CFD simulation of the near-neutral atmospheric boundary layer

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CFD simulation of the near-neutral atmospheric boundary layer: New temperature inlet profile consistent with wall functions

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Abstract

Accurate Computational Fluid Dynamics (CFD) simulations of Atmospheric Boundary Layer (ABL) flow are essential for a wide range of applications, including atmospheric heat and pollutant dispersion. An important requirement is that the imposed inlet boundary conditions should yield vertical profiles that maintain horizontal homogeneity (i.e. no streamwise gradients) in the upstream part of the computational domain for all relevant parameters, including temperature. Many previous studies imposed a uniform temperature profile at the inlet, which has often led to horizontal inhomogeneity of the temperature profile. This study presents a new temperature inlet profile that can yield horizontal homogeneity for neutral and near-neutral ABL conditions when used in combination with the Standard Gradient Diffusion Hypothesis (SGDH) and a temperature wall function. The horizontal homogeneity by this profile is verified by 2D Reynolds-Averaged Navier-Stokes (RANS) CFD simulations performed with the standard k-ε turbulence model and the SGDH. The approach in this paper can be extended to other types of wall functions and other RANS closure schemes for Reynolds stresses and turbulent heat fluxes.

1. Introduction

Computational Fluid Dynamics (CFD) is increasingly used to analyze transport processes in the Atmospheric Boundary Layer (ABL) (Ayotte, 2008; Blocken, 2018; Blocken et al., 2007; Blocken and Carmeliet, 2004; Choi, 1993; Huang et al., 2005; Jeanjean et al., 2016; Kato et al., 1992; Luo and Li, 2011; Miller et al., 2013; Murakami et al., 1999; Pearlmutter et al., 1999; Sini et al., 1996; Sumner et al., 2010; Tominaga and Stathopoulos, 2013; Toparlara et al., 2017a; Vardoulakis et al., 2003). While CFD offers the capability of obtaining whole-field data under controlled conditions, the accuracy and reliability of the results require an appropriate selection of many parameters including computational model geometry, computational domain, computational grid, boundary conditions, turbulence model, near-wall treatment, discretization schemes and convergence criteria. In this perspective, CFD simulations of atmospheric flow processes have greatly benefited from a wide range of generic best practice guidelines (Blocken and Gualtieri, 2012; Casey and Wintergerste, 2000; Roache, 1997; Roy, 2005; Tucker and Mosquera, 2001) and applied best practice guidelines tailored to CFD simulations of ABL flow (Blocken, 2015; Franke et al., 2007; Richards and Hoxey, 1993; Tominaga et al., 2008).

CFD studies investigating wind flow in the ABL typically focus on an Area of Interest (AoI) that can consist of a group of explicitly modeled buildings and other obstacles such as trees (Fig. 1). The AoI is located in the central part of the domain, the dimensions of which are based on best practice guidelines (Blocken, 2015; Franke et al., 2007; Tominaga et al., 2008). The ABL flow is imposed at the inlet boundary and while traveling towards the AoI, in the upstream part, the vertical ABL profiles should ideally be absent of pressure gradients and horizontally homogenous (fully developed) (Ludwig and Sundaram, 1969; Raine, 1974). Horizontal homogeneity refers to the absence of streamwise gradients in the vertical profiles of mean wind velocity, turbulence properties, temperature, etc.

In the upstream and downstream parts of the domain, i.e. outside the AoI, obstacles such as buildings and trees are generally not modeled explicitly (i.e. with their actual shape and size) but implicitly, by assigning appropriate roughness parameters to the wall-type ground boundary. This is typically performed using wall functions, for mean velocity, turbulence properties and temperature, which represent the...
effect of the wall on these flow parameters in the wall-adjacent cells. Two types of wall functions exist: (1) \( y_0 \)-type wall functions, in which roughness is implemented via the aerodynamic roughness length \( y_0 \); and (2) \( k_S \)-type wall functions, in which roughness is implemented via the equivalent sand-grain roughness height \( k_S \). \( y_0 \) can be estimated using the updated Davenport roughness classification (Wieringa, 1992) (Table 1).

The parameter \( k_S \) originates from Nikuradse's experiments in roughened pipe flows (Nikuradse, 1933). Compared to \( y_0 \), \( k_S \) historically refers to roughness at much smaller scales. Even though \( y_0 \) represents the roughness of features relevant for \( ABL \) flow, wall functions commonly used in commercial CFD codes such as ANSYS Fluent (ANSYS Inc, 2013) and open-source CFD codes such as OpenFOAM (OpenFOAM Foundation, 2013) include roughness specifications based on \( k_S \). Both codes contain the Standard Wall Functions (SWF) by Launder and Spalding (1974) and their roughness modification by Cebeci and Bradshaw (1977), which is based on two parameters: (1) the roughness height \( k_S \) and (2) the roughness constant \( C_S \). Therefore, the remainder of this paper will focus on \( k_S \)-type wall functions, although the methodology can easily be extended to \( y_0 \)-type wall functions.

