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MODELLING DIABATIC ATMOSPHERIC BOUNDARY LAYER USING A RANS CFD CODE WITH A K-EPSILON TURBULENCE CLOSURE

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Abstract: In this paper, we present a specific methodology developed to simulate a diabatic (stable or unstable situations) atmospheric Surface Layer (SL) with a CFD approach using the RANS equations closed by a k-ε turbulence model. This study has been carried out with the CFD software Fluent, but the results presented are of more general interest. In a first part, we propose a set of vertical profiles for velocity, potential temperature, pressure, turbulent kinetic energy and turbulent dissipation rate in a diabatic SBL and we discuss the consistency of these profiles with the equations solved in a RANS CFD code with a k-ε turbulence model. We show that a parameterization for σ_k and σ_ε can improve this consistency. In the second part, we describe a set of boundary conditions used to simulate a steady homogeneous SL. In the last part, we discuss some results which illustrate the ability of the present approach to reproduce and maintain the different profiles predicted by the Monin-Obukhov similarity theory.

Key words: *diabatic surface layer, Monin-Obukhov similarity theory, CFD simulations, k-ε turbulence model*

INTRODUCTION

Modelling of pollutant dispersion over industrial areas implies the description of the flow around buildings or complex obstacles. Thanks to the continual increase of computers performances, it is possible today to simulate this flow around obstacles using CFD models employing RANS equations (Fluent, Phoenics, StarCD…). But a challenging issue in this kind of models is the parameterization of atmospheric processes, particularly those associated with thermal stratification. If one can find several works in the literature on the application of these models in neutral stability conditions (Richards P.J. and R.P. Hoxey, 1993; Blocken B. *et al.*, 2007; Hargreaves D.M. and N.G. Wright, 2007), the particular case of stable and unstable conditions has been less studied and requires very close attention. Duynkerke P.G. (1988), in his famous paper, proposes a modification of the k-ε model constants in order to match the physical characteristics of the atmospheric surface layer in neutral and stable conditions. Huser A. *et al.* (1997) apply this parameterization but show that their inlet turbulence profiles do not maintain with distance and that turbulence increases in the case of stable stratification, which is certainly due to the lack of buoyancy effects in the turbulent kinetic energy (TKE) equation for k. Pontiggia M. *et al.* (2009) and Freedman F.R. and M.Z. Jacobson (2003) have treated the problem of the inconsistency between the k and ε profiles and the conservation equations for k and ε, by adding a source term in the turbulent dissipation rate (TDR) equation for ε or by providing a non-constant formulation for the $c_{\varepsilon 1}$ parameter.

But these different works leave some questions unanswered:

- Firstly, it is sometimes believed in the engineering CFD community that the modelling of the atmospheric stability processes is not required to study short domains less than 1 or 2 km and that inlet stratified velocity and turbulence profiles are sufficient to reproduce the atmospheric stability. It has seemed necessary to us to demonstrate that a full and consistent treatment of the stratification is a condition to model properly flow and turbulent dispersion.
- In a diabatic boundary layer, the vertical momentum equation generates a pressure profile which departs from the constant pressure outflow condition which is generally used in CFD codes. We will show in this article how to describe this pressure profile in order to define an appropriate downwind boundary condition for the stable or unstable cases.
- In a surface layer, one of the main assumptions is that the fluxes of momentum and energy remain constant with altitude. But this condition will not be satisfied by using symmetry or Dirichlet condition at the top of the domain, as it is done in all the papers reviewed. The constant fluxes assumption requires a "flux condition" at the ground and at the top of the computational domain. We will discuss in this paper how to impose these conditions.
- The question of the inconsistency of the k and ε profiles will be discussed further in order to evaluate some criteria for the necessity to make specific modifications of the set of constants for the k-ε model.

In the first section, we derive all the equations used in the parameterization of the surface boundary layer. In the second section, we present the integration of these conditions in the CFD calculation. Then in the last section we discuss some numerical results obtained by application of this methodology.

