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Numerical simulation of atmospheric flows using general purpose CFD solvers

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Introduction

The numerical investigation of atmospheric flows were intensively developed, since computers have been applied for solving such complex numerical problems. ENIAC was the first electronic general purpose computer, and an atmospheric simulation was among the first successful computations executed on this revolutionary machine. The last few decades have seen considerable technological advances in computer sciences, which enables the possibility of detailed numerical simulation of micro- and meso-scale atmospheric phenomena. Since the spatial resolution is approaching to the lower scales with the increasing computational capacity, more and more details should be considered in order to their influence on the flow field. These details, such as the geometry of buildings and structures, generate turbulence and modify the flow patterns on smaller scales. General purpose CFD solvers handle the geometrical constraints pliantly, although representing the physical flavor of atmospheric flows is still a challenge.

The present research focused on the numerical simulation of micro- and meso-scale atmospheric flows using general purpose CFD solvers. There is a developing demand in civil engineering practice for the accurate description of small scale atmospheric phenomenon, inasmuch as the sustainable development is getting more and more important, hence the constructions should be suitable in environmental and energetics point of view as well. Several engineering problems are connected to the atmospheric processes, such as the analysis of optimal wind farm design and city ventilation, calculation of wind load on buildings and structures, furthermore the prediction of pollutant dispersion. Consequently, the study deals with the adaptation of commonly used solvers in engineering practice, the development, verification and validation of models and approaches, furthermore the elaboration of the modeling procedure. The work is divided into four parts, whose cover the four main problem investigated in this research.

The first problem is focused on the boundary conditions used for the simulation of flows within the neutral atmospheric boundary layer (ABL). The objective requires physically correct boundary conditions, whose are representative for the entire ABL. While the atmosphere is bounded by the ground from below, the lower boundary is always considered as a rough surface. In the engineering practice, the rough wall functions are used for modeling the effects of the surface roughness, using the sand grain roughness and the roughness parameter for characterizing the quality of the surface. On the other hand, in the description of the neutral atmospheric boundary layer, the quality of the surface is characterized by the roughness length, according to the meteorological terminology. For this reason, the application of the rough wall function available in general purpose solvers together with the atmospheric profiles is problematic, while the fully developed inlet profiles degenerates along the domain, even in case of flat terrain with homogeneous roughness, which results inhomogeneous boundary layer. To overcome this problem developments should be carried out on the rough wall functions and on the turbulence model, in order to reproduce the homogeneous ABL.

The second problem is focused on the simulation of flows over complex terrain. A turbulence model developed and applied for resolving the homogeneous, neutral ABL are not appropriate for inhomogeneous boundary layers develop over complex terrain. The solution is a generalized turbulence model, which is valid for mixed boundary layers.

The third problem is formed on the simulations of urban canopy layers. In the simulations of urban flows, the geometry of the buildings can be considered in the course of spatial discretization, but it implies high computational costs, since the required spatial resolution ($\sim$0.1 - 10 m) results unmanageably high number of cells, in particular for larger domains. The spatial resolution of limited area atmospheric models used for meteorological purposes ($\sim$100 - 10000 m) does not allow to take into consideration the geometrical features of the buildings, but the effects of the built-up environment could be realized in the calculations via parametrizations. These two scale should be converged to each other, since the computational costs should be reduced, but the important flow features should be resolved in order to achieve reasonable results with feasible computational requirements.

The last main part has several portion, since the simulation of atmospheric flows implies several problem specific task, such as the geometrical representation of the complex terrain, the setup of boundary conditions, the definition of the surface roughness and other surface specific parameters, furthermore the mesh generation considering the formers. These tasks are different from the general tasks of the engineering practice, thus a specialized methodology is required.

Results and discussion

As it is mentioned above, the research is compartmentalized four problem, whose are discussed in the following. The methods, approaches and models developed to get a solution for these problems are introduced together with their results.