Horizontal homogeneity of ABL flow requires consistency between the inlet profiles, the wall functions, the computational grid and the turbulence model. Richards and Hoxey (1993) proposed a set of RANS inlet profiles for ABL flow based on aerodynamic roughness length \( y_0 \) (Davenport, 1961; Wieringa, 1992) to be used in combination with the standard \( k-\varepsilon \) turbulence model (Jones and Launder, 1972) and with \( y_0 \)-type wall functions. Blocken et al. (2007) derived the consistency relationship between \( k_S \) and \( y_0 \) such that the Richards and Hoxey profiles could also be used in combination with \( k_S \)-type wall functions. Further studies towards consistency with different model parameters were published by Gorle et al. (2009), Yang et al. (2009) and Parente et al. (2011). These studies all focused on the neutral ABL. Contributions for non-neutral (stable or unstable) ABL flow were made by Pontiggia et al. (2009) and by Pieterse and Harms (2013) based on \( y_0 \) and the Monin-Obukhov Length \( \lambda \) (m) with similarity functions. The profiles for mean wind speed, turbulent kinetic energy and turbulence dissipation rate proposed by Richards and Hoxey (1993) (Eqs. (1)–(3) in this paper) are valid for neutrally stratified Atmospheric Boundary Layer (ABL) flows. Strictly, these profiles are applicable for isothermal simulations. However, two situations can be distinguished where these profiles have to be used in conjunction with the energy equation. Situation (i) is a situation in which the large-scale ABL has neutral stratification but where convective heat transfer is important in the study, however the spatial scale of this heat transfer and/or the temperature differences involved are not such that they change the stratification of the ABL. Examples are the convective heat transfer at building surfaces, due to building exhaust or car exhaust gas, thermal effects on pollutant dispersion, or convective heat transfer at part of the Earth’s surface that is shielded from solar radiation or long-wave nocturnal cooling by clouds. Situation (ii) is as situation (i) but where the spatial scale of the heat transfer and/or the temperature differences are such that they do cause some minor changes in the ABL stratification (near-neutral ABL). In these two situations, the Richards and Hoxey (1993) profiles of \( U \), \( k \) and \( \varepsilon \) can and will be used but also the energy
equation needs to be solved. For these situations, the present paper presents a new temperature inlet profile consistent with wall functions.

When horizontal homogeneity is of concern, this should also be the case for the temperature profile imposed at the domain inlet. Franke et al. (2007) proposed to use measured temperature profiles as inlet boundary condition. This was done in several previous studies (e.g., Gracik et al., 2015; Kwak et al., 2011; Liu et al., 2015). However, such measurement of vertical temperature profiles are generally not available. Therefore, the vast majority of CFD simulations of urban microclimate have imposed a uniform temperature inlet profile (e.g., Allegrini et al., 2015a, 2015b; Ashie and Kono, 2011; Baik et al., 2012; Bo-ot et al., 2012; Bottolo et al., 2014; Chen et al., 2009; Dimoudi et al., 2014; Dimoudi and Nikolopoulou, 2003; Girgis et al., 2016; Gromke et al., 2015; Haghighat and Mirzaei, 2011; Hsieh et al., 2010; Kim et al., 2014; Maragkogiannis et al., 2013; Ooka et al., 2008; Peng et al., 2015; Pillai and Yoshie, 2012; Qu et al., 2012; Toparlar et al., 2017b, 2015; Vidrigh and Medved, 2013). Some other studies used dedicated temperature profiles for different thermal stability conditions based on $y_0$ and the Monin-Obukhov Length $L$ (m) (Panofsky and Dutton, 1984; Pieterse and Harms, 2013; Pontiggia et al., 2009). However, these studies were focused on stable or unstable stratified ABLS, without a particular focus on near-neutral ABL flow. The present study presents a new temperature inlet profile for neutral and near-neutral ABL flow that is consistent with the standard wall functions, incorporates surface roughness characteristics and satisfies the horizontal homogeneity of temperature in combination with the standard $k$-$\varepsilon$ turbulence model (Jones and Lauder, 1972). As such, this study represents the extension of the appropriate set of boundary conditions by Richards and Hoxey (1993) into the heat transfer arena.

### 2. Horizontal homogeneity problems for temperature

#### 2.1. Isothermal conditions

The problem with the horizontal inhomogeneity with $k$-$\varepsilon$-type wall functions was investigated by Blocken et al. (2007) by simulating ABL flow in a 2D computational domain with the 2D Reynolds-Averaged Navier-Stokes (RANS) equations, the standard $k$-$\varepsilon$ turbulence model and the inlet profiles by Richards and Hoxey (1993):

$$U(y) = \frac{u^*}{k} \ln \left( \frac{y + y_0}{y_0} \right)$$

(1)

$$k(y) = \frac{u^*}{\sqrt{C_p}}$$

(2)

$$\varepsilon(y) = \frac{u^*}{k(y + y_0)}$$

(3)

where $U$ is the mean wind speed, $y$ the height above ground, $u^*$ the ABL friction velocity, $y_0$ the aerodynamic roughness length, $k$ the von Karman constant, $C_p (=0.09)$ a model constant and $\varepsilon$ the turbulence dissipation rate. At the outlet, zero static gauge pressure was imposed and at the top, a symmetry plane with zero normal velocity and zero normal gradients of all flow parameters was imposed. Since imposing a symmetry condition at the top boundary can also cause unintended streamwise gradients in the vertical flow profiles, especially