PARAMETERIZATION OF THE SURFACE BOUNDARY LAYER

Surface boundary layer assumptions

The atmospheric Surface Layer is commonly associated with several assumptions which are listed below:

- The flow is oriented along the x direction and the mean vertical velocity is null:
$$\overline{v} = \overline{w} = 0 \qquad (1)$$
- The vertical turbulent fluxes (Reynolds stresses and heat flux) are constant with respect to altitude throughout all the surface layer (Garratt J.R., 1992) :

$$\begin{cases} \overline{u'w'} = cste = -u_*^2 \\ \overline{w'\theta'} = cste = \dfrac{H_0}{\rho_0 C_p} = -u_*\theta_* \end{cases} \tag{2}$$

It allows to postulate that the surface layer is steady (stationarity $\partial/\partial t = 0$).

- The Monin-Obukhov similarity theory predicts that the dimensionless gradients of velocity and potential temperature only depend on z/L_{MO} (Garratt J.R., 1992):

$$\begin{cases} \dfrac{\kappa z}{u_*}\dfrac{\partial \overline{u}}{\partial z} = \phi_m(\zeta) \\ \dfrac{\kappa z}{\theta_*}\dfrac{\partial \overline{\theta}}{\partial z} = \phi_h(\zeta) \end{cases} \quad \text{where} \quad \zeta = \frac{z}{L_{MO}} \quad \text{and} \quad L_{MO} = -\frac{\rho_0 C_p \theta_0 u_*^3}{\kappa g H_0} \tag{3}$$

where H_0 is the ground sensible heat flux, u_* the friction velocity and L_{MO} the Monin-Obukhov length. ϕ_m and ϕ_h are the Monin-Obukhov universal functions for which one can find analytical expressions in Garratt, J.R. (1992).

- The turbulence satisfies a local equilibrium within the surface layer (Tennekes, H. and J. L. Lumley, 1972):

$$P + B = \varepsilon \quad \text{with} \quad \begin{cases} P = -\overline{u'w'}\dfrac{\partial \overline{u}}{\partial z} = \text{ shear TKE production} \\ B = \dfrac{g}{\theta_0}\overline{w'\theta'} = \text{ thermal TKE production/destruction} \\ \varepsilon = \text{ turbulent dissipation rate} \end{cases} \tag{4}$$

- Influence of buoyancy effects in the momentum equation can be taken into account using the Boussinesq approximation, which consists of assuming that the density ρ is constant except in the buoyancy term of the momentum equation:

$$\rho \approx \rho_0 = cste \tag{5}$$

$$\text{except for the term } (\rho - \rho_0)g \approx -\rho_0\beta(\theta - \theta_0)g \quad \text{with} \quad \beta \approx \frac{1}{\theta_0} \quad \text{for an ideal gas} \tag{6}$$

Conservation equations

When using the assumptions (1) to (6), the Reynolds Averaged Navier-Stokes (RANS) equations of conservation for the mass, horizontal momentum and energy are easily verified. The vertical momentum equation reduces to:

$$\frac{\partial \overline{P}}{\partial z} = -\rho_0\beta(\theta - \theta_0)g \qquad \text{with} \qquad \overline{P_{abs}} = \overline{P} + P_0 - \rho_0 g z \tag{7}$$

where $\overline{P}$ is defined as a difference between absolute and hydrostatic pressure. $\overline{P}$ is often used in CFD codes instead of $\overline{P_{abs}}$ in order to improve numerical accuracy. Integration of equation (7) will give the vertical profile of $\overline{P}$ in the SBL (see equation (12)). One can notice that $\overline{P}$ is constant for the neutral case, where $\theta = \theta_0$.

***k*-ε turbulent closure**

In order to model the turbulent fluxes, we use in this work a k-ε turbulent closure, defined by:

$$\begin{cases} \overline{u'w'} = -K_m \dfrac{\partial \overline{u}}{\partial z} \\ \overline{w'\theta'} = -K_h \dfrac{\partial \overline{\theta}}{\partial z} \end{cases} \quad \text{with} \quad K_m = c_\mu \frac{k^2}{\varepsilon} \quad \text{and} \quad K_h = \frac{K_h}{\Pr_t} \tag{8}$$

where k is the turbulent kinetic energy, ε is the turbulent dissipation rate and K_m and K_h are the turbulent diffusivity of momentum and heat. k and ε are given by two conservation equations :

- Turbulent kinetic energy equation:

$$\underbrace{\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_k}\frac{\partial k}{\partial z}\right)}_{D} + P + B - \varepsilon = 0 \tag{9}$$

where D is the diffusion term. As discussed later, equation (9) is not necessarily consistent with equation (4) if k is not a constant.

