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ATMOSPHERIC BOUNDARY LAYER FLOW SIMULATIONS WITH OPENFOAM USING A MODIFIED K-EPSILON MODEL CONSISTENT WITH PRESCRIBED INLET CONDITIONS

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Abstract. *Two-equation models for the turbulent stress in the Reynolds-averaged Navier Stokes (RANS) equations are the most common turbulence modeling approach applied to atmospheric boundary layer (ABL) flows, mainly owing to their low computational cost. However, these models are known to generate streamwise gradients in the flow variables. As the flow approaches obstacles within the computational domain, even a small streamwise deviation of the flow variables from their inlet boundary conditions may have a non-negligible impact on the flow prediction. Over the years, previous work has addressed this issue in multiple ways, including a reduction of the computational domain upwind of the obstacle and new formulations for the wall functions that are consistent with the inlet boundary conditions. In this work, we implement a non-standard* $k-\epsilon$ *model in OpenFOAM-v2112 that is appropriate to simulate ABL flows. Results show that the inlet boundary conditions are largely preserved throughout the entire computational domain. Our implementation relies heavily on the previous work of Parente, A., Gorlé, C., van Beeck, J. and Benocci, C., 2011. "Improved* $k-\varepsilon$ *model and wall function formulation for the RANS simulation of ABL flows". Journal of Wind Engineering and Industrial Aerodynamics, Vol. 99, No. 4, pp. 267–278.*

Keywords: *Atmospheric Boundary Layer, OpenFOAM, k-*ε *model, CFD*

1. INTRODUCTION

The flow modeling underlying the lower part of the troposphere, the so-called the atmospheric boundary layer (ABL), over urban and complex areas, is usually performed within a Computational Fluid Dynamics (CFD) approach. The most common fluid flow models available are the Reynolds-averaged Navier Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS). The last two modeling approaches are more accurate than the RANS model, but the computational cost required by LES and DNS are considerably higher. Therefore, the numerical simulations of the flow over the urban canopy are usually performed using the RANS model associated with a two-equation turbulence model. However, RANS models have a known discrepancy between the inlet profiles prescribed for the wind velocity, turbulent kinetic energy (TKE) and turbulent kinetic energy dissipation rate (TDR), and the approaching flow just before the obstacles inside the computational domain. The reported non-homogeneity of the profiles is due to an inconsistency between the profiles for the wind velocity, TKE, and the TDR defined at the inlet boundary condition and the wall function formulation for rough surfaces.

In one of the seminal works concerning this subject, (Richards and Hoxey, 1993) claimed that horizontal homogeneity, which implies that all the stream-wise gradients of all variables should be zero, is hard to achieve and it can only exist away from obstacles. According to the authors, to avoid such gradients in the flow variables, it is indispensable that the inlet velocity, the turbulence profiles, the surface shear stress and the turbulence model should be in equilibrium. Thus, they proposed a new $k-\varepsilon$ turbulent model adapted to simulate the ABL flow. In a later work, (Blocken *et al.*, 2007) discussed these reported unintended stream-wise gradients, its negative consequences for the simulations and suggest remedial measurements to improve the simulations of the neutral ABL flow. (Yang *et al.*, 2009) proposed a set of inflow boundary conditions for the standard $k-\varepsilon$ model to simulate the neutral ABL flow. Such boundary conditions were theoretically derived to model an equilibrium ABL flow. Their premise is based on the hypotheses that to model an equilibrium ABL using the CFD approach requires the inflow boundary conditions to satisfy the set of model equations. The model considers a decrease in the inlet TKE profile with the height, which is more likely to reproduce full-scale measurements than the TKE profile proposed by (Richards and Hoxey, 1993), which is constant with height. (Parente *et al.*, 2011b,a) proposed an improvement of the wall function for the turbulence production developed by (Richards and Hoxey, 1993), avoiding the recurrently related over-prediction of the TKE on the wall. They also proposed modified

$k-\varepsilon$ turbulence model to enable the use of arbitrary sets of fully developed profiles at the inflow portion of the domain. Posteriorly, (Balogh *et al.*, 2012) proposed a comparison of the performances of the models developed in (Parente *et al.*, 2011b) and (Parente *et al.*, 2011a) using the softwares Ansys Fluent and OpenFOAM. According to the authors, the OpenFOAM code showed a great potential to simulate ABL flows and, compared to a commercial code, it provided better results with a comparable numerical effort.

