall. If we have a measurement near the wall (in case for example the problem has also been modelled in a wind tunnel) then we compare the numerical results with the measurement.
- 4) Then we construct a denser grid and the simulation and the subsequent comparison between the numerical results and the measurement is repeated.
- 5) This iterative process is repeated until satisfactory agreement between the numerical results and the measurements is reached.

If however we do not have a quality assured measurement at a location of interest then the process from step 3 and onward differs:

- 3) We extract results for a scalar of interest like a vertical u - component profile from the ground up to the roof level inside a street and quite close to any of the walls (let's assume the leeward).
- 4) Then we construct a denser grid and we compare the results from the two different grids. Normally there will be a disagreement between the two.

5) Then we repeat the same process until the disagreement in the results between two consequent steps is satisfactory small.

Only then we declare the specifications of a grid as assured.

B.1.5. Time step choice

The choice of the appropriate time step when performing a numerical simulation should also be considered: we usually use some fraction of the characteristic velocity over some characteristic length scale. At the same time we are careful to satisfy the Courant-Friedrichs-Lewy stability criteria.

Usually, smaller time steps will lead to definite convergence but will require a lot more of computing time. At the other hand significantly higher time steps cannot guarantee a higher quality of results.

B.1.6. Convergence criteria sensitivity

By experience we have found that for most applications (at least most engineering ones) convergence of the scaled residuals down to 10^{-5} should be OK (this applies to all three codes). However, depending on the complexity of the problem under investigation and also on the goal of the numerical study (in other words on what we want to measure and where), we have found by experience that a convergence criterion study for some problems is necessary. The process is essentially the same as the one described in step 4. Starting with larger residuals convergence criteria (10^{-3}) we perform a series of numerical simulations by gradually reducing them (10^{-4} , 10^{-5} and so on) until the disagreement between two subsequent steps is sufficiently small. One should bear in mind that convergence down to very small criteria results in largely increased computing time. Therefore, with respect to the choice of the convergence criteria, the requirement should be to obtain quality results in the least possible computing time.

These are the general guidelines of the procedure that we usually follow. We have found that it helps a lot to adequately reduce numerical errors in a relatively wide range of applications.

B.2. Practice of CFD simulation at IFT, University of Siegen

The Department of Fluid and Thermodynamics (IFT) at the University of Siegen, Germany, conducts CFD simulations in the built environment, using the following practise.

Grid generation software: ANSYS ICEM CFD (V4.0 – V4.3)

CFD code: FLUENT (V6.0 – V6.3)

Applications: up to now only comparisons of flow fields with wind tunnel experiments (mostly from CEDVAL database); RANS with constant fluid properties; analysis of

- turbulence models
- domain size
- grid resolution

- rough wall boundary conditions
- Best practice based on:
- ERCOFTAC BPG (Casey & Wintergerste, 2000)
 - AIJ BPG (Mochida et al., 2002, Yoshie et al., 2005)
 - COST C14 recommendations (Franke et al., 2004)

B.2.1. Turbulence models

Simulations are always started with the standard k- ϵ model, due to its very good stability. Depending on the application different models are then additionally tested:

- Realizable k- ϵ model for pedestrian wind environment, see Blocken et al. (2004)
- Renormalization group k- ϵ model for pressures on buildings, see Wright & Easom (1999)
- Reynolds stress model(s) (RSM) with and without wall damping for both applications (LRR-IP, SSG models are available in FLUENT)

B.2.2. Domain size

The domain size is very application-dependent. For single buildings we use the recommendations of Hall (1997) if the height and width are not too different. Otherwise we use a domain height of $6H_{\max}$ and the span-wise extent is determined by applying the aspect ratio of the building to the domain (Blocken et al., 2004). In front of the building we use as a minimum $5H_{\max}$ and behind the building $15H_{\max}$. For multiple buildings we only have experience with wind tunnel experiments where we use the tunnel geometry as height and width.

B.2.3. Grid

One important boundary condition is the available memory of the computers. Always using double precision we are therefore restricted to app. $2.3 \cdot 10^6$ cells to be able to use RSM models. As most applications in the urban environment are geometrically rather simple we never used anything but a block structured grid, sometimes with local refinement. The resolution at the ground is not only determined by the non-dimensional wall distance but mainly by the roughness height. This is the greatest weakness of commercial CFD codes from mechanical engineering applications as they use normally the sand grain roughness, which is app. 30 times the hydrodynamic roughness length z_0 in the wall function approach. Another criterion is the height of the positions where the flow is analysed. For pedestrian winds the fourth cell should be at app. 2m. For building heights and street resolution we use ten cells as minimum, as also recommended by Bartzis et al. (2004). Finally the expansion ratio of the grid is kept below 1.5, normally 1.2 is the maximum. Up to now we performed grid sensitivity tests with at least three grids only qualitatively. At the moment we start analysing the grid convergence with Richardson extrapolation.

