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A COMPARATIVE STUDY OF NEUTRAL ATMOSPHERIC BOUNDARY LAYER FLOW AND DISPERSION USING NON-STANDARD RANS MODELS IN OPENFOAM AND ANSYS FLUENT

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Abstract. *In this work we investigate the implementation of a non-standard RANS k-ε model in OpenFOAM and Ansys Fluent, previously proposed in the literature, in order to accurately simulate ABL flows with obstacles. The model consists of the addition of a source term in the turbulent kinetic energy dissipation equation of the RANS $k - \varepsilon$ model, which has the effect of inhibiting the development of stream-wise gradients in empty domains. In the presence of obstacles the model is supplemented by the use of a blending function, with the aim of smoothly deactivating the source term. Simulation results are compared to the CEDVAL A1-1 and A1-5 reference wind tunnel experiments. Our results show that both velocity profiles and source concentration distributions are satisfactorily reproduced by simulations, however turbulent kinetic energy is consistently overpredicted. Similar accuracy is observed between OpenFOAM and Ansys Fluent model implementations.*

Keywords: *k-ε model, computational fluid dynamics, atmospheric boundary layer, atmospheric dispersion, OpenFoam, Ansys Fluent.*

1. INTRODUCTION

Atmospheric boundary layer (ABL) flow and dispersion modeling is a challenging task owing to underlying phenomena such as the complex wind flow patterns, chemical reactions and removal processes. These difficulties increase largely when flow and dispersion occur over complex topographies, such as urban regions. Short-term atmospheric flow and dispersion models applied to urban regions have been broadly explored in the past decades. Large Eddy Simulations (LES), such as in Zheng *et al.* (2021) and the Direct Numerical Simulations (DNS) (Coceal *et al.*, 2007) provide more accurate results, but they are usually impractical due to their prohibitive computational cost. On the other hand, Reynolds Averaged Navier-Stokes (RANS) based-models, such as the standard two equation k-epsilon model are most commonly applied to both atmospheric flow and dispersion modeling (Saleh *et al.*, 2022). The main reason for their frequent use is their comparative low computational cost. However, the available RANS models exhibit some drawbacks recurrently reported in the literature. First, there is an incompatibility among the inlet profiles for the flow variables such as the velocity field, turbulent kinetic energy, turbulence dissipation rate and the standard wall functions (Parente *et al.*, 2011b). This inconsistency appears in the solution as an undesired stream-wise gradient in the flow variables. In addition, near buildings and obstacles, the RANS models tend to overpredict the turbulence levels (Parente *et al.*, 2011b). Several remedies have been proposed in the literature, such as the introduction of wall function formulations consistent with the inlet boundary conditions and improvements in the representation of the surface roughness and flows around obstacles (Parente *et al.*, 2011a,b). In this work, we investigate the addition of source terms in the RANS equations in order to address the aforementioned inconsistencies along with different blending functions that turn off added source terms near buildings and obstacles. The model implementation is performed within the framework of the CFD open-source code OpenFOAM (Weller *et al.*, 1998) and the commercial software Ansys Fluent, while simulation predictions are compared to wind tunnel data from the CEDVAL experiments A1-1 and A1-5 (Leitl, 1998).

The paper is structured as follows. In §2 we provide a brief summary of the theoretical underpinnings of the introduction of a source term in the turbulent kinetic energy dissipation equation and the use of blending functions to modulate the source term, as well as present the pollutant dispersion modeling. In §3 we describe the computational setup and numerical methods used to solve the flow equations. In §4 we present and discuss the main findings regarding our use of blending functions in the simulations of CEDVAL A1-1 and A1-5 wind tunnel experiments. Finally, in §5 we give our concluding remarks and steps in future work.

2. FLOW AND DISPERSION MODELING

Following Richards and Hoxey (1993), an incompressible, horizontally homogeneous, statistically stationary, two-dimensional ABL flow can be described assuming:

H.1 constant shear stress τ,

H.2 null vertical component of the velocity,

H.3 constant pressure along the stream-wise (x) and the vertical (z) directions, respectively.