In this work, we implement and explore modifications to the $k-\varepsilon$ model previously reported in the literature to address the inconsistency, within the framework of the CFD open-source code OpenFOAM. In order to validate our simulations, we use the wind tunnel experiment CEDVAL A1-1 (Leitl, 1998). This work constitutes the first step towards an open-source code solution, freely available to the community. The next step is to develop enhancements to include new formulations and non-neutral ABL flow and also atmospheric dispersion modeling.

2. MATHEMATICAL MODELS

Consider the ABL flow over a flat surface, with no obstacle and no changes on the meteorological conditions. In addition, no heat surface fluxes are considered. Assuming an incompressible, horizontally homogeneous and stationary state, the two-dimensional ABL can be described by the following hypotheses:

- constant shear stress,
- null vertical component of the velocity,
- constant pressure along the stream-wise (x) and the vertical (z) directions, respectively.

The $k-\varepsilon$ model is used to model turbulence. This model consists of the transport equations for the TKE (k) and the TDR (ε). The considerations above lead to equations for momentum, k and ε given respectively by Eqs. (1), (2) and (3).

$$\mu_T \frac{\partial u}{\partial z} = \tau = \rho u_*^2 \ , \tag{1}$$

$$\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_k}\frac{\partial k}{\partial z}\right) + G_k - \rho\varepsilon = 0 \ , \tag{2}$$

$$\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right) + \frac{\varepsilon}{k}C_{\varepsilon_1}G_k - \frac{\varepsilon^2}{k}\rho C_{\varepsilon_2} = 0 \ , \tag{3}$$

where $u_* \equiv \sqrt{\tau/\rho}$ is the friction velocity, C_{ε_1}, C_{ε_2}, σ_k, σ_ε, and C_μ are the model empirical constants defined originally by Launder and Spalding (1974). In addition, ρ is the air density, u is the wind velocity component in the x direction and μ_T is the turbulent viscosity. In the $k-\varepsilon$ model, the turbulent viscosity is defined as,

$$\mu_T \equiv \rho C_\mu \frac{k^2}{\varepsilon} \ . \tag{4}$$

Finally, the mechanical production of TKE term G_k is given by,

$$G_k = \mu_T \left(\frac{\partial u}{\partial z}\right)^2 \ . \tag{5}$$

In this work, we follow to a large extent the suggested modifications in the standard $k-\varepsilon$ model proposed by Parente *et al.* (2011a). These are briefly outlined next.

Under the assumption of equilibrium between production and dissipation in Eq. (2), we arrive at the following expression for the TDR:

$$\varepsilon = k\sqrt{C_\mu}\frac{\partial u}{\partial z} \ . \tag{6}$$

By combining Eqs. (1), (4) and (6), we obtain a relation for C_μ,

$$C_\mu(z) = \frac{u_*^4}{k(z)^2} \ , \tag{7}$$

where the dependence on the z-coordinate has been made explicit. This variable $C_\mu(z)$ guarantees a constant shear-stress throughout the boundary layer and was first proposed by Gorlé *et al.* (2009).