### Table 1

**Updated Davenport roughness classification (Wieringa, 1992).**

<table>
<thead>
<tr>
<th>Aerodynamic roughness length ($y_0$) (m)</th>
<th>Landscape description</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0002 (sea)</td>
<td>Open sea or lake (irrespective of the wave size), tidal flat, snow covered flat plain, featureless desert, tarmac and concrete, with a free fetch of several kilometers.</td>
</tr>
<tr>
<td>0.005 (smooth)</td>
<td>Featureless land surface without any noticeable obstacles and with negligible vegetation; e.g. beaches, pack ice without large ridges, moras, and snow-covered or fallow open country.</td>
</tr>
<tr>
<td>0.03 (open)</td>
<td>Level country with low vegetation (e.g. grass) and isolated obstacles with separations of at least 50 obstacle heights; e.g. grazing land without windbreaks, heather, moor and tundra, runway area of airports.</td>
</tr>
<tr>
<td>0.1 (roughly open)</td>
<td>Cultivated area with regular cover of low crops, or moderately open country with occasional obstacles (e.g. low hedges, single rows of trees, isolated farms) at relative horizontal distances of at least 20 obstacle heights.</td>
</tr>
<tr>
<td>0.25 (rough)</td>
<td>Recently-developed ‘young’ landscape with high crops or crops of varying height, and scattered obstacles (e.g. dense shelterbelts, vineyards) at relative distances of about 15 obstacle heights.</td>
</tr>
<tr>
<td>0.5 (very rough)</td>
<td>&quot;Old&quot; cultivated landscape with many rather large obstacle groups (large farms, clumps of forest) separated by open spaces of about 10 obstacle heights. Also, low large vegetation with small inter- spaces, such as bushland, orchards, young densely-planted forest, landscape totally and quite regularly covered with similar-size large obstacles, with open spaces comparable to the obstacle heights; e.g. mature regular forests, homogenous cities or villages.</td>
</tr>
<tr>
<td>1.0 (closed)</td>
<td>Centers of large towns with mixture of low-rise and high-rise buildings. Also, irregular large forests with many clearings.</td>
</tr>
<tr>
<td>2.0 (chaotic)</td>
<td>For these situations, the present paper presents a new temperature inlet profile consistent with wall functions.</td>
</tr>
</tbody>
</table>
near the top of the domain, the simulations by Blocken et al. (2007) imposed fixed values in the top layer cells for $U$, $k$ and $\epsilon$, which were calculated with Eqs. (1)–(3). At the ground, a wall type boundary was specified with the standard wall functions (Launder and Spalding, 1974), with $k_0$-type roughness modification and employing the consistency relationship derived by Blocken et al. (2007) for the commercial CFD code ANSYS Fluent:

$$k_0 = \frac{9.793 y_0}{C_5}$$

(4)

where the value $9.793$ is the empirical wall constant $\varepsilon$ (–). Blocken et al. (2007) demonstrated that the above-mentioned conditions in combination with the standard $k$-$\varepsilon$ model provide the required horizontal homogeneity of $U$, $k$ and $\epsilon$ for neutral ABL flow. Their study however did not consider heat transfer.

### 2.2. Thermal conditions

To illustrate the problem of horizontal inhomogeneity of temperature, CFD simulations of ABL flow are performed with the 2D RANS equations, the standard $k$-$\varepsilon$ turbulence model and the Standard Gradient Diffusion Hypothesis (SGDH) for turbulent heat flux closure. The computational domain has dimensions $L \times H = 5000 \times 500 \text{ m}^2$ (Fig. 2). It is discretized in the streamwise direction with 500 cells of equal length ($10 \text{ m}$) and in the vertical direction with 46 cells of varying height. The height of the center-point of the first cell above the ground boundary $y_p$ is $0.287 \text{ m}$. The grid consists of 46000 rectangular cells and is identical to the one by Blocken et al. (2007).

At the inlet, the ABL profiles (Eqs. (1)–(3)) are imposed. The von Karman constant ($\kappa$) used in the profiles is determined by the equation provided by Richards and Hoxey (1993):

$$\kappa = \sqrt{\frac{C_s - C_2}{1}} \sqrt{C_p}$$

(5)

where the model constants are $C_s = 1.22$, $C_1 = 1.44$ and $C_2 = 1.92$, which leads to $\kappa = 0.4187$. At the outlet, zero static gauge pressure is imposed. The top boundary of the domain is specified as symmetry, with zero normal velocity and zero normal gradients for all the variables. Similar to the methodology followed by Blocken et al. (2007), fixed values of $U$, $k$ and $\epsilon$, calculated with Eqs. (1)–(3) are imposed at the top layer cells (Fig. 2) to avoid unintended streamwise gradients in the vertical flow profiles.