Under the hypotheses above, Parente *et al.* (2011b) developed a model with consistent prescribed inlet profiles for velocity u, turbulent kinetic energy (TKE-k) and turbulent dissipation rate (TDR-ε), resulting in homogeneous profiles for the flow variables in an empty domain, at the expense of the addition of a source term in the equation for the TDR. The inlet profiles are given by,

$$u_{\text{inlet}} = \frac{u_*}{\kappa} \ln\left(\frac{z+z_0}{z_0}\right) , \tag{1}$$

$$k_{\text{inlet}} = A \ln(z+z_0) + B , \tag{2}$$

$$\varepsilon_{\text{inlet}} = \sqrt{C_\mu(z)} k_{\text{inlet}} \frac{du_{\log}}{dz} , \tag{3}$$

with fitting constants A, B and the roughness length z_0. These inlet profiles are consistent with the following set of equations for momentum, TKE and TDR,

$$\mu_T \frac{\partial u}{\partial z} = \tau = \rho u_*^2 , \tag{4}$$

$$\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_k}\frac{\partial k}{\partial z}\right) + G_k - \rho\varepsilon = 0 , \tag{5}$$

$$\frac{\partial}{\partial z}\left(\frac{\mu_T}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right) + \frac{\varepsilon}{k} C_{\varepsilon_1} G_k - \frac{\varepsilon^2}{k}\rho C_{\varepsilon_2} = S_\varepsilon , \tag{6}$$

where ρ is density, $u^* = \sqrt{\tau/\rho}$, is the friction velocity, G_k is the production of TKE and C_{ε_1}, C_{ε_2}, σ_k, σ_ε are empirical model constants defined originally by Launder and Spalding (1974). The turbulent viscosity μ_T, the added source term S_ε and a variable C_μ are defined as,

$$\mu_T \equiv \rho C_\mu \frac{k^2}{\varepsilon} , \tag{7}$$

$$S_\varepsilon \equiv \frac{\rho u_*^4}{(z+z_0)}\left[\frac{(C_{\varepsilon_2} - C_{\varepsilon_1})\sqrt{C_\mu}}{\kappa^2} - \frac{1}{\sigma_\varepsilon}\right] , \tag{8}$$

$$C_\mu(z) \equiv \frac{u_*^4}{k_{\text{inlet}}^2} , \tag{9}$$

where κ is the von Kármán constant.

In OpenFoam, the no-slip condition is set for the velocity at the wall and the wall adjacent centroid values are specified for ε, G_k, μ_T and k_p according to,

$$\varepsilon_p = \frac{u_*^3}{\kappa(z_p+z_0)} , \tag{10}$$

$$G_{kp} = \frac{\rho u_*^3}{\kappa(z_p+z_0)} , \tag{11}$$

$$\mu_{Tp} = \rho u_* \kappa (z_p+z_0) , \tag{12}$$

$$k_p = A \ln(z_p+z_0) + B , \tag{13}$$

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 the source term in Eq. (8) is identically zero at the wall adjacent cell centroid,

$$\sigma_\varepsilon = \frac{\kappa^2}{(C_{\varepsilon_2} - C_{\varepsilon_1})\sqrt{C_\mu(z_p)}} \ . \tag{14}$$

This step eliminates the need to assign σ_ε. The model constants are presented in Tab. 1. This methodology has been implemented in OpenFOAM and Fluent and results have been previously reported in Salazar and Albani (2022).

Table 1. Model parameters. u_* and z_0 are obtained from the CEDVAL A1-1/A1-5 experiment (Leitl, 1998). A and B are fitting parameters for the k inlet boundary condition (Eq. 2) obtained considering the CEDVAL datasets, depending of the flow problem considered.