- Turbulent dissipation rate equation:

$$\frac{\partial}{\partial z}\left(\frac{K_m}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial z}\right)+c_{\varepsilon 1}\frac{\varepsilon P}{k}-c_{\varepsilon 2}\frac{\varepsilon^2}{k}=0 \tag{10}$$

without any term for the buoyancy effects, as suggested by Duynkerke P.G. (1988). Some authors (Pontiggia M. *et al.*, 2009; and Freedman F.R. and M.Z. Jacobson, 2003) suggest to add a buoyancy term in the ε equation but the necessity of this term is not clear. That is why we decided to omit it in this study but one can notice that the use of this term would not change significantly the methodology proposed.

The use of the *k*-ε model requires values for the constant c_μ, σ_k, σ_ε, $c_{\varepsilon 1}$ and $c_{\varepsilon 2}$. In order to simulate realistic atmospheric values of the TKE in the surface layer ($k/u_*^2 \approx 5.5$, after Garratt, 1992), it is necessary to use the modified constant set proposed by Duynkerke P.G. (1988) and corrected to satisfy equation (19):

Table 1. Duynkerke constants for the *k*-ε model

c_μ	σ_k	σ_ε	$c_{\varepsilon 1}$	$c_{\varepsilon 2}$
0.033	1.0	2.38	1.46	1.83

Set of equations for the vertical profiles

Integration of equations (3) gives the classical logarithmic velocity and temperature profiles:

$$\begin{cases}\overline{u}(z)=\dfrac{u_*}{\kappa}\left[\ln(z/z_0)-\psi_m(\zeta)\right]\\[2mm] \overline{\theta}(z)=\theta_0+\dfrac{\theta_*}{\kappa}\left[\ln(z/z_T)-\psi_h(\zeta)\right]\end{cases} \tag{11}$$

where ψ_m and ψ_h are the integrated universal functions of the Monin-Obukhov theory.

Integration of (7) using (11) provides:

$$\overline{P}(z)=-\frac{\rho_0 g\theta_*}{\kappa\theta_0}\int_0^z\left[\ln(z/z_T)-\psi_h(\zeta)\right]dz \tag{12}$$

With equations (2), (3) and (4), one can derive the profile of the turbulent dissipation rate ε:

$$\varepsilon(z)=\frac{u_*^3}{\kappa z}\phi_m(\zeta)\left[1-\frac{\zeta}{\phi_m(\zeta)}\right] \tag{13}$$

Combining equations (2), (8) and (13) gives the profile of the turbulent kinetic energy *k*:

$$k(z)=\frac{u_*^2}{\sqrt{c_\mu}}\sqrt{1-\frac{\zeta}{\phi_m(\zeta)}} \tag{14}$$

Finally, equations (8), (13) and (14) provide the profile of the momentum turbulent diffusivity:

$$K_m(z)=\frac{u_*\kappa z}{\phi_m(\zeta)} \tag{15}$$

This set of solutions has been used by several authors cited in the introduction to define the upwind boundary conditions for a CFD calculation of a diabatic surface layer. The main problem with these equations is that the complete equation (9) for *k* and the equation (10) for ε have not been used to derive this solution and then, these conservations equations have no reason to be satisfied. This inconsistency will be discussed in the next section.

Consistency with the equation of *k*

As mentioned by Freedman and Jacobson (2003), the consistency between equations (9) and (4) implies that the diffusion term *D* of (9) should be equal to zero. If σ_k is a constant, one can show that D cannot be null, except for the neutral case. Freedman and Jacobson suggest that, though *D* is different from zero, its value does not exceed $10^{-3}(P + B)$. In fact, this comparison seems not to be the most appropriate in this case. We propose to evaluate the ratio between *D* and the TKE *k*, which can be interpreted as the inverse of a characteristic time t_k for *k* to vary significantly from the "pseudo" equilibrium value given by equation (13). An approximate expression of t_k can be derived near the ground:

$$t_k=\left|\frac{k}{D}\right|\approx\left|\frac{2L_{MO}\sigma_k}{u_*\kappa}\right| \quad \text{for} \quad \zeta=\frac{z}{L_{MO}}=1 \tag{16}$$

For example, with L_{MO} = 50 m and u_* = 0.25 m.s^{-1}, the characteristic time t_k for *k* to vary significantly from (13) when using equation (9) is about 1000 s. More generally, one can predict that for studying an atmospheric SBL in a short domain (< 1km), an inflow boundary condition based on equation (14) for k will remain almost constant when using a *k*-ε turbulence model with a constant σ_k. For larger domains, we suggest introducing a non-constant parameterization of σ_k, in order to ensure the local equilibrium (4).