The aerodynamic roughness length ($y_0$) is specified as $0.1 \text{ m}$. At the ground, the $k_0$-type standard wall functions (Cebeci and Bradshaw, 1977; Launder and Spalding, 1974) are imposed. Simulations are performed with the commercial CFD code ANSYS Fluent (ANSYS Inc. 2013) that implicitly requires that the condition $y_P > k_0$ is satisfied. Note that although physically, as stated by ANSYS, this condition makes sense because fluid flow cannot be solved below the roughness (i.e. in the solid), Blocken et al. (2007) stated that mathematically this condition does not need to be satisfied, as the roughness $k_0$ is not modeled explicitly and the ground surface is often modeled as a flat surface. Regardless, the simulations performed in this study satisfy the requirement $y_P > k_0$ as $y_P = 0.287$ and $k_0 = 0.25 \text{ m}$. The appropriate roughness relationship (Eq. (4)) is satisfied by imposing $C_S = 3.9172$.

In line with the approach employed in the majority of previous CFD simulations of atmospheric heat transfer, temperature is introduced to the domain by a uniform vertical profile, in this case $T = 300 \text{ K}$. At the ground boundary, a constant heat flux of $q_{wall} = 200 \text{ W/m}^2$ is applied to create a non-isothermal simulation case. Second order discretization schemes are employed for all equations. The material properties for air at $300 \text{ K}$ are specified as: $p = 1.177 \text{ kg/m}^3$, $C_P = 1004.9 \text{ J/kg K}$, $\lambda = 0.0262 \text{ W/m K}$ and $\mu = 1.846 \times 10^{-5} \text{ kg/ms}$.

The simulations are considered converged when all residuals showed no further decrease with increasing number of iterations. At the end of the simulations, the scaled residuals had reached values of $10^{-11}$ for continuity, $10^{-16}$ for $x$-velocity, $10^{-17}$ for $y$-velocity, $10^{-15}$ for $k$ and $\epsilon$ and $10^{-16}$ for energy. This simulation with the uniform temperature profile at the inlet will be denoted as “case-T-uniform” for the remainder of this paper.

Fig. 3 demonstrates that the horizontal inhomogeneity of $U$, $k$ and $\epsilon$ is quite well satisfied as the maximum inhomogeneity error is $2.9\%$ for $U$ at $y/H = 0.002$, $4.1\%$ for $k$ at $y/H = 0.005$ and $5.4\%$ for $\epsilon$ at $y/H = 0.031$. However, the temperature profile imposed at the inlet cannot be sustained along the length of the domain, leading to noticeable inhomogeneity. The maximum inhomogeneity error (error$_{T}$) is $11.4 \text{ K}$ at $T_{wall}$ (at $y = 0$) and $2.2 \text{ K}$ for $T_P$ (temperature at $y_P (0.287 \text{ m})$). The deviation in temperature is less distinct in the upper parts of the domain. The results show that imposing a uniform temperature profile, although being a common approach in CFD studies on ABL flows, can lead to substantial temperature inhomogeneity. Note that the inhomogeneity would even be higher if the simulations were performed with a higher heat flux at the ground boundary.

The inhomogeneity in the vertical profiles of temperature occurs because of the mismatch (first-order discontinuity) between the uniform temperature inlet profile and the temperature wall function, as will be shown later. Therefore, a new and consistent temperature inlet profile will be derived in the next section.

![Fig. 2. 2D computational domain and grid (number of cells: 46,000).](image-url)
3. Derivation of an appropriate temperature inlet profile

3.1. Energy equation and standard wall function

In CFD simulations of ABL flow with heat transfer, generally two equations for heat transfer are employed. The first is the common convection-diffusion equation or energy equation:

\[
\frac{\partial T}{\partial t} = \nabla \cdot (\alpha \nabla T) - \nabla \cdot (\bar{v} T) + R
\]  

with \( T \) the temperature, \( t \) the time, \( \alpha \) the thermal diffusivity, \( \bar{v} \) the velocity vector and \( R \) a term representing sources/sinks. Eq. (8) is employed in all the computational cells within the domain. The second is the wall function (WF) that is used to calculate the temperature \( T_p \) at the center of the wall-adjacent cell \( y_p^* \):

\[
T^* = \frac{(T_{wall} - T_p) \rho C_p u^*}{q_{wall}}
\]  

where \( T^* \) is the dimensionless friction temperature. The term \( \frac{q_{wall}}{\rho C_p u^*} \) is commonly referred to as the scaling temperature \( T^* \) (Panofsky and Dutton, 1984). For incompressible flows (\( \nabla \cdot u = 0 \)), \( T^* \) is calculated based on the non-dimensional thermal sublayer thickness \( y^*_T \), which can be different from \( y^* \), which is calculated as the following:

\[
y^* = \frac{\rho u y}{\mu}
\]  

\[
y^*_T = \frac{\rho u^* y}{\mu}
\]  

\[
y^*_T = Pr \ln (Ey^*_T) + P
\]  

where \( Pr \) is the molecular Prandtl number (\( \approx 0.707 \) for air at 300 K), \( Pr_t \) is the turbulent Prandtl number (\( \approx 0.85 \) in this study (ANSYS Inc, 2013; Kays, 1994)), \( E \) (\( \approx 9.793 \)) is an empirical constant used in the near-wall description of the velocity profile (Lauder and Spalding, 1974) and \( P \) is a term based on an experimental work by Jayatilleke (1966). The value

Fig. 3. Vertical profiles of (a) \( U \), (b) \( k \), (c) \( \varepsilon \) normalized with \( u^* = 0.938 \) m/s and (d) temperature difference with respect to \( T (10, \text{inlet}) = 300 \) K for inlet, \( x = 0.1 \) L, \( x = 0.5 \) L and \( x = 0.9 \) L. Results are based on the simulation with uniform temperature at the inlet (case-T-uniform).
of $y_\text{fl}^*$ is the $y^*$ value at which Eq. (11) and Eq. (12) intersect (Fig. 4).