Parameter	Value	Units
u_*	0.377	m/s
z_0	0.0007	m
A	-0.0437/-0.0345	m^2/s^2
B	0.3548/0.4905	m^2/s^2
κ	0.4892/0.4130	-
C_{ε_1}	1.44	-
C_{ε_2}	1.92	-
σ_ε	1.9472/1.72301	-
σ_k	1.0	-

In the flow region affected by obstacles, hypotheses H.1-H.3 cannot be made and Eqs. (4-6) are no longer an adequate model for the flow. In order to circumvent this issue, an approach proposed by Parente *et al.* (2011a) that allows a gradual transition between the smooth and the disturbed ABL flow is used. A measure of the deviation from the inlet profile is considered by the introduction of a blending metric Δ. Following Parente *et al.* (2011a); Longo *et al.* (2017), the source term S_ε and C_μ are then rewritten to provide a smooth transition between the undisturbed and disturbed flow regime according to the following formulations,

1. Polynomial

$$\phi = \phi_{\text{std}} + (1 - \Delta^\alpha)(\phi_{\text{hom}} - \phi_{\text{std}}), \tag{15}$$

2. Sinusoidal

$$\phi = \phi_{\text{std}} + [1 - 0.5(1 + \sin\Delta_*)]^\alpha\,(\phi_{\text{hom}} - \phi_{\text{std}}), \tag{16}$$

$$\Delta_* = \pi \max(\Delta - 0.5, -0.5) \ , \tag{17}$$

where ϕ represents S_ε or C_μ, and Δ is the choice of a blending metric. The subscripts hom and std stand for the homogeneous values of these variables, given by Eqs. (8) and (9) and the values for the standard $k-\varepsilon$ model, namely $S_\varepsilon = 0$ and $C_\mu = 0.09$, respectively. The following options for the blending metric are investigated,

$$\Delta_u = \min\left[\left(\frac{u - u_{\text{inlet}}}{u_{\text{inlet}}}\right), 1\right] \ , \tag{18}$$

$$\Delta_k = \min\left[\left(\frac{k - k_{\text{inlet}}}{k_{\text{inlet}}}\right), 1\right] \ , \tag{19}$$

$$\Delta_{k,u} = \max[\Delta_u, \Delta_k] \ . \tag{20}$$

The pollutant dispersion is modeled by the partial differential equation,

$$u \cdot \nabla C - \nabla \cdot (K_{\text{eff}} \nabla C) = S_C(\mathbf{x}), \tag{21}$$

where u is the velocity, K_{eff} is the diffusion coefficient given. by $K_{\text{eff}} = \mu/Sc + \mu_T/Sc_T$. Further, μ and Sc are the laminar viscosity and Schmidt numbers, respectively. The turbulent counterparts are denoted by μ_T and Sc_T. Solution of Eq. (21) provides the steady-state spatial distribution of a species concentration C for any position $\mathbf{x}$ over the computational domain Ω for a source distribution $S_C(\mathbf{x})$.

3. COMPUTATIONAL SETUP

The computational domain is shown in Fig. 3. The domain is defined as the region $\Omega = \{(x, y, z) \mid x \in$ [-1.05,4.05], $y \in$ [-0.3125,0], $z \in$ [0,1.0] m$\}$ and the block center is located at position $(x, y, z) = (0, 0, 0)$, with a height of 0.125 m, width of 0.075 m and length of 0.1 m. The total number of cells in the mesh is 2418800, with refinement near solid surfaces, such that the distance to the centroid closest to any solid surface is 7.5×10^{-4} m. For the CEDVAL A1-5 problem there are two sources located on the leeward side of the block, each with an area of 1.3×10^{-4} m^2 and flow rate of 2.76×10^{-6}m^3/s. More details about the geometry and position of the dispersion sources can be found in Leitl (1998). The boundary conditions are given in Table 2.

Both in OpenFOAM and Fluent, second order upwind schemes were used for discretization of the convective terms and gradients were discretized by cell limited least squares. The SIMPLE algorithm was used for pressure-velocity coupling. The flow is modeled as incompressible.