Consistency with the equation of ε

As mentioned above, equation (13) for ε as been derived without using the conservation equation (10). In the assumption of a homogeneous and steady SL, it is required that the solution (13) will be solution of (10). Introducing (13) into (10) gives the condition:

$$T = \frac{\partial}{\partial z}\left(-\frac{Ri'}{\sigma_\varepsilon Ri}\right) + \frac{1}{L_{MO}^2}\frac{\sqrt{1-Ri}}{Ri^2}\left(\frac{c_{\varepsilon 2}\sqrt{c_\mu}}{\kappa^2}Ri - \frac{1}{\sigma_{\varepsilon,N}}\right) = 0 \tag{17}$$

$$\text{with} \quad Ri = \frac{\zeta}{\phi_m(\zeta)}, \quad Ri' = \frac{dRi}{d\zeta} \tag{18}$$

$$\text{and} \quad \sigma_{\varepsilon,N} = \frac{\kappa^2}{\left(c_{\varepsilon 2} - c_{\varepsilon 1}\right)\sqrt{c_\mu}} \tag{19}$$

In the neutral case, this equation is satisfied by "adjusting" the value of the constant $\sigma_{\varepsilon,N}$ as given by equation (19). In the diabatic case, it is no longer possible to satisfy equation (17) with a constant value of σ_ε. In order to quantify the "disequilibrium" of equation (10) using the solution (13), we estimate the ratio ε / T which can be interpreted as a characteristic time t_ε for ε to vary significantly from (13). An approximate expression of t_ε can be derived near the ground:

$$t_\varepsilon = \left|\frac{\varepsilon}{T}\right| \approx \left|\frac{\kappa L_{MO}\sigma_k}{c_{\varepsilon 2}\sqrt{c_\mu}\,u_*}\right| \quad \text{for} \quad \zeta = \frac{z}{L_{MO}} = 1 \tag{20}$$

For example, with L_{MO} = 50 m and u_* = 0.25 m.s^{-1}, the characteristic time t_ε for ε to vary significantly from (13) when using equation (10) is about 240 s. More generally, one can predict that for studying an atmospheric SL even on a relatively short distance (> 100 m), solution (13) for the turbulent dissipation rate will not maintain with distance when using a *k*-ε turbulence model with a constant σ_ε. Therefore we suggest introducing a non-constant parameterization of σ_ε.

PARAMETERIZATION IN A RANS CFD SIMULATION

In this section, we detail the settings used in the CFD code Fluent to simulate a diabatic surface layer.

Equations solved

The equations solved are the standard RANS equations with the incompressible and Boussinesq assumptions. The energy conservation was treated, considering the potential temperature instead of the simple temperature. The *k*-ε turbulence closure was used in the form of equations (8) to (10), using non-constant parameterizations for σ_k and σ_ε, to ensure consistency as discussed above. These parameterizations depend on the sign of the stratification (stable or unstable).

Inlet Dirichlet condition

On the upwind boundary, we impose the vertical profiles given by equations (11), (13) and (14).

Ground and top flux boundary conditions

In order to preserve the momentum and heat fluxes through the thickness of the domain, it is necessary to impose these fluxes on the ground and top boundaries. At the ground, we use a wall function based on the rough logarithmic law for the velocity (see Blocken B. *et al.*, 2007) and we specify the sensible heat flux H_0 (positive or negative). At the top of the domain, it is necessary to add opposite fluxes. To do that, we define a shallow numerical layer (20 m) in which we add volumic source terms for the momentum and energy equations, so that the integrals of these volumic sources equilibrate the ground fluxes.

Non-uniform pressure outflow condition

In order to satisfy the vertical equilibrium of the momentum equation with buoyancy effects, it is necessary to specify an outflow pressure condition with a variation of pressure with height, derived from equation (12) by integration of the Monin-Obukhov universal functions.

The parameterization based on these different conditions was implemented and tested with the commercial CFD software Fluent 6.3. Some results are presented in the next section.