In Section 2, it was shown that the uniform temperature profile cannot yield consistency between the energy equation (Eq. (8)) and the SWF (Eq. (12)). Fig. 4 demonstrates the cause of this inconsistency by plotting a representative curve based on the energy equation and the SWF (Eq. (11) and Eq. (12)). When the wall function and energy equation do not exhibit first-order continuity in point $y_\text{fl}^*$, horizontal inhomogeneity will result. The focus of the following sub-section is on establishing consistency by means of first-order continuity between the energy equation and the temperature SWF by means of an appropriate temperature inlet profile.

3.2. Appropriate temperature inlet profile

An appropriate temperature inlet profile can be obtained by matching the energy equation and the temperature SWF equation while demanding a horizontally homogeneous flow. Focusing on the steady RANS equations ($\frac{\partial \bar{T}}{\partial t} = 0$) and in absence of heat sources/sinks, ($R = 0$), Eq. (8) can be simplified to:

$$\nabla \cdot \left( \bar{T} \nabla \bar{T} \right) = \nabla \cdot (\alpha \nabla \bar{T})$$

(13)

which can be written in open form as:

$$\left( \frac{\partial \bar{T}}{\partial x} + \frac{\partial \bar{T}}{\partial y} + \frac{\partial \bar{T}}{\partial y} \right) = \alpha \left( \frac{\partial \bar{T}}{\partial x} + \frac{\partial \bar{T}}{\partial y} \right)$$

(14)

where $\bar{u}$ and $\bar{v}$ denote the x-component and the y-component of mean velocity, respectively, $\bar{T}$ denotes the mean temperature and $\bar{u} \bar{T}$ and $\bar{v} \bar{T}$ denote the turbulent heat fluxes. In a horizontally homogenous flow $\bar{v} = 0$ , hence Eq. (14) becomes:

$$\left( \frac{\partial \bar{T}}{\partial x} + \frac{\partial \bar{T}}{\partial y} + \frac{\partial \bar{T}}{\partial y} \right) = \alpha \left( \frac{\partial \bar{T}}{\partial x} + \frac{\partial \bar{T}}{\partial y} \right)$$

(15)

The SGDH assumes that the turbulent heat fluxes are proportional to the gradients of mean temperature:

$$\bar{u} \bar{T} = -\alpha \frac{\partial \bar{T}}{\partial x} \bar{v} \bar{T} = -\alpha \frac{\partial \bar{T}}{\partial y}$$

(16)

where $\alpha$ is the turbulent thermal diffusivity ($m^2/s$):

$$\alpha = \frac{\nu_I}{Pr_I}$$

(17)

$\nu_I$ is the kinematic turbulent viscosity and $Pr_I$ is the turbulent Prandtl number (=0.85 in this study). Combining Eq. (15) ad Eq. (16) yields:

$$\frac{\partial T}{\partial x} = \alpha \left( \frac{\partial T}{\partial x} + \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial y} \left( \alpha \frac{\partial T}{\partial y} \right)$$

(18)

Demanding horizontal homogeneity of the mean temperature $\left( \frac{\partial \bar{T}}{\partial x} = 0 \right)$, Eq. (18) can be expressed as:

$$\frac{\partial}{\partial y} \left( \alpha \frac{\partial T}{\partial y} \right) = 0$$

(19)

$$\frac{\partial}{\partial y} \left( \frac{\partial T}{\partial y} + \alpha \frac{\partial T}{\partial y} \right) = 0$$

(20)

The relationship between the vertical temperature gradient and the wall heat flux $q_{wall}$ (W/m²) is:

$$q_{wall} = -\lambda \frac{\partial T}{\partial y}$$

(21)

where $\lambda$ denotes the turbulent thermal conductivity (W/mK). Dividing both sides of Eq. (21) with ($\rho C^v$):

$$\frac{q_{wall}}{\rho C^v} = -\frac{\lambda \frac{\partial T}{\partial y}}{\rho C^v}$$

(22)

By implementing Eq. (17) in Eq. (23):

$$\frac{q_{wall}}{\rho C^v} = -\frac{\nu_I}{Pr_I} \frac{\partial T}{\partial y}$$

(24)

$$\frac{q_{wall}}{\rho C^v} = -\frac{\nu_I}{Pr_I} \frac{\partial T}{\partial y}$$

(25)

where $\nu_I$ is the dynamic turbulence viscosity, which for the standard k-ε turbulence model can be expressed as:

$$\nu_I = \rho C^v \frac{k^2}{\varepsilon}$$

(26)