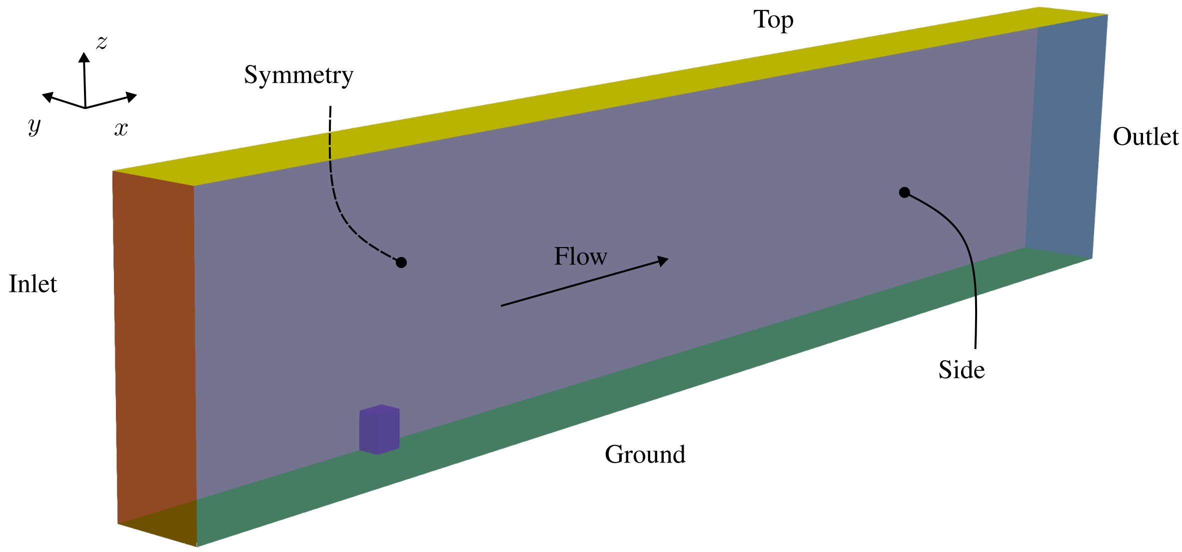


Figure 1. Computational domain.

4. RESULTS

4.1 CEDVAL A1-1

OpenFOAM and Fluent simulation results for the streamwise velocity u and TKE are compared to CEDVAL A1-1 experimental data in Figures 2 and 3. The reference velocity U is used to normalize these variables. From these figures we can see that simulation results are close to each other and that agreement for the velocity component u is much better than for TKE, even when we use the $\Delta_{k,u}$ blending metric. Especially for the profile upstream of the block ($x = -0.04$ m), there is a significant overestimation of TKE in the simulations. The use of different blending metrics did not have a significant effect on the results for these profiles.

In order to better assess the prediction capabilities of the non-standard $k - \varepsilon$ blending function approach, we compare simulation results to TKE data measured along different planes.

The experimental results for plane $y = 0$ m are shown in Figure 4(a), while the OpenFOAM results are shown in Figure 4(b), where the Δ_u metric was used. From these figures it is evident that the simulation significantly overpredicts the TKE in the region immediately upstream of the obstacle. This trend is observed also in the near wake region of the obstacle. A quantitative measure of the errors over this plane is given in Fig. 4(c). In spite of general trends being relatively well predicted, errors over a great extent of the plane lie in the range of 10% to 100%.

The experimental results for plane $z = 0.035$ m are shown in Figure 5(a), while the Fluent results are shown for comparison in Figure 5(b), where the Δ_* metric was chosen. Again, we see that the simulation over predicts the TKE in the region immediately upstream of the obstacle. On the other hand, the simulation fails to capture the higher values of TKE seen in the experimental data, near the side of the obstacle. A quantitative measure of the errors over this plane is given in Fig. 5(c). The error magnitudes for the z plane are somewhat smaller than observed in the y plane, but more notably the extent of the largest error regions is reduced.

Table 2. Boundary conditions for solution variables. Standard solver nomenclature has been used in the table.