To overcome the problems originated from the parametrization of rough wall functions, an alternative formulation is derived for the calculation of roughness parameters by imposing first-order matching between the velocity given by the inlet profile and the wall function at the wall adjacent cell. Under the assumption that the regime is fully rough, a modified roughness constant and equivalent sand grain roughness are calculated using the physical roughness and the wall distance of the first cell centroid. This approach has the advantage that its application does not require modifications on the wall function, thus it can be applied directly in most of the general purpose CFD solver. It should be noted that its application could be limited by the given roughness constant range of the solver. The deteoriation of the inlet profiles in streamwise direction yielded the motivation to the development and implementation of a consistent set of inlet and wall boundary conditions. The STD k-ε turbulence model is taken as a basis and modified according to make it valid for the entire homogeneous neutral atmospheric boundary layer (HBL), namely to ensure the conformity between the model, the wall functions and the inlet boundary conditions. This approach is extended above the boundary layer thickness, with a novel profile formulation including a four parameter turbulent kinetic energy profile to achieve better correspondence between the boundary conditions and experimental profiles. The consequential source terms of the extended approach are derived for ensuring the validity of the turbulence model within and above the boundary layer. The boundary conditions, wall functions and the implemented HBL k-ε model are validated against theoretical profiles at full scale, and against measurements at laboratory scale from three different data sets obtained via wind tunnel experiments. Results indicate that the novel set of boundary conditions reproduces the measured profiles for all examined cases, as indicated by correlation coefficients above 0.8. This improvement is pronounced compared to the formerly suggested boundary conditions, where the correlation coefficients of the turbulent kinetic energy profiles had the values of 0.119, 0.416 and -0.785 by turns, and whose are improved by the new method to 0.822, 0.966 and 0.941, respectively. Moreover, the extended model ensures the stream-wise homogeneity of the velocity and turbulence profiles at the inlet and outlet sections of the domain, even above the boundary layer thickness.

In order to simulate inhomogeneous ABL flows develops over complex terrain, the HBL k-ε model is further developed, to achieve that its formalism is applied in those regions, where the boundary layer is considered as homogeneous, but in case of streamwise inhomogeneities caused by the complex terrain, the STD k-ε model is applied. The new model, the so-called ABL k-ε model provides continuous smooth blending between the formalisms, which based on the normalized velocity difference between its simulated and theoretical value. The rate of transition is described by a sinusoidal power function with a supplemental threshold offset, which required in order to avoid pseudo blending caused by small numerical discrepancies next to the wall in former blending functions. The optimal value for the exhibitor N of this function is determined in the course of different flow simulations over complex terrain. Out of the examined integer values, the best results were obtained with $N = 3$. The ABL k-ε model is validated against measurements at laboratory scale and full scale as well, using the optimal blending exhibitor. The calculated velocity agreed well with the measurements at both laboratory and full scale, while reasonable agreement is found for the turbulent kinetic energy. In order to measure the improvement produced by the ABL k-ε, its results are compared to results obtained by the formalisms can be found in the literature. These are proved oneself to be significantly better than the results obtained by using the formerly suggested formalisms. The improvement on the hit rate was around 10–15% for the velocity and 10–20% for the turbulent kinetic energy, thanks to the application of the new approach. According to the recommendation can be found in the literature, the Kato-Launder modification, the Yap correction, furthermore the Murakami-Mochida-Kondo (MMK) model are implemented to enhance the performance of the ABL k-ε model in the simulations of flow where stagnation and separation appears. The effects of these are investigated on the cases used for the former validation. At laboratory scale, the application of these modifications decreased the hit rates with 1–2% for both the velocity and turbulent kinetic energy. At full scale, the application of the Kato-Launder modification with the Yap correction are not produce remarkable improvement, but the MMK model resulted a significant improvement reaching the 100% hit rate value for the velocity. In order to further extend the examination of the ABL k-ε model, a quantitative comparison is carried out between the results obtained by ANSYS-Fluent and OpenFOAM general purpose solvers. The OpenFOAM solver provided significantly better results with similar computational costs. The simulations, using the original in-built models of the solvers, gives similar quantitative results, although these are worse than the results obtained with the new approach. As it is identified, the differences are originated from the way of the implementation. While the OpenFOAM is an open source C++ library, the implementation of a model is straightforward. Contrarily the ANSYS-Fluent commercial solver can be only modified via user defined functions, moreover, the source of the model formalisms are not accessible, therefore the potential of the strict implementation is limited.