In order to solve equations (1)-(3), appropriate boundary conditions are required. As a starting point we begin by considering the well-known log-law inlet condition for velocity,

$$u = \frac{u_*}{\kappa} \ln\left(\frac{z + z_0}{z_0}\right) , \tag{8}$$

where κ is the von Kármán constant and z_0 is the aerodynamic roughness length. Combining the results from Eqs. (7), (6) and the analytical derivative $\partial u/\partial z$ from Eq. (8), we obtain a relation for ε,

$$\varepsilon = \frac{u_*^3}{\kappa(z + z_0)} . \tag{9}$$

The equation above for ε is consistent with the velocity profile given by Eq. (8) and satisfies the requirement of equilibrium between production and dissipation of TKE within the ABL. However, in order to satisfy the TKE equation, the first term in Eq. 2 must be identically zero, i.e.,

$$\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_k}\frac{\partial k}{\partial z}\right) = 0 . \tag{10}$$

Substitution of Eqs. (4), (7) and the analytical derivative $\partial u/\partial z$ from Eq. (8) in Eq. (10) yields, after integration,

$$k = A \ln{(z + z_0)} + B , \tag{11}$$

where A and B are numerical constants that can be fitted to experimental data.

At this stage we have arrived at a set of consistent inlet boundary conditions for u, k and ε given by Eqs. (8), (11) and (9), respectively. Furthermore, these guarantee that Eqs. (1) and (2) are identically satisfied. Substitution of the previous results in Eq. (3) shows that an addition of a source term S_ε is required in order to satisfy the equality. This term is given by,

$$S_\varepsilon = \frac{\rho u_*^4}{(z + z_0)}\left[\frac{(C_{\varepsilon_2} - C_{\varepsilon_1})\sqrt{C_\mu}}{\kappa^2} - \frac{1}{\sigma_\varepsilon}\right] \tag{12}$$

With this we conclude the overview of the modeling steps given in Parente *et al.* (2011a).

In order to avoid the unintended stream-wise gradient in the flow variables, the default wall function formulation implemented in OpenFOAM was also modified. Here our formulation departs from the work of Parente *et al.* (2011a). In our formulation, the no-slip condition is set for velocity at the wall and the wall adjacent centroid values are specified for ε, G_k, μ_T and k_p according to,

$$\varepsilon_p = \frac{u_*^3}{\kappa(z_p + z_0)} , \tag{13}$$

$$G_{kp} = \frac{\rho u_*^3}{\kappa(z_p + z_0)} , \tag{14}$$

$$\mu_{Tp} = \rho u_* \kappa(z_p + z_0) , \tag{15}$$

$$k_p = A \ln{(z_p + z_0)} + B , \tag{16}$$

where the sub-index p indicates values evaluated at the first wall-adjacent cell centroid. These equations assume a constant stream-wise experimentally prescribed value of u_* and a prescribed value of k_p fitted from experimental data. They are consistent with the modeling assumptions made for the interior flow.

Finally, it is worth mentioning that we choose the model constant σ_ε such that source term in Eq. (12) is identically zero at the wall adjacent cell centroid,

$$\sigma_\varepsilon = \frac{\kappa^2}{(C_{\varepsilon_2} - C_{\varepsilon_1})\sqrt{C_\mu(z_p)}} . \tag{17}$$

This step eliminates the need to define σ_ε. However, we also obtain good results when using the standard value for σ_ε, as will be shown.

3. COMPUTATIONAL SETUP AND METHODS

The ABL flow developing in the conditions described previously can modeled as a two-dimensional flow before any obstacle is reached. Figure 1 shows the computational domain for the simulations. In this work, we numerically model the

CEDVAL wind tunnel Experiment A1-1(Leitl, 1998). The computational domain has the same height as the wind tunnel data, H=1 m, and the same length, L=4 m. The grid size was the same as the used in Parente *et al.* (2011a), i.e. 71 cells in the vertical direction and 400 cells in the horizontal direction. The height of the wall adjacent cell is 0.005 m, with the centroid at $z_p = 0.0025$ m. The domain is uniformly discretized in the flow direction. The simulation parameters and the boundary conditions are given in Tables 1 and 2, respectively.

