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REVIEW AND INTERCOMPARISONS OF PARAMETERISATIONS AND BOUNDARY CONDITIONS FOR RANS AND LES CFD SIMULATIONS OF ATMOSPHERIC FLOW AND DISPERSION

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Abstract: Computation Fluid Dynamics (CFD) is now currently used in different operational context to simulate the atmospheric flow and the dispersion of pollutants over a complex built terrain, with resolved buildings and obstacles, as in urban or industrial area. Most of these applications involve RANS (Reynolds Averaged Navier-Stokes) approaches but the LES (Large Eddy Simulation) approach is also beginning to be commonly used for research works and for applied studies and industrial cases. Nevertheless, the definition of a parameterisation and boundary conditions to correctly describe the atmospheric boundary layer (ABL) are critical both for RANS and LES models and requires a particular attention. In the current work, we reviewed different methodologies used in the literature for RANS approaches during the last 30 years, and we performed a sensitivity study and a comparison of this different methodologies. We are also interested in the applicability and generalisation of these methodologies for LES approach.

Key words: *CFD, boundary conditions review, RANS, LES.*

INTRODUCTION

One source of uncertainties in CFD simulations is directly related to boundary conditions, e.g. inflow profiles, ground roughness, etc. The proper setting of boundary conditions enable to reduce numerical errors and correctly interpreted the final results. Although decades of studies, this subject is still open due to the extremely complexity of the ABL.

The current CFD review is divided into two main parts. The first one is dedicated to parameterisation and boundary conditions for RANS and the second is related to LES model. The last part is dedicated to the conclusions.

PARAMETERISATION AND BOUNDARY CONDITIONS FOR RANS MODEL

The work of Richards and Hoxey, (1993) could be considered as a fundamental reference for the ABL modelling. It represents a clear guideline to deal with this challenging problem and laid the foundations for more recent and complex models. We are interested to study the bottom part of the ABL, also known as surface boundary layer (SBL) or atmospheric surface layer. According to the previous authors the flow in this region should normally be modelled as a homogeneous flow. Therefore velocity and turbulence profiles, commonly associated with k-ε turbulence model, needs to produce homogeneous conditions. Ludwing and Sundaram, (1969) have suggested the basic conditions for simulate the SBL. Without considering how the flow is generated, a suitable model for the SBL should be related to a flow that is fully aerodynamically rough, horizontally homogeneous, and relatively free from any pressure gradients. A direct consequence of fully aerodynamic roughness is that the shear stress should be dominated by the Reynolds stresses. Moreover, the harder characteristic to achieve is the horizontal homogeneity. This condition can exist only in regions remote from any kind of obstructions and impose that the streamwise gradient of all variables are zero. Many numerical works (Yang et al., 2009; Tian et al., 2018) have underlined that the use of empirical equations for inflow boundary conditions, e.g. power law for velocity or polynomial fit for experimental turbulence kinetic energy, changes rapidly in the inlet region of the domain. The flow near the surface tends to accelerate considerably before been retarded by the influence of obstacles. In order to avoid this problem, it is very important that the inlet velocity and turbulence profiles, the ground shear stress and the turbulence model should be in equilibrium. Nevertheless, Hargreaves and Wright, (2007) have demonstrated that the latter conditions are not enough to produce a sustainable SBL. In order to reproduce a sustainable SBL, the computational approach needs additional modifications to the wall function and the top boundary conditions.

In steady incompressible 2-D flow modelling of SBL with the k-ε turbulence model, the existence of homogeneous flow has the following implications. Firstly the vertical velocity is zero, then the pressure is constant. Thirdly, the shear stress is constant as shown in equation (1).

$$\tau_w = \mu_t \frac{\partial u}{\partial z} = \rho u_*^2 \tag{1}$$

Finally the turbulent kinetic energy k and its dissipation rate ε satisfy their respective conservation equations. The latter equations are satisfied by the Richards and Hoxey profiles (R&H) for velocity, k and ε as illustrated in the set of equations (2). The current analysis is strictly related to a neutral SBL.

$$u(z) = \frac{u_*}{\kappa} ln\left(\frac{z + z_0}{z_0}\right), \qquad k = \frac{u_*^2}{\sqrt{C_\mu}}, \qquad \varepsilon(z) = \frac{u_*^3}{\kappa(z + z_0)} \tag{2}$$

The friction velocity is usually computed thanks to a specific velocity U_{ref} at a reference height z_{ref}. The desired equilibrium is reached only if the k-ε model coefficients are settled properly. The original coefficients (Launder and Sharma, 1974) proposed by default in many CFD codes does not conserve the profiles along the domain. In fact, the main constrain derives from the transport equation of the turbulence dissipation rate ε, which imposes:

$$\sigma_\varepsilon = \frac{\kappa^2}{(C_{\varepsilon 2} - C_{\varepsilon 1})\sqrt{C_\mu}} \tag{3}$$

Table 1. k-ε coefficients

	$\boldsymbol{\sigma_k}$	$\boldsymbol{\sigma_\varepsilon}$	$\boldsymbol{C_{\varepsilon 1}}$	$\boldsymbol{C_{\varepsilon 2}}$	$\boldsymbol{C_\mu}$
Launder and Sharma, (1974)	1.0	1.3	1.44	1.92	0.09
Hargreaves and Wright, (2007)	1.0	1.11	1.44	1.92	0.09
Duynkerke, (1988)	1.0	2.38	1.46	1.83	0.033

In this way, as shown in Table 1, Hargreaves and Wright, (2007) and Duynkerke, (1988) have proposed two valid set of coefficients which respect the constraint of equation (3).