CFD SIMULATION RESULTS

The simulation domain used is 2D domain of 20 km length and 500 m height. This height was constant for convenience even if the validity of the surface layer assumptions is limited to one tenth of the atmospheric boundary layer height. Consequently, results will have to be observed with this restriction.

Simulations for different stability conditions (stable, neutral and unstable) were performed in order to evaluate the conservation of the upwind boundary condition along such a domain. We illustrate these results on figure 1 for a stable condition (H_0 = -15 W.m^{-2} and u_* = 0.4 m.s^{-1}). One can observe that the vertical inlet profiles remain perfectly preserved along the 20 km of the domain.

In order to evaluate the idea that one can reproduce stratification effects only by using upwind profiles defined by equations (11), (13) and (14), we made a simulation without any specific treatment of the atmospheric thermal stratification effects: no energy equation solved, no variable pressure condition at the outlet, no thermal flux at the ground and at the top of the domain. Figure 1 demonstrates that such a parameterization is not appropriate to maintain the stratified upwind profiles, even for a short distance after the domain inlet. This rapid evolution is mainly due to the local disequilibrium of the TKE conservation equation in which the lack of buoyancy effects makes k evolve rapidly.

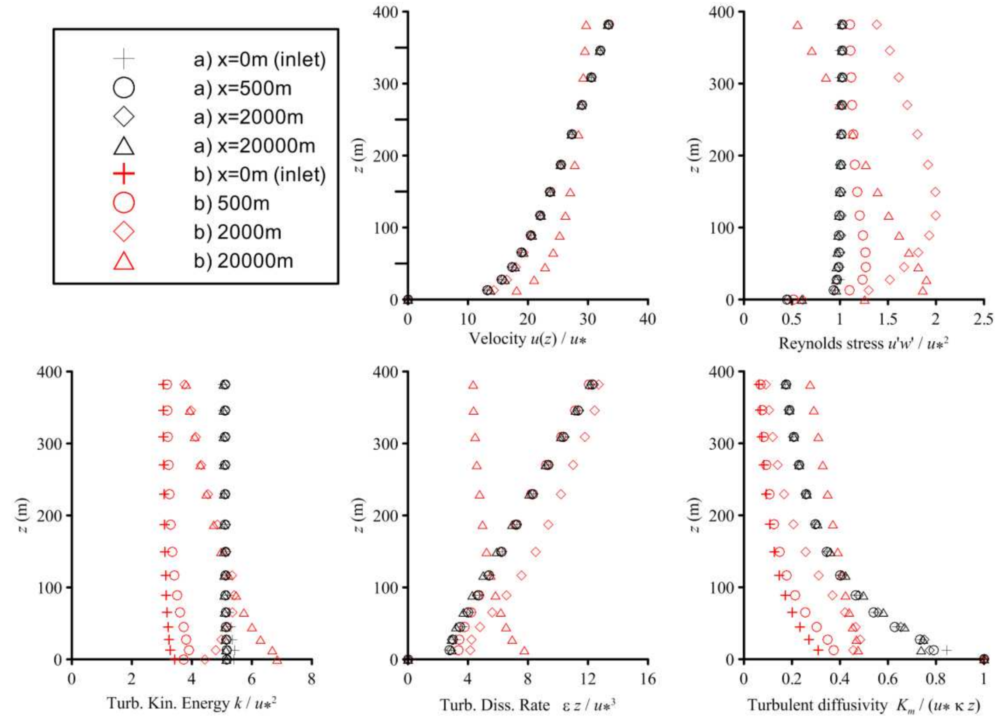

Figure 1. Vertical profiles of pressure, velocity, Reynolds stress, k and ε for different position in the simulation domain. a) Black profiles correspond to our methodology. b) Red profiles correspond to a RANS / k-ε simulation without thermal stratification parameterization.

CONCLUSION

In this work, we have proposed an analysis of the application of a RANS CFD approach with a k-ε closure to the simulation of a diabatic atmospheric surface layer. We discuss the consistency of the upwind turbulence profiles with conservation equations for k and ε and we propose an approach to modify the outlet pressure condition and to include a top flux condition in order to satisfy the main physical patterns of the surface layer. The results illustrate the ability of our approach to maintain the inlet profiles and the problems encountered if no parameterization is used for the stratification effects.

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