Boundary Condition	Variable	OpenFoam	Fluent
Inlet	u	Eq. (1)	Eq. (1)
	k	Eq. (2)	Eq. (2)
	ε	Eq. (3)	Eq. (3)
	p	zeroGradient	
	μ_T	Eq. (7)	Eq. (7)
	C	fixedValue = 0	Specified Value = 0
Outlet	u, k, ε	inletOutlet (convective)	Pressure Outlet
	p	fixedValue = 0 Pa	Gauge pressure = 0 Pa
	μ_T	Eq. (7)	
	C	zeroGradient	Specified Value = 0
Top	u	fixedShearStress, Eq. (4)	Symmetry
	k, ε, p	zeroGradient	Symmetry
	μ_T	Eq. (7)	Symmetry
	C	zeroGradient	Symmetry
Symmetry	$u, k, \varepsilon, p, \mu_T, C$	symmetry	Symmetry
Ground	u	noSlip	No Slip
	k_p	Eq. (13)	
	ε_p	Eq. (10)	
	G_{kp}	Eq. (11)	
	p	zeroGradient	
	μ_{Tp}	Eq. (12)	
	C	zeroGradient	Specified Flux = 0
Side	u, p, k, ε, μ_T	slip	Symmetry
	C	zeroGradient	Symmetry
Block	u	noSlip	No Slip
	k	kLowReWallFunction	
	ε_p	epsilonWallFunction	
	p	zeroGradient	
	μ_T	nutUSpaldingWallFunction	
	C	zeroGradient	Specified Flux = 0

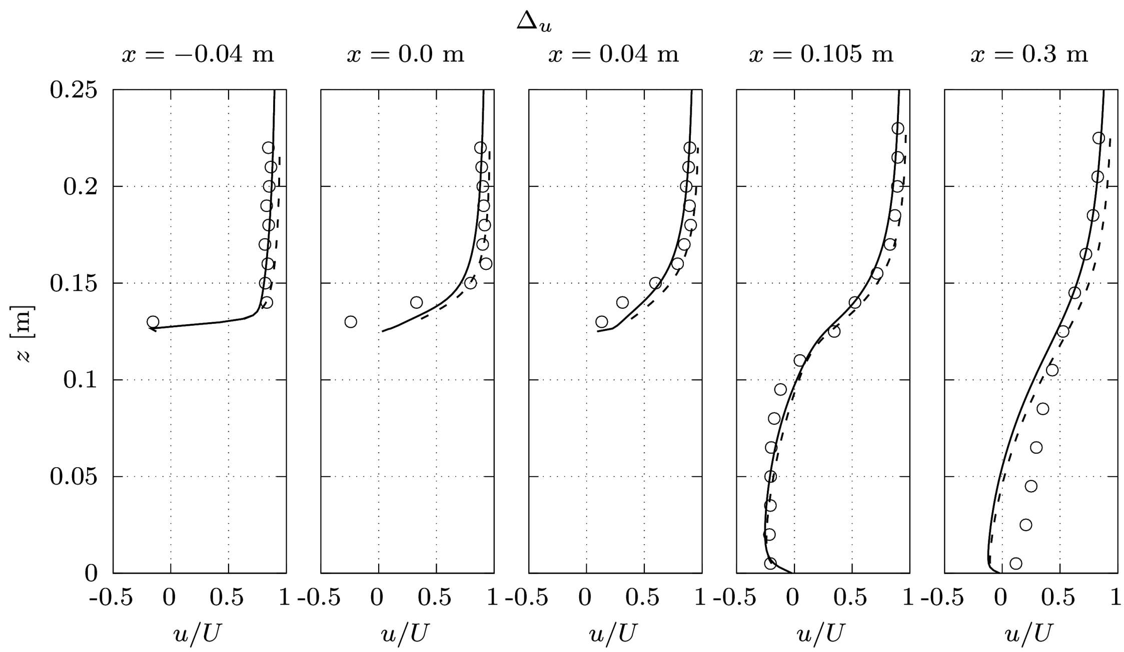


Figure 2. Normalized vertical velocity profiles along different streamwise positions in the CEDVAL A1-1 wind tunnel experiment - Δ_u blending function. ○ Experiment, —— OpenFOAM, - - - - Fluent.