The incompressible steady-state solver simpleFoam, available within OpenFOAM, was used to solve the resulting system of linear equations (Weller *et al.*, 1998). Modifications to the standard $k-\varepsilon$ model and custom boundary conditions are available at `https://labcc@bitbucket.org/labccopenfoam/kepsilon.git`, along with configuration files and instructions that enable reproduction of all results presented here.

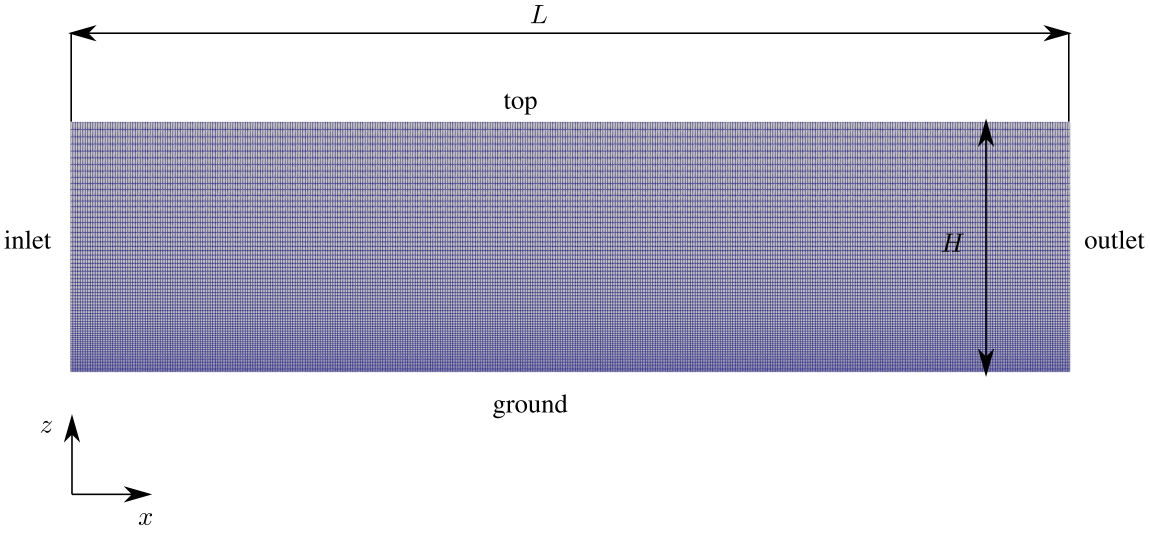


Figure 1: Two-dimensional computational mesh with boundaries.

Parameter	Value	Units
u_*	0.377	m/s
z_0	0.0007	m
A	-0.0346	m^2/s^2
B	0.4906	m^2/s^2
κ	0.413	-
C_{ε_1}	1.44	-
C_{ε_2}	1.92	-
σ_ε	Eq. (17)	-
σ_k	1.0	-

Table 1: Model parameters. u_* and z_0 are obtained from the CEDVAL A1-1 experiment (Leitl, 1998). A and B are fitting parameters for the k inlet boundary condition (Eq. 11) obtained considering the CEDVAL datasets A1-1. The value for κ was calculated from $u_* = u_{\text{ref}}\kappa / \ln\left[\left(z_{\text{ref}} + z_0\right)/z_0\right]$, where $u_{\text{ref}} = 6$ m/s at z_{ref}=0.5 m.