Dealing with the third problem, a scale adaptive hybrid modeling method is developed for combining the advantages of the parametrization schemes applied in the meteorological practice, and the explicit geometrical modeling, resolving its features applied in CFD approaches. The substance of this method is that the porous drag force approach is applied in the marginal regions for simulate the effects of the buildings and the vegetation, while the geometry of building blocks, or even some selected buildings can be considered explicitly via mesh refinement in the regions, where the flow features are important in the analysis point of view. A special meshing procedure is developed, which allows the separation of the regions with different surface coverage, furthermore provide continuous transition between the coarser mesh applied in marginal regions and the finest applied in the target area of the analysis. The porous drag force approach specialized for atmospheric flows is implemented in the ANSYS-Fluent general purpose solver, in the form of additional source terms in the transport equations of momentum, turbulent kinetic energy and its dissipation rate. The source terms are computed based on the local cell values of the field variables, furthermore the canopy parameters specified automatically in each cells at the initialization. The scale adaptive hybrid method is validated against up-scaled wind tunnel measurements, where it was applied together with the clearly explicit and implicit approaches. The results of the clearly explicit method are above the validation limit (66%) for both streamwise and vertical velocity components with the hit rate of 75.44% and 77.21%, respectively. The resulted hit rate for turbulent kinetic energy just fall below the limit with 64.84%. The explicit results are fairly similar to the former simulation results obtained with the MISKAM solver at the measurement tower placed in the middle of the target area, although their agreement with the measurements is not satisfactory. The local velocity results of the hybrid and explicit method is similar in the target area, however, the hybrid approach requires much less computational resources, namely one in five. The layer averaged velocity results show good agreement among the three different approaches within the canopy layer, although slight differences can be observed above, which proves that implicit approach are able to represent the effects of the canopy at larger scales. The approach verified against theoretical profiles in a practical application as well, which demonstrate the its potential in field of real engineering problems.

For the problem specific tasks of atmospheric simulations are brought up from the last problem, the methodology of their procedure is developed. In order to simplify the setup of the lateral boundary conditions, the accommodation of the domain extension with the so-called relaxation zone is proposed. In this zone, which frames the target area, the relief as well as the surface coverage parameters are connected with a smooth transition to the constant terrain height and surface parameters defined at the lateral boundaries of the domain. It does not only facilitate the setup, but improves the numerical stability and convergence of the calculations. According to facilitate the preparation of domain geometry, recommendations are given for the extended size of the computational domain and for the selection of map projection with respect to the location and size of the target area, furthermore the features and properties of the relief. The recommended size of the extension is corroborated by a series of numerical simulation, while the recommendations for the applicable map projections are based on practical considerations. Mesh generation methods are developed for the efficient and automatic meshing for domains with complex terrain geometry, and with separated regions with different surface coverage, producing task specific meshes. The terrain relaxation is built in this mesh generation framework. The methodology for the preparation and execution of atmospheric simulations is developed and applied successfully in different case studies. This methodology serve as a guideline for solving atmospheric problems in the engineering practice.

New scientific results

1. Thesis: Boundary conditions for atmospheric simulations

A novel wall function parametrization is derived for rough walls can be used in atmospheric simulations. A former approach is extended with a realizable set of inlet conditions, including a novel turbulent kinetic energy profile. The source terms required for the simulation of homogeneous neutral ABL is derived. The turbulence model, which applies the extended approach and called HBL k-ε is implemented in the OpenFOAM general purpose CFD solver and validated against measurements, together with the formerly suggested approaches for comparison.

a) In order to overcome the problems originated from the parametrization of rough wall functions, alternative formulation is derived for the calculation of the roughness constant and the sand grain roughness. This approach has the advantage that its application does not require modifications on the wall function, which is commonly used in CFD solvers.

b) The consistent set of inlet boundary conditions and wall functions are implemented in the OpenFOAM simulation system. The STD k-ε turbulence model in OpenFOAM is modified according to make it valid within the homogeneous neutral atmospheric boundary layer (HBL), namely to ensure the conformity between the model and the boundary conditions [1, 2]. This former approach is extended above the boundary layer thickness, with a novel inlet profile formulation including a four parameter turbulent kinetic energy profile. The source terms of the extended approach are derived for ensuring the validity of the turbulence model within and above the boundary layer [3]. The extended turbulence model is called as HBL k-ε.

c) The boundary conditions, wall functions and the implemented HBL k-ε model are validated against theoretical profiles at full scale, and against measurements at laboratory scale. Results indicate that the novel set of boundary conditions reproduces the measured profiles for all examined cases, as indicated by correlation coefficients above 0.8. This improvement is pronounced compared to the formerly suggested boundary conditions. Moreover, the extended model ensures the streamwise homogeneity of the velocity and turbulence profiles, as it is shown by the matching at the inlet and outlet sections of the domains, even above the boundary layer thickness [3].