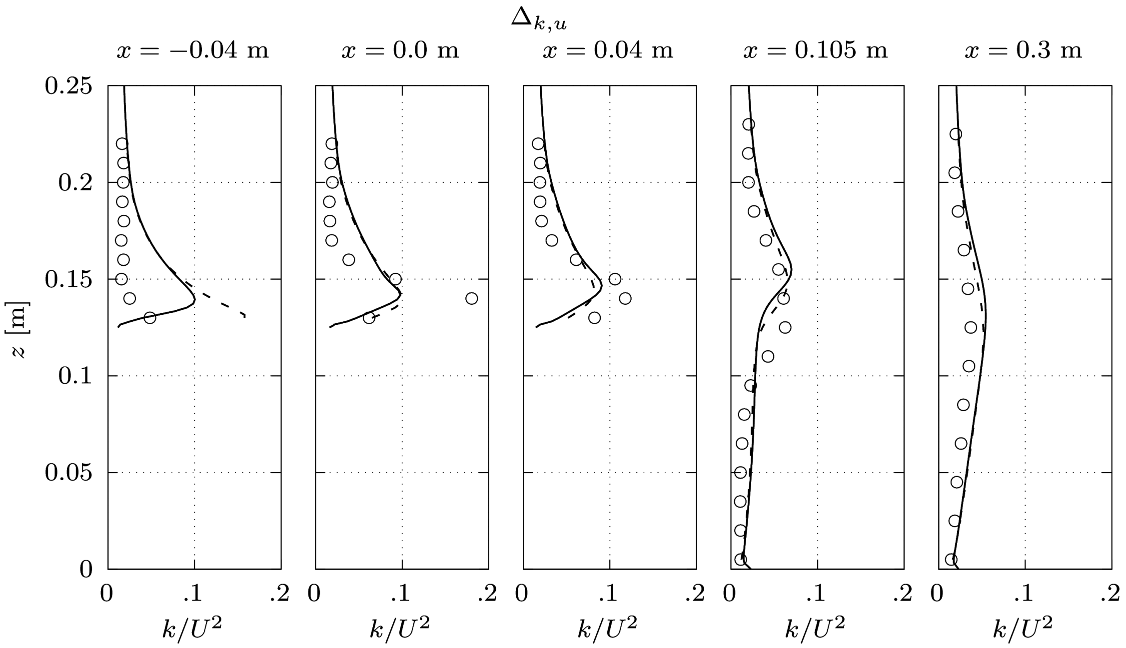
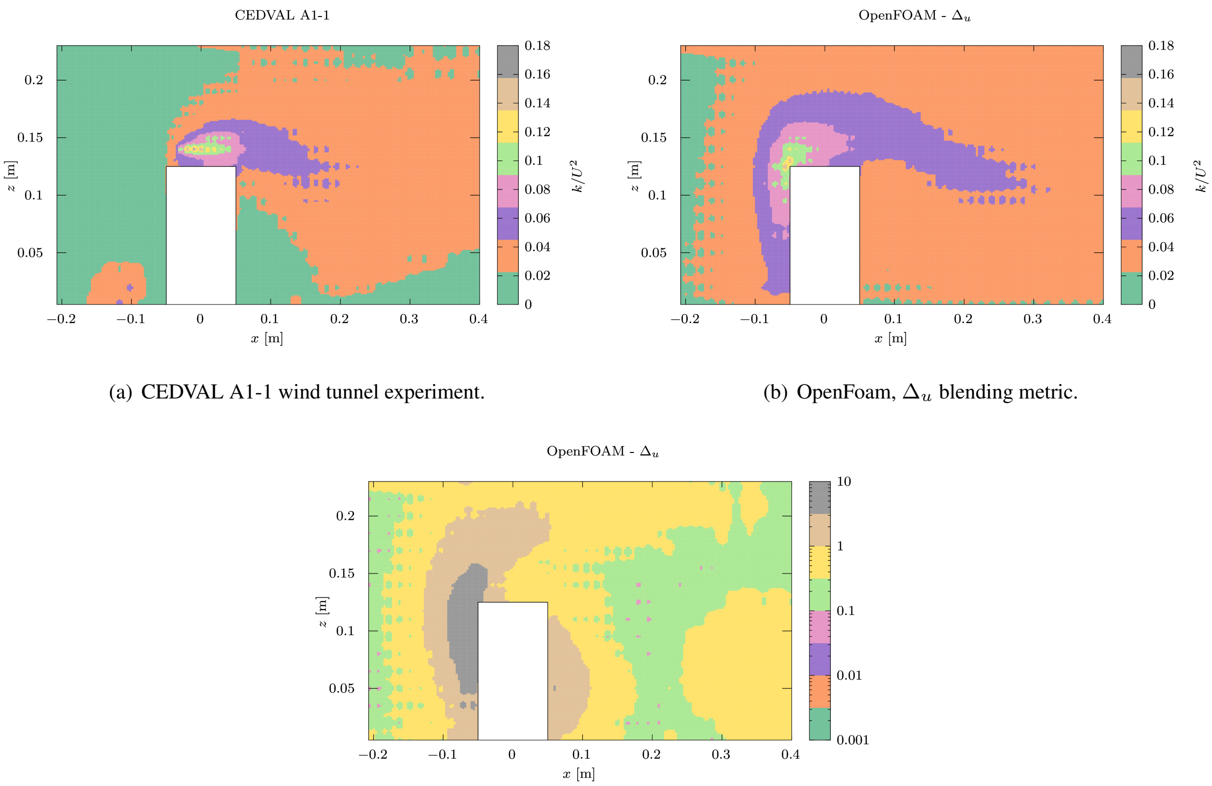