Combining Eq. (25) and Eq. (26) yields:

$$\frac{q_{wall}}{\rho C^v} = -\rho C^v \frac{k^2}{\varepsilon} \frac{\partial T}{\partial y}$$

(27)

Inserting the profiles of $k$ and $\varepsilon$ by Richards and Hoxey (1993) (Eq. (2) and Eq. (3)) in Eq. (27) gives:
Substituting $y = y_P$ in Eq. (36) yields Eq. (42) hence guaranteeing zeroth order continuity. The matching of the first derivatives of Eq. (36) and Eq. (42) at $y_P$ yields:

$$
\frac{\partial}{\partial y} \left( y + y_E \right) = \frac{\partial}{\partial y} \left( \frac{y + y_U}{y_0y_P} \right)
$$

(43)

This implies that the matching of the first derivatives can be satisfied when $y_P \gg y_0$. Usually, CFD studies focusing on ABL flow consider computational grids where $y_P > y_0$ since the typical values of $y_0$ representing landscape features (Table 1) are smaller than the grid sizes used in the CFD simulations of ABL flow. To understand the relationship between the temperature ABL profile (Eq. (36)) and the wall function profile (Eq. (42)) at the matching point $y_P$, profiles are generated with varying $y_0$ values while keeping the $y_P$ fixed at 0.287 m.

In Fig. 5, the profiles generated for $y_0 = 0.01$ m, $y_0 = 0.1$ m and $y_0 = 1.0$ m are demonstrated. The zeroth order matching of the profiles at $y_P$ is satisfied for all the cases. It is noticeable that while keeping the $y_P$ fixed, with increasing $y_0$, the shape of the profile at the matching point ($y_P$) is deflected. Fig. 5c demonstrates the first derivative of temperature with respect to height and the discontinuity of temperature change $(\frac{dT}{dy})$ at the matching point ($y_P$) is clearly noticeable for cases with higher $y_0$ values.

With the good matching of the profiles, the appropriate temperature boundary condition for the CFD simulations of ABL flow with the wall functions can be expressed as:

$$
T(y) = T_{wall} - \frac{T_P}{\kappa} \ln \left( \frac{y + y_0}{y_0} \right)
$$

(46)

4. Verification of horizontal homogeneity for temperature

In CFD simulations of ABL flow, inlet profiles, such as the one for the mean wind velocity (Eq. (1)), are commonly generated by specifying a reference wind velocity $U_{ref}$ at a reference height $y_{ref}$. Similarly, the newly derived temperature profile can be used by imposing a reference temperature $T_{ref}$ at a reference height $y_{ref}$. To test the horizontal homogeneity of the new temperature ABL profile (Eq. (46)), an additional set of CFD simulations is performed. Apart from the temperature profile imposed at the inlet, all other simulation settings are kept the same as in Section 2 (case-T-uniform). The profile is generated assuming an air temperature of 300 K at a reference height of $y_{ref} = 10$ m. Together with a $u^* = 0.938$ m/s, $C_p = 1004.9$ J/kg.K and $\rho = 1.177$ km$^2$/m$^3$, the constant heat flux at the ground boundary $q_{wall} = 200$ w/m$^2$ yields $T_i = 0.18$ since $T_i = \frac{q_{wall}}{\rho c_p}$. Simulations are performed with 12000 iterations. This simulation is denoted as case-T-ABL.

Fig. 6 shows the resulting vertical profiles at three positions in the domain together with the inlet profiles. Now, not only the vertical profiles of $U$, $k$ and $\varepsilon$ show good horizontal homogeneity, but also the vertical profile of $T$. The maximum inhomogeneity error ($\text{error}_T$) is 0.02 K for $T_{wall}$ and 0.01 K for $T_P$ (at $y = y_P = 0.287$ m). As opposed to the common approach of using uniform temperature profiles at the inlets, using the new temperature profile (Eq. (46)) leads to a homogenous temperature field. Note this homogeneity can only be achieved when the flow parameters $U$, $k$ and $\varepsilon$ also show horizontal homogeneity. For that, the appropriate roughness relationship by Blocken et al. (2007) should be satisfied.
5. Discussion

5.1. Comparison with measured profiles

Ideally, the newly derived temperature profile should be compared with measured near-surface temperature profiles in neutral and near-neutral atmospheric stratification where also information about terrain roughness, friction velocity, surface heat fluxes etc. is provided. Due to the scarcity of such data to allow such a comparison, in the present section, only a very preliminary comparison is made between the theoretical temperature profile and temperature profiles obtained from a variety of measurements, under conditions ranging from near-neutral to very non-neutral. This comparison is not intended to be a validation or verification of the theoretical profile, rather it is intended to show that the theoretical profile can exhibit a good degree of similarity to actual measured profiles, under a wide range of conditions.

The comparison of the theoretical profile to measured vertical temperature profiles in ABL flows reported by previous studies entails some challenges. As the profile expressed in this study requires the specific values of $T_{wall}$, $y_0$ and $T_*$, the measurement studies should have reported these values at the time of the measurements to conduct an exact comparison. Among the identified studies that reported measured vertical temperature profiles, none has listed these required values altogether. Therefore, instead of conducting a strict validation study, the profile is compared with measured profiles by specifying best-fit values for $T_{wall}$, $y_0$ and $T_*$ to reproduce each measurement case.