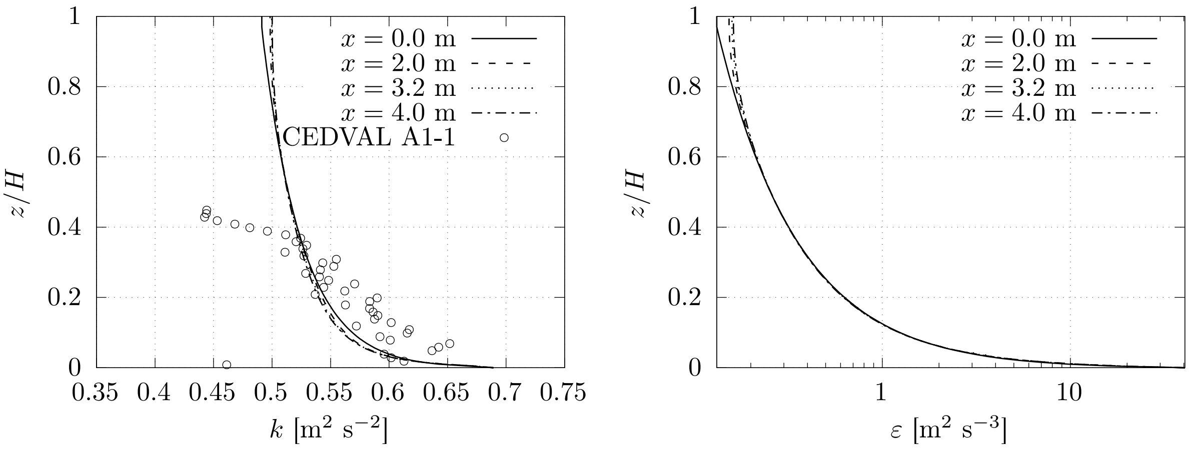
4. RESULTS

Figure 2 shows profiles for the solution variables at several downstream positions. It is apparent that profiles are maintained approximately constant throughout the computational domain, as desired. Only near the top boundary, where a zero-gradient condition is applied for k, ε and p, do the simulation results deviate more significantly from prescribed inlet conditions. The velocity profile (Figure 2d) is practically indistinguishable at different downstream positions. For this variable a constant shear-stress boundary condition was applied (see Table 2). Also shown is the CEDVAL experimental data for the TKE in Fig. 2a, from which the constants A and B listed in Table 1 were obtained.

The effect on the choice of σ_ε is not significant, as is seen in Fig. 3. Here we compare results from the standard value of σ_ε=1.3 with the value calculated from Eq. (17), which gives σ_ε=1.72.

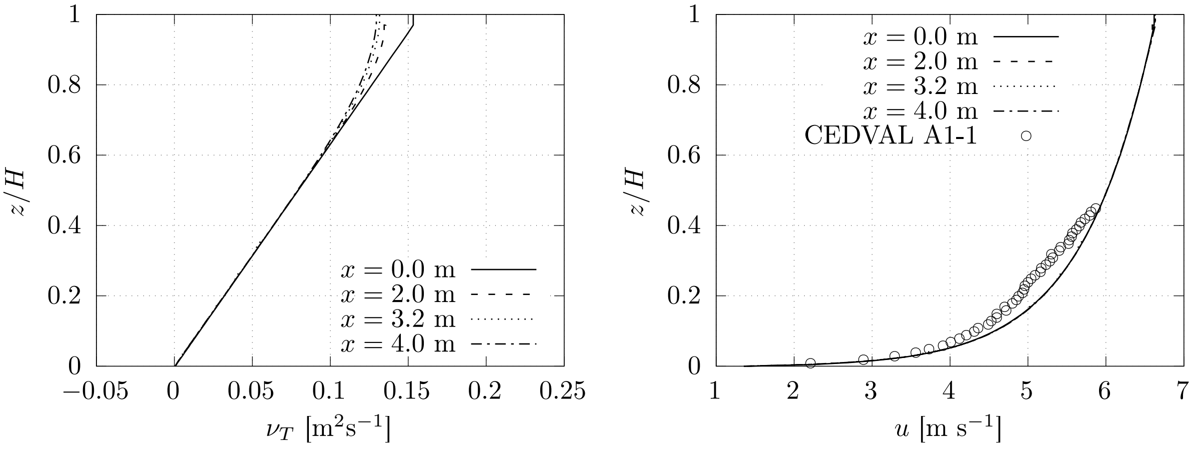
Boundary Condition	Variable	Description
Inlet	u	Eq. (8)
	k	Eq. (11)
	ε	Eq. (9)
	p	zero-gradient
	μ_T	calculated from Eq. (4)
Outlet	u, k, ε	outlet (convective)
	p	uniform fixed value
	μ_T	calculated from Eq. (4)
Top	u	Constant shear-stress, Eq. (1)
	k, ε, p	zero-gradient
	μ_T	calculated from Eq. (4)
Ground	u	no-slip
	k_p	Eq. (16)
	ε_p	Eq. (13)
	G_{kp}	Eq. (14)
	p	zero-gradient
	μ_{T_p}	Eq. (15)