Figure 3. Normalized TKE profiles along different streamwise positions in the CEDVAL A1-1 wind tunnel experiment - $\Delta_{k,u}$ blending function. ○ Experiment, ——— OpenFOAM, - - - - Fluent.

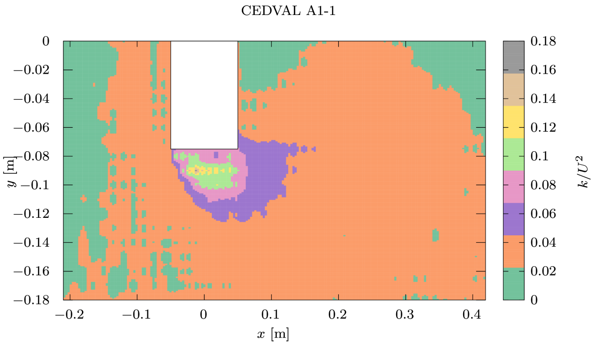


(a) CEDVAL A1-1 wind tunnel experiment.

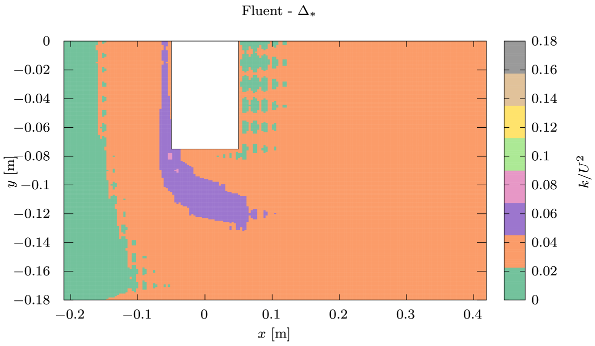
(b) OpenFoam, Δ_u blending metric.

(c) Normalized TKE relative errors.