The comparison is visualized in Fig. 7. Three of the profiles were measured during the famous Wangara experiment (Clarke, 1971; Hess et al., 1981). The specific data for the Wangara day-33 was considered in various studies in the past (Arya, 2005; Mahrt et al., 1979; Mahrt and Lenschow, 1976) and the measured temperature profiles on this specific day were reported for 09:00, 12:00 and 15:00 h. The profile generated to fit the Wangara day 33 (9:00 h) data is established by specifying $T_* = -0.61$, $y_0 = 0.1$ m and $T_{wall} = 272$ K. The temperature profile fitted to the one reported by Angevine et al. (2001) is generated by imposing $T_0 = -0.25$, $y_0 = 0.51$ m and $T_{wall} = 283.5$ K. The value imposed for the $y_0$ is explicitly stated by Angevine et al. (2001). The profile reported was measured at Cabauw (the Netherlands) for multiple days at the sunrise and the values were averaged over these measurement days. Segal et al. (1991) conducted measurements of flow above snow and snow-free areas to investigate snow breeze. The study reported two vertical temperature profiles over two terrains, with and without snow cover. The fitted profiles are specified by imposing $T_0 = -0.63$, $y_0 = 0.03$ m, $T_{wall} = 286$ K and $T_* = 0.02$, $y_0 = 0.03$ m, $T_{wall} = 298.6$ K corresponding to the cases with and without snow, respectively.

The comparisons show that overall, the new analytical profile derived in the present study exhibits a good degree of similarity to the temperature profiles measured in the respective prior studies, even though there are some differences between the fitted profiles and the measured profiles in the surface layer, especially below 200 m height. The differences between the fitted profiles and the measured profiles are more significant in cases with a larger vertical temperature gradient (i.e. for non-neutral ABL cases). On the other hand, the fitted profiles can represent the measured profiles of near-neutral ABL cases, such as Segal et al. (1991) (without snow) and Wangara day 33 12:00 h with much less deviations.

5.2. On the effect of turbulent Prandtl number and von Karman constant

The turbulent Prandtl number ($Pr_t$) is a non-dimensional parameter denoting the ratio of momentum eddy diffusivity to heat transfer eddy diffusivity (Eq. (17)). It can be challenging to determine the exact value of $Pr_t$ since dedicated efforts are required to measure turbulent shear stress and turbulent heat flux as well as velocity and temperature gradients occurring in boundary layers. Various studies in the past investigated or modeled $Pr_t$ values used in the literature. Ceci (1973) produced a numerical model for predicting $Pr_t$ while comparing the model results with earlier measurement studies. The study concluded that even though a value of 0.9 is commonly used, in some particular cases, higher values such as $Pr_t = 1.22$ can be more reasonable. Kays (1994) reviewed several studies aimed at quantifying $Pr_t$ and listed the findings, which reported $Pr_t$ in the range of 0.73–0.92. A similar finding on the $Pr_t$ values ranging from 0.72 to 1.00 was reported in the review study by Leclerc and Foken (2014). Up until here in the present paper, a $Pr_t = 0.85$ is imposed for all the profiles. In Fig. 8, the effect of changing $Pr_t$ on the temperature profile is shown for $Pr_t = 0.72$, $Pr_t = 0.85$, $Pr_t = 1.00$ and $Pr_t = 1.22$ while keeping all the other parameters the same as in Section 4 ($T(10) = 300$ K, $T_* = 0.18$, $y_0 = 0.1$ m). It is noticeable that within the range of previously reported $Pr_t$ values and considering the thermal conditions imposed in Section 4, the temperature profile can shift approximately 1.1 K at 500 m height. The changes in temperature from different $Pr_t$ values are lower close to the ground level, than the changes in the upper levels. Future studies on urban climatology can focus on determining a suitable $Pr_t$ value which can be applicable for use in urban microclimate simulations.

The von Karman constant ($\kappa$) is imposed in this study as 0.4187 in accordance with Eq. (4), which is based on the model constants of the standard $k$-$\varepsilon$ turbulence model. Högström (1996) investigated several relevant parameters in the atmospheric surface layer, including the von...
Karman constant. The study provided a list of appropriate $\kappa$ values reported in prior studies, which was in the range of 0.35–0.65. The majority of the studies reported $\kappa$ values in the range of 0.39–0.42 and Högström (1996) listed several reasons for the deviations found in studies with $\kappa$ values outside of the 0.39–0.42 range. The new temperature profile is not influenced significantly within the $\kappa$ range of 0.39–0.42. Even though the deviations in the $\kappa$ value affects the profile to a lesser extent compared to other parameters (i.e. $P_r_t$), CFD studies using the temperature profile should consider imposing an appropriate $\kappa$ based on the turbulence model chosen since its effect on mean wind speed and turbulence parameters might be significant.