B.2.4. Numerical approximations

For app. the first 100 iterations we use first order upwind for the interpolation within the convective terms and then switch to second order upwind for the final solutions. On the finest grid we sometimes make calculations with the QUICK scheme for

comparison. Until now we never found a big difference. Gradients are calculated with a second order scheme (second order on equidistant grids).

B.2.5. Convergence criteria

Scaled residuals are used as standard in FLUENT. The L_1 norm of the residual in every cell is computed. For the continuity scaling is performed with the maximum value of the norm during the first five iterations. For the other variables scaling is done with the sum of the products between the central coefficients (a_p) and the cell values of the variables. We normally prescribe 10^{-6} as convergence criterion for all variables. It is often impossible to reach these values due to the fact that we often start our calculation on the finer grids with the results of the coarser grids. Therefore continuity is already relatively well converged within the first five iterations and the residuals then are not reduced substantially. But we always monitor the variables of interest at least at critical positions.

B.3. Practice of CFD simulation with MISKAM

This approach is based on German VDI guideline (VDI, 2005), the MISKAM hand book (Eichhorn, 2004) and experiences obtained by

- National Environmental Research Institute (M. Ketzler, R. Berkowicz),
- Department of Fluid Mechanics, Budapest University of Technology and Economics (BME) (I. Goricsán, M. Balczó),
- Lohmeyer Consulting Engineers (Th. Flassak),
- MISKAM developer J. Eichhorn

This should mainly be a reminder as in daily life a modeller needs a very brief and concise checklist when he applies a model. That does not at all exclude the need to read the full guideline and hand book in the initial phase.

B.3.1. Computational domain

Height H:

- Choice of H large enough to keep the blockage ratio smaller than 10 % (VDI, 2005).
- The height of the largest building may not exceed 30% of the domain height, H (Eichhorn, 2004).
- Recommendation for H about 500 m, since variable results have been found for smaller heights (Ketzler et al., 2000).
- A somewhat sharper criterion than above: H should be at least 6 times as much as the characteristic building height H_b . Blockage ratio is to be kept below 3% (Franke et al., 2004).

Horizontal dimensions:

Borders around the investigated area would be approximately $10H_b$ (H_b is the characteristic height of the buildings) or 400 m (Lohmeyer, 2005).

If only one wind direction is investigated, $5H_b$ distance between inflow boundaries and investigated area is enough, and $10H_b$ is necessary to the outflow boundaries.

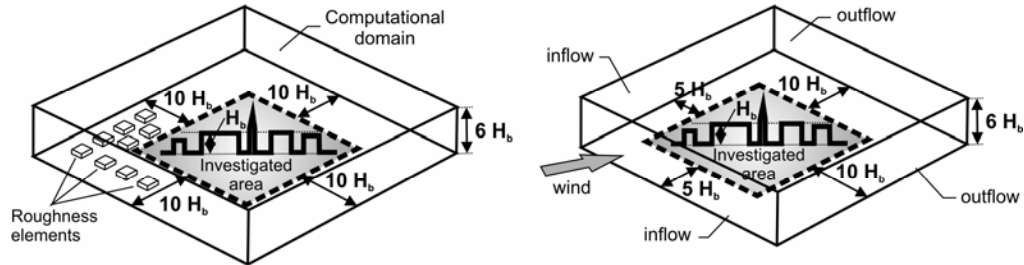


Figure 1: MISKAM boundaries in multidirectional and one directional simulation if the roughness around the investigated area is homogeneous

Roughness elements (block buildings with height of H_b) can be used in the border area located around the investigated area if the roughness around the investigated area is homogeneous. This method is acceptable to simulate the effect of neighbouring buildings (quarters). For multidirectional simulation tall buildings, outside the investigated area, have to be included if their distance to the border of the investigated area is less than 10 building heights. For one-directional simulation: include buildings in case the distance is less than 2 building heights if building is down stream, 10 building heights if upstream.