Hargreaves and Wright, (2007) highlights the importance of wall functions and top boundary condition. A standard treatment of a rough wall could not be appropriate when we simulate an SBL because it is quite common to have the y^+ value of the first bottom cell outside the range of 30 to 300 that is recommended to apply the logarithmic law of the wall. If we use a commercial CFD code, it is important to take into account the error due to the use of a wall function with a standard roughness model and the need of a manual correction, e.g. through a User Defined Function. Open-source codes, like OpenFOAM, allow to correct directly the source code of the wall functions, as Richards and Hoxey made. However, with respect to the standard wall functions used by Hargreaves and Wright, (2007), OpenFOAM provides wall functions based on standard roughness model with good performances also outside of the logarithmic regions, as shown by Figure (1). Open-source codes could also present the wall function correction suggested by Hargreaves and Wright, (2007). Figure (2) illustrates the result induced by the latter approach. The performances of both the approaches are almost the same. Some slight difference is found near the wall due to the peak of the turbulent kinetic energy. On the other hand, the top boundary condition is important to preserve the profiles in the higher part of the domain. The standard suggestions regard the imposition of a constant shear stress of ρu_*^2, but it is also possible to impose a constant velocity (Tian et al., 2018) or a fixed gradient to the velocity and turbulent profiles, being defined thanks to a known expressions. The latter technique is applied in the results of Figure (1) and (2).

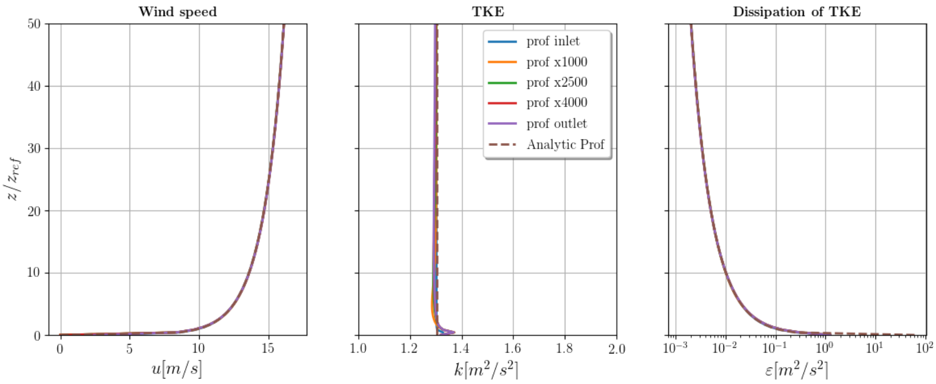

Figure 1. Evolution of velocity, turbulent kinetic energy and dissipation of turbulent kinetic energy profiles along 2D domain of 5 km and with z_{ref} of 6 m. Overall setting: Hargreaves and Wright, (2007). The intermediate profiles are at 1 km, 2.5 km and 4 km. The ground wall function uses a standard roughness model, available in OpenFOAM.

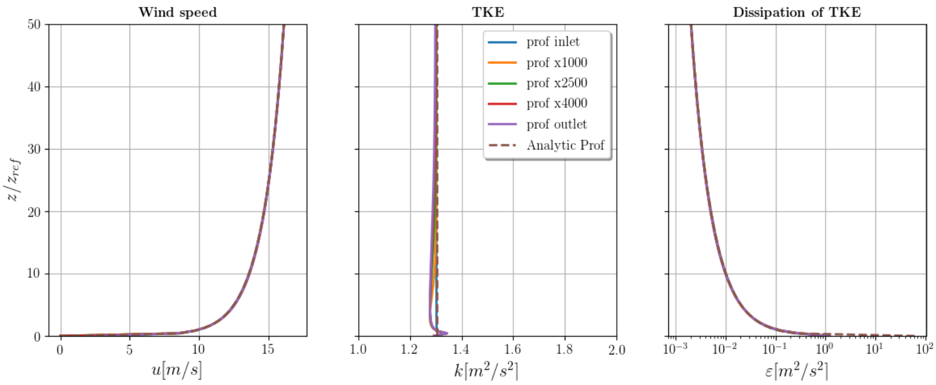

Figure 2. Evolution of velocity, turbulent kinetic energy and dissipation of turbulent kinetic energy profiles along 2D domain of 5 km and with z_{ref} of 6 m. The ground wall function uses a Hargreaves and Wright, (2007) correction.