5.3. Differences from other temperature profiles

This study is aimed to extend the set of “appropriate boundary conditions” specified by Richards and Hoxey (1993) with a new inlet temperature profile. The profiles by Richards and Hoxey (1993) and the profile expressed in the present study are essentially valid for neutral and near-neutral atmospheric conditions. Some other temperature profiles are sometimes expressed in terms of temperature roughness ($y_0T$) with the following (Leclerc and Foken, 2014):

$$T(y) = T(y_0T) - \frac{T_{in}}{\kappa} \ln \left( \frac{y}{y_0T} \right)$$

(47)

However, commonly used CFD tools, such as ANSYS Fluent and OpenFOAM, consider only a single roughness parameter in the calculations of the wall functions, which is the aerodynamic roughness length $y_0$. Therefore, imposing $y_0T$ is generally not an applicable method for CFD studies.

Consideration of atmospheric stability in CFD simulations is an issue out of the scope of the present paper. Pontiggia et al. (2009) focused on developing boundary conditions aimed to be valid for changing stability conditions, using the following equation as the temperature profile:

$$T(y) = T_{wall} + \frac{T_{in}}{\kappa} \left[ \ln \left( \frac{y}{y_0} \right) + \phi_e \frac{\varphi^2}{\varphi} - 1 \right] - \frac{g}{C_p} (y - y_0)$$

(48)

In comparison to the new temperature profile specified in the present study (Eq. (42)), the $P_r_t$ term is not used in the profile by Pontiggia et al. (2009) and the rate of temperature change is calculated with the
similarity function $\phi_m(z) - 1$, which depends on height and on the Monin-Obukhov length. A similar profile was presented and used by Pieterse and Harms (2013) in the following form:

$$T(y) = T_{wall} + \frac{T_r - T_*}{\kappa} \ln \left( \frac{y}{y_0} \right) - \Psi_m \left( \frac{z}{L} \right)$$

where $\Psi_m$ is the integrated form of the similarity function. Both profiles (Eq. (46) and Eq. (47)) are specified for non-neutral ABL cases whereas the focus of the temperature profile presented in this paper is on neutral and near-neutral ABL flow and it is an extension of the profiles by Richards and Hoxey (1993).

5.4. Limitations and future perspectives

The derivation of the new temperature profile is based on the profiles of $U$, $k$ and $\varepsilon$ specified by Richards and Hoxey (1993) and on the SGDH. These profiles are specified for neutral atmospheric conditions and similarly, the temperature profile derived in this study is considered to be valid for neutral or near-neutral atmospheric conditions only.

The profiles defined by Richards and Hoxey (1993) are analytical solutions to the standard $k-\varepsilon$ turbulence model but they have also been
used in various studies in the past with different turbulence models (Blocken, 2015; Franke et al., 2007; Tominaga et al., 2008). Similarly, the temperature profile determined in this study can be used in simulations performed with other turbulence models. In such cases, it is recommended to carefully monitor any eventual temperature inhomogeneity by performing a simulation in an empty computational domain, prior to embarking on the actual modeling study.

In CFD simulations performed with the commercial CFD code ANSYS Fluent, it is necessary to ensure that $y_P > k_S$. In Section 3.2 of this study, another condition was specified as $y_P > k_S$ to ensure the smooth transition of the temperature profile at the middle of the wall-adjacent cell. Since typical vertical $y_P$ values are much smaller than typical $k_S$ values, this condition is more lenient compared to the condition of $y_P > k_S$. In majority of the cases, when the $y_P > k_S$ condition is satisfied, most likely the condition of $y_P > y_0$ will also be satisfied because the appropriate roughness relationship (Blocken et al., 2007) $k_S = \frac{9.793 \text{Re}^{1/2}}{u_*}$ dictates a $k_S$ which is, for a $C_s$ of 1, one order of magnitude larger than $y_0$.

Future studies using the temperature profile presented in this paper should ensure the proper implementation of the inlet profiles by Richards and Hoxey (1993) and the appropriate roughness relationship presented by Blocken et al. (2007) as otherwise flow inhomogeneity might occur. In particular, when the temperature profile is to be used in combination with flow profiles other than the ones stated by Richards and Hoxey (1993), the development of the vertical temperature profile in the computational domains should be carefully checked. If the simulation results lead to any temperature inhomogeneity, deviations from the inlet profiles should be reported and considered carefully while processing the results.

6. Summary and conclusions

CFD studies investigating physical occurrences within the Atmospheric Boundary Layer (ABL) have benefited from the advances in computational capabilities, the establishment of best practice guidelines and appropriate boundary conditions. An important requirement of the CFD simulations is that the imposed boundary conditions should yield vertical profiles that maintain horizontal homogeneity (i.e. no streamwise gradients) for all relevant parameters, including temperature.

Currently, CFD simulations of ABL flow can satisfy the horizontal homogeneity of mean wind velocity and turbulence parameters thanks to the development of appropriate boundary conditions and roughness relationships. As for temperature, many previous studies impose a uniform temperature profile at the inlet, which can lead to temperature inhomogeneity. In this paper, a new temperature inlet profile is derived that can yield horizontal homogeneity for neutral and near-neutral ABL conditions when used in combination with the standard $k$-$

The verification of this profile with regards to horizontal homogeneity is demonstrated through 2D Reynolds-Averaged Navier-Stokes (RANS) simulations performed with the standard $k$-$

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