Table 2: Boundary conditions for solution variables u, k, ε, and pressure p. Although strictly speaking we are modelling a zero-pressure gradient flow, for computational domains this is not possible. Therefore, we set the pressure at the outlet and adopt a zero-gradient boundary condition at the inlet. The non-zero resulting pressure-gradient is small in magnitude.



(a) Turbulent kinetic energy k

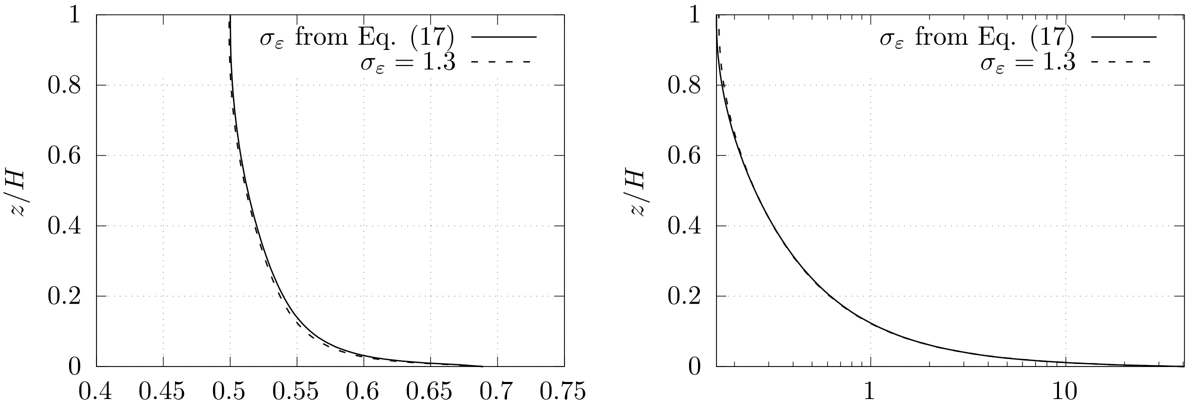
(b) Turbulent kinetic energy dissipation rate ε