The R&H profiles are usually used as inlet conditions. Nevertheless, we often work outside the SBL and its hypothesis. In fact, the assumption of constant kinetic energy k is not in agreement with wind-tunnel data (Nironi et al., 2015), where a variation of k with respect to height is observed. Yang et al. (2009) proposed a new set of inlet profiles, considering that k profile is a function of height. However, this approach produce an inconsistency with the k-ε model equations. Consequently, Gorle et al., (2009) proposed particular formulations for C_μ and σ_ε constants to ensure streamwise homogeneity in the new condition. One solution to equilibrate inlet profiles different from the Richards and Hoxey's ones are to introduce variable coefficients for the k-ε model. An alternative to variable coefficients which have different expressions according to the set of profiles treated, is the solution proposed by Parente et al. (2011). For the ε transport equation, the σ_ε coefficient could be maintained constant if a source term, shown in equation (4), is added to the transport equation.

$$S_\varepsilon(z) = \frac{\rho u_*^4}{(z+z_0)^2}\left(\frac{(C_2 - C_1)\sqrt{C_\mu}}{\kappa^2} - \frac{1}{\sigma_\varepsilon}\right) \tag{4}$$

The presence of a source term does not require the calculation of σ_ε. The current source self-adapts to the characteristics of SBL under investigation. Assuming a turbulent kinetic energy which vary with height, it is suggested to add a source term also in the k transport equation of the form:

$$S_k(z) = \frac{\rho u_* \kappa}{\sigma_k}\left((z+z_0)\frac{\partial k}{\partial z}\right) \tag{5}$$

The formulation of the source term is valid for any shape of k inlet profile, as long as the k gradient in vertical direction is specified. More recently, Tian et al., (2018) have present a more extensive review of the good practice to numerically simulate the SBL. The treatment of empirical and variable inlet profiles, which usually are not in equilibrium with the turbulent model equations, represent a challenging problem especially in cases of stable and unstable conditions of the ABL. Vendel, (2011) used the approach of variable coefficients for the k-ε model in order to equilibrate the different stability conditions of the ABL based on Gryning et al. (2007) approach.

Summarising, the use of inlet profiles different from R&H profiles highlight that it is important to re-equilibrate the k-ε equations. It could be done thanks to variable coefficients for the turbulence models or with the introduction of a source term in the transport equations of the turbulent kinetic energy and of its dissipation rate. Furthermore, it is fundamental to use appropriates wall functions and top boundary conditions to obtain a sustainable SBL.

BOUNDARY CONDITIONS FOR LES MODEL

When LES is chosen to solve the flow, the main issues concerning the SBL simulation are the boundary conditions, while the parameterisation of turbulence model plays a less important role with respect to RANS cases. In fact, a time-varying velocity field has to be specified at the inflow boundary using an appropriate inflow generator. Moreover, a suitable model that accounts for surface roughness needs to be employed. Therefore, inlet and wall boundary conditions have to be treated carefully. The inflow generators could be grouped into two classes (Tabor and Baba-Ahmadi, 2010): precursor simulation methods and synthetic methods. On the other hand, with respect to the roughness modelling, Vasaturo et al., (2018) have suggested a classification into three families of methods. The first method explicitly model the roughness elements. The second one uses momentum forcing terms. The last take into account the ground roughness though the prescription of shear stress at the wall.

In this part of our research, we are interested to the Vortex Method (VM), which made part of the inlet synthetic methods, and roughness models related to wall stress methods and wall functions. According to Mathey et al., (2006) and Vasaturo et al., (2018), the VM seems to present a good compromise between applicability to industrial cases and the stability-accuracy combination. Indeed, the precursor methods guarantee higher performances but with an unsustainable computational cost for industrial applications. Whereas, inside the family of synthetic methods, the Random Flow Generator is easier to implement but it suffers from problems linked to the decay of turbulence along the domain.

Resolving the near-wall dynamics directly is a no feasible path for industrial application because it could imply to have a grid adjacent to the wall of y^+ dimension less than 1. Consequently, a wall stress model or a wall function, which takes into account wall roughness, represents a good alternative. In this case, modelling the near-wall dynamics allow to work in the logarithmic layer ($20 \leq y^+ \leq 200$), (Sagaut, 2006). Wall function is applied when a hybrid method (RANS-LES) is used. Particular attention is given to Detached-Eddy Simulation (DES) that could be able to lighten the computational cost not only close to the wall but also in other regions of the domain where is not required so much accuracy.

CONCLUSIONS

The parameterisation of RANS model and the correct choice of its boundary conditions could take advantage of a big amount of works which have found different ways to simulate SBL in a proper way. On the other hand, LES model could face some difficulties related to computational cost for industrial and applied studies. For this reason a further research on hybrid methods and efficient inflow generators could give a fundamental contribution. Finally, the lack of works related to the different stability conditions of the ABL will lead us to better investigate this topic.

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