Note: For the calculation of domain sizes and blockage ratio, also those 1 or 5 cells should be considered, which can be added to each domain side in horizontal directions (using Menu item ‘MISKAM version’ in WinMISKAM)

B.3.2. Grid resolution

Horizontal resolution:

- The horizontal resolution in street canyons should be ≤ 2 m, at least 6 - 8 nodes would be necessary in street canyons (Eichhorn, 2004).
- Resolution of buildings: at least 3 nodes would be necessary in every direction in case of buildings located in the investigated area (VDI, 2005).
- Accuracy of building geometry in the investigated area should be of about 1 m, to avoid large errors at the projection of the building shapes to the computational grid. If the grid is fine enough, inclined roofs can be also modelled (Eichhorn, 2004).
- Accuracy of buildings outside of the investigated area can be less, ≤ 20 % is enough or simulated by roughness elements. Roof modelling is not necessary (Eichhorn, 2004).

Vertical resolution:

- Fine vertical resolution (cells < 10 m) up to $3H_b$ (at least 12 layers; VDI, 2005).
- Higher resolution near the ground (≤ 1 m) especially in case of ground sources (e.g. traffic).
- Investigated points have to be situated at least in $4z_0$ height (VDI, 2005).

Horizontal and vertical resolution:

- between the building or the surface and the investigated cell at least 2 cells are required (VDI, 2005).
- The minimum distance between the investigated cell and the border area might be 10 cells (Eichhorn, 2004).
- The investigated point (cell) cannot be in cells containing source or neighboured to source cell (Eichhorn, 2004).
- The vertical and horizontal expansion ratio of the cells should not exceed 1.2 (VDI, 2005).

B.3.3. Other MISKAM options

Turbulence closure: k - ε turbulence closure is the only choice in newer MISKAM versions.

Roughness lengths:

- On the ground: Choice of z_0 according to the table in Eichhorn (2004), but it might not exceed 25% of the height of the lowest cell.
- Walls and roofs: z_0 of 1-5 cm suggested (Eichhorn, 2004).

Stability criterion:

- Wind field calculation: steady state
- Dispersion calculation: S2 should be used by default. In cases, where investigated points are near to the source and are expected to have high concentrations, S1 stability criterion is also adequate (shorter CPU time), e.g. in street canyons with line source. Use of the S2 stability criterion is advisable in all other cases, e. g. for long-distance pollution transport (Eichhorn, 2004).

Smolarkiewicz correction steps at dispersion calculations:

- To decrease the numerical diffusion of the upwind scheme, this option is useful, e.g. for point source simulations (Eichhorn, 2004).
- If statistical values are computed: the upwind scheme (without correction steps) is sufficient.

Roughness initial profile:

- Corresponding to the terrain from 0.1 to 0.5 m, but z_0 must not exceed the 25% of the height of lowest cell (i.e. maximal 0.15 m; VDI, 2005).

B.3.4. Meteorology

For annual mean concentration statistics

- reference height of 100 m and reference wind velocity of 5-10 m/s might be used (Lohmeyer, 2006).

In general cases

- reference wind velocity and reference height can be chosen according to the available meteorological data.

B.3.5. Traffic produced turbulence

For MISKAM calculations close to roads, the effect of traffic produced turbulence on the dispersion has to be considered, especially for low wind speeds. Several scaling methods suitable for calculation of time series or statistical values from CFD code results have been investigated (Ketzler et al., 2001). The so-called TPT scaling is recommended. WinMISKAM allows the user to choose a scaling proportional to a power of the wind speed (usually 0.35) below a threshold (usually 3-4 m/s), the so called VDI scaling.

B.3.6. Stability

- Using MISKAM under stable conditions is proposed just with great caution due to the not validated stability module. High stability (1K/100m) can cause irrational vertical velocity profiles.
- When using lower stability (0.5K/100m), a high reference height has to be chosen (e.g. top boundary height) to avoid irrational high velocities at large heights.

B.3.7. Known Problems

As known, at wind field calculations MISKAM uses first order upwind scheme with high numerical diffusion.

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- to develop a coherent and structured quality assurance procedure for these type of models,
- to provide a systematically compiled set of appropriate and sufficiently detailed data for model validation work in a convenient and generally accessible form,
- to build a consensus within the community of micro-scale model developers and users regarding the usefulness of the procedure,
- to stimulate a widespread application of the procedure and the preparation of quality assurance protocols which prove the ‘fitness for purpose’ of all micro-scale meteorological models participating in this activity,
- to contribute to the proper use of models by disseminating information on the range of applicability, the potential and the limitations of such models,
- to identify the current weaknesses of the models and data bases,
- to give recommendations for focussed experimental programmes in order to improve the data base and
- to give recommendations for the improvement of present models and, if necessary, for new model parameterisations or even new model developments.



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