(c) Turbulent viscosity profile ν_T

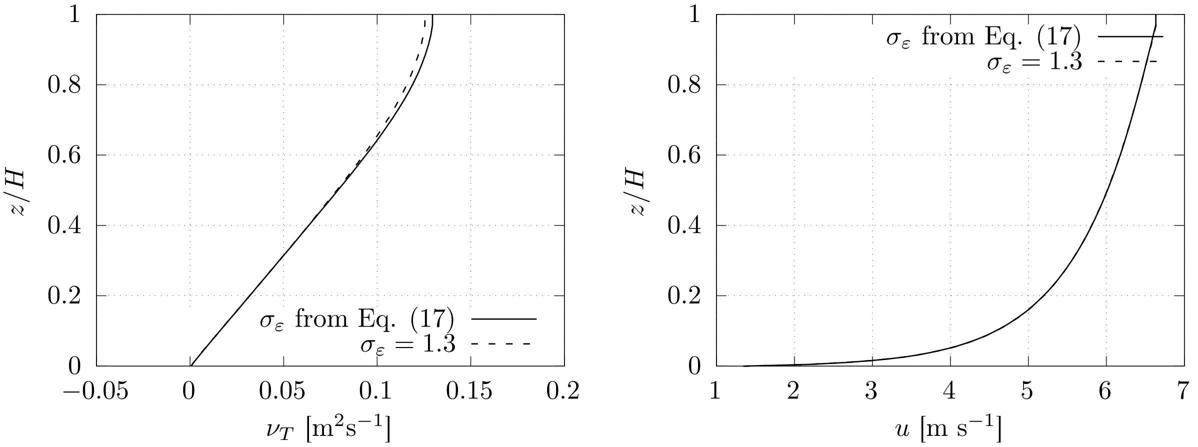
(d) Turbulent velocity profile u

Figure 2: Vertical profiles of solution variables at different downstream positions of the ABL.



(a) Turbulent kinetic energy k

(b) Turbulent kinetic energy dissipation rate ε



(c) Turbulent viscosity profile ν_T

(d) Turbulent velocity profile u

Figure 3: Vertical profiles of solution variables at the domain outlet ($x = 4.0$ m) obtained by using different values for σ_ε.

In order assess the effect the modifications outlined above have accomplished, in Fig. 4 we show the TKE profile obtained with the atmBoundaryLayer class in OpenFOAM-v2112[1]. This is the class we have used as a starting point. The figure shows how the TKE profile decays as the flow progresses downstream. If we had specified an inlet condition for TKE, this would be lost by the time the flow encountered any obstacle in the computational domain. Other profiles are less affected.

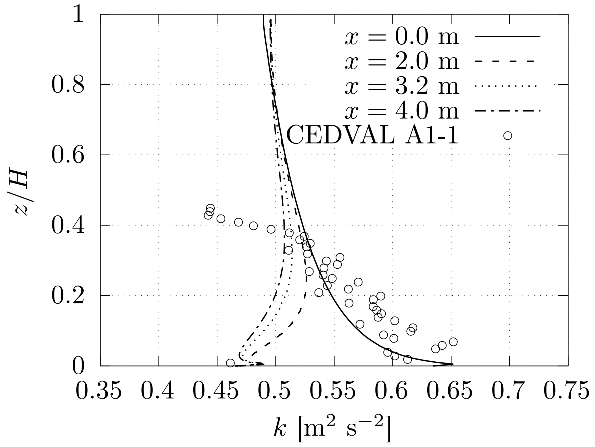


Figure 4: Turbulent kinetic energy k from the atmBoundaryLayer class in OpenFOAM-v2112.

5. CONCLUSIONS

A modified $k - \epsilon$ model proposed by Parente *et al.* (2011a,b) for the neutral ABL has been implemented in the open-source software OpenFOAM-v2112. Our implementation differs with respect to treatment of wall conditions, for which a novel boundary condition for the TKE has been implemented. The main features of this model are a variable C_μ and the addition of a source term $S\varepsilon$ to the TDR equation, which when combined lead to a consistent set of prescribed inlet conditions that do not evolve significantly in the flow direction. There is a slight deviation from prescribed inlet conditions at the upper boundary of the computational domain, owing the zero-gradient boundary condition for k and ε. However, the deviation is small and does not affect these flow variables near the surface level. In addition, the longitudinal component of velocity is practically constant throughout the entire domain. This is a necessary modeling step towards realistic simulations of obstacles and dispersion processes in ABL flows. There is a significant advantage of this implementation when compared to the atmBoundaryLayer class currently implemented in OpenFOAM-v2112.

The main advantage of solving ABL flow problems with OpenFOAM is the flexibility of the open-source implementation, allowing the inclusion of custom boundary conditions, such as the wall functions implemented in the present work, modifications of model equations and even entire flow solvers. This is not possible when using commercial software such as the Ansys Fluent. The current model along with instructions on how to reproduce the results presented here are availlable at `https://labcc@bitbucket.org/labccopenfoam/kepsilon.git`.

6. ACKNOWLEDGEMENTS

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