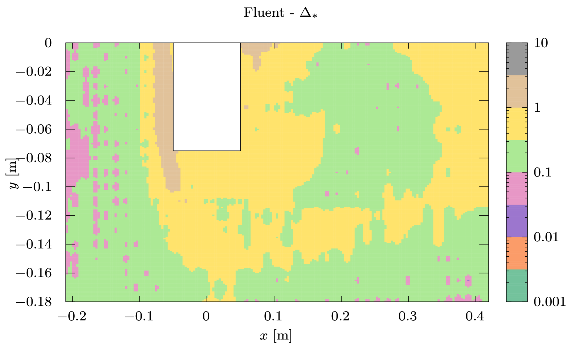
Figure 4. Normalized TKE along for the $y = 0$ m plane



(a) CEDVAL A1-1 wind tunnel experiment.



(b) Fluent, Δ_* blending metric.



(c) Normalized TKE relative errors.

Figure 5. Normalized TKE for the $z = 0.035$ m plane.

4.2 CEDVAL A1-5

In the CEDVAL A1-5 experiment, scalar sources are placed on the leeward side of the obstacle, near the ground. Measurements were acquired for the same planes considered previously, $y = 0$ and $z = 0.035$ m. Details of the measurement techniques and setup are found in Leitl (1998). The normalized concentration K is defined according the following equation,

$$K = \frac{C}{C_S}\frac{UH^2}{Q_S} \ , \tag{22}$$

where C_S is the source concentration, H is obstacle height and Q_S is the volumetric flow rate of the source.

CEDVAL A1-5 measurements for the $z = 0.035$ m are shown in Fig. 6(a). OpenFOAM simulation data is shown in Fig. 6(b). It can be seen that the OpenFOAM simulation shows good agreement with the experimental data, which is encouraging for use in predictions of pollutant dispersion for real-world applications. Similar accuracy is also observed in the $y = 0$ m plane, but not shown here.

5. CONCLUSIONS AND FUTURE WORKS

In this paper we have implemented the non-standard k-ε model with blending functions proposed by Parente *et al.* (2011b,a); Longo *et al.* (2017) in both OpenFOAM and Ansys Fluent, and made comparisons to experimental measurements from the CEDVAL wind tunnel experiments. Our results confirm prior studies that found an over prediction of TKE by simulations. On the other hand, the numerical model predictions for pollutant dispersion is promising. Moreover, we find that our implementations in OpenFOAM and Fluent show similar accuracy. Care has been take in order to use equivalent discretization schemes and solver settings. Future work will be aimed towards extending the formulation to non-neutral ABL conditions and the formulation of alternate blending functions. The code and data required to reproduce the data in this paper can be found at `https://bitbucket.org/labccopenfoam/kepsilonabl`.

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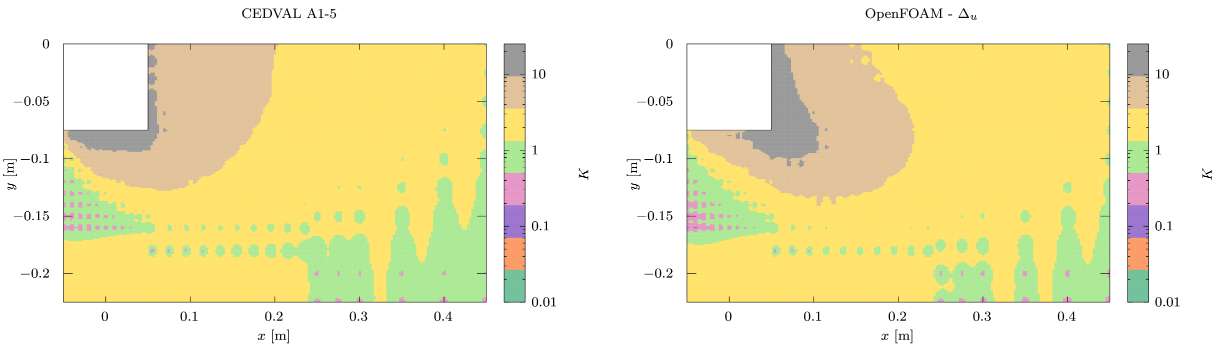

(a) CEDVAL A1-1 wind tunnel experiment.

(b) OpenFOAM, Δ_u blending metric.

Figure 6. Normalized concentration K for the $z = 0.035$ m plane

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