2. Thesis: Modeling atmospheric flows over complex terrain

The HBL k-ε model is generalized in order to simulate both homogeneous and inhomogeneous ABL flows over complex terrain. A novel sinusoidal blending function formulated for the universal model called ABL k-ε. The ABL k-ε model are validated against measurements. The recommended modification on the turbulence model for flows with stagnation and separation, can be found in the literature, are implemented into the generalized model, and the effectiveness of these are investigated on different cases.

a) The HBL k-ε turbulence model is generalized to achieve that in the homogeneous regions of the boundary layer the formalism of HBL model is applied, and it is continuously blended to the STD model formalism in those inhomogeneous regions, where the velocity field is strongly affected by the complex geometry. The generalized, so-called ABL k-ε model applies smooth blending between the formalisms, which based on the normalized velocity difference between its simulated and reference value. The rate of the transition is described by a sinusoidal power function. The optimal value for the exhibitor of the power function N is determined in the course of different flow simulations over complex terrain. Out of the examined integer values, the best results were obtained with $N = 3$ [1, 2, 4].

b) The ABL k-ε model is validated against measurements at laboratory scale and full scale, using the optimal blending exhibitor. The results are compared to the ones obtained by the formerly suggested approaches. The calculated velocity agreed well with the measurements at both laboratory and full scale, while reasonable agreement is found for the turbulent kinetic energy. The present results is proved oneself to be significantly better than the results obtained by using the former approaches [1, 2, 4].

c) According to the recommendation can be found in the literature, the Kato-Launder modification, the Yap correction, furthermore the MMK model are implemented to enhance the performance of the ABL k-ε model in the simulations of flows, where stagnation or separation appears. The effectiveness of these are investigated in detail on 3D cases at both laboratory and full scale. The investigation shown that the application of the Kato-Launder modification and the Yap correction are not produce remarkable improvement, but the MMK model resulted a significant improvement at full scale [1, 2, 4].

3. Thesis: Scale adaptive modeling approach for urban flows

A novel scale adaptive, hybrid method is developed for the simulations of atmospheric flows in urban canopy layers, implemented in a general purpose solver, validated against measurements and verified on a practical engineering application.

a) The novel hybrid method is developed, which combines the advantages of the implicit porous drag force approach, applied at larger scales, and the explicit modeling of the geometry, resolving its features applied in CFD approaches. The substance of this method is that the porous drag force approach is applied in the marginal regions of the domain for describe the effects of the buildings and the vegetation, while the geometrical features of the urban environment are considered via mesh refinement in the target area, which is the most important in the aspect of the analysis. A special meshing procedure is developed, which allows the separation of the regions with different surface coverage, furthermore provide continuous transition between the coarser mesh applied in marginal regions and the finest applied in the target area of the analysis[5, 6].

b) The porous drag force approach specialized for atmospheric flows, and implemented in the ANSYS-FLUENT general purpose solver. The scale adaptive hybrid method is validated against up-scaled wind tunnel measurements, and applied together with the clearly explicit and implicit approaches for comparison. The layer averaged velocity results showed good agreement among the three different approaches within the canopy layer, while slight differences are observed above. The velocity results of the hybrid and explicit method were matching in the target area, however, the hybrid approach requires much less computational resources. The novel method verified against theoretical profiles in a practical application, which demonstrates the potential of the approach in field of real wind engineering problems [5, 6].

4. Thesis: Methodology of atmospheric simulations

The methodology of atmospheric CFD simulations is developed, which focuses on those problem specific tasks, whose are different from the general tasks in the engineering practice. These tasks are the geometrical realization of the complex terrain, the definition of the lateral boundary conditions and surface parameters, furthermore the mesh generation process and turbulence modeling.

a) For the simplified setup of the lateral boundary conditions, the usage of a domain extension with the so-called relaxation zone is proposed. In this zone, which frames the target area, the relief as well as the surface coverage parameters are connected with smooth transition to the constant terrain height and surface parameters defined at the lateral boundaries of the domain. It does not only facilitate the setup, but improves the numerical stability and convergence of the calculations [7, 5, 6].

b) Recommendations are given for the extended size of the computational domain and for the selection of map projection with respect to the location and size of the target area, furthermore the features and properties of the relief. The recommended size of the extension is corroborated by a series of numerical simulation, while the recommendations for the applicable map projections are based on practical considerations.

c) Mesh generation methods are developed for the efficient and automatic meshing of domains with complex terrain geometry, and with separated regions with different surface coverage. The terrain smoothing and the formation of the relaxation zone is built in this mesh generation framework [7, 5, 6].

d) The methodology for the preparation and execution of atmospheric simulations is developed and applied successfully in different case studies (see e.g. [6, 2, 1, 8, 4]), using novel approaches for turbulence modeling. This methodology serves as a guideline for solving atmospheric problems in the engineering practice.

Publications for thesis points

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