Hazardous gas dispersion: a CFD model
accounting for atmospheric stability classes

M. Pontiggia, M. Derudi, R. Rota*

* To whom correspondence should be addressed email renato.rota@polimi.it

Politecnico di Milano, Dipartimento di Chimica, Materiali, Ingegneria Chimica “Giulio
Natta”, via Macinelli 7, 20131 Milano - Italy

Key – words: CFD; Turbulence modeling; gas dispersion; atmospheric stability; safety.

Abstract

Nowadays Computational Fluid Dynamics (CFD) is rapidly imposing itself also in the
industrial risk assessment area, replacing integral models when particular situations,
such as those involving complex terrains or large obstacles are involved. Thanks to the
increasing CPU power, geometrically complex environment can be simulated giving
reliable predictions of the obstacles influences on the gas dispersion behaviour.
Nevertheless, commercial CFD codes do not provide specific turbulence model for
simulating atmospheric stratification effects, which are usually accounted for in integral
models by the well-known stability-class approach. In this work a new approach able to
account for atmospheric features in CFD simulations has been developed and validated
by comparison with available experimental data.
1 Introduction

Risk assessment of hazardous gaseous releases is an important task in the process industry safety, since this type of scenario can lead to large consequences: the cloud of hazardous products can be carried by wind even for kilometres maintaining its concentration high enough to represent an hazard both for environment and human health. Dense gas clouds, which are characterized by a negative buoyancy, maximize the negative effects both in terms of distance and duration of the hazardous cloud since they fall to the ground, where wind speed decreases and the dilution with air is reduced. A release can behave like a dense gas cloud for several, often concurring, reasons: the high molecular weight of the substance (which makes the gas cloud denser then air even at atmospheric conditions), the low temperature, or the presence of aerosols.

The interest in this kind of analysis has brought, in the early 1980s, to the execution of large-spill trials and to the development of simulation mathematical models that are currently used for loss prevention purposes in chemical and process industries [1] [2]. Some of them, like DEGADIS, SLAB, ALOHA and UDM are among the most popular and widely used models in safety engineering applications [3] [4]. These tools are characterized by lumped mathematical models, usually one-dimensional, and account for some physical phenomena using semi-empirical relations whose coefficients are tuned on field test data (for example, the obstacles geometry is summarized in a couple of parameters, the surface roughness and displacement height) [5]. Since the experimental set-up of the field trials usually do not involve any relevant obstacle, these models consequently provide good results only in open field conditions.

In order to simulate more complex geometries and to analyze the effect of large obstacles on gas dispersion, computational tools based on fluid dynamics methods
(commonly known as Computational Fluid Dynamics or CFD codes) have been applied. This approach allows for performing full three-dimensional analysis, and to predict velocity, temperature and concentration fields. While assuring more detailed results, it requires a larger amount of resources both in term of CPU time and analyst skill. CFD results have been successfully validated against experimental field data [6], lab scale trials [7] and they have been also used for complex geometries analysis, such as urban canyons [8].

However, particular attention in CFD simulations has to be paid to turbulence modelling. The effect of the turbulent fluctuations can be modelled through the RANS (Reynolds Averaged Navier-Stokes) approach, or fully simulated through Direct Numerical Simulation (DNS). The DNS is very resources-demanding and, nowadays, can be applied only to very simple cases. An intermediate solution is represented by Large Eddies Simulations (LES) that simulate only larger eddies (down to Kolmogorov scale) and use models for simulating the effects of isotropic dissipating eddies. Although LES is less demanding than DNS, it is still quite demanding in complex scenarios. Consequently, RANS still represents a good compromise between results accuracy and computational efforts. The most popular closure model for the RANS approach is the k-ε two-equations model, since it assure reasonable results and good stability [9].

RANS-CFD models are currently implemented in commercial codes, which are multi-tasking instruments mainly developed for confined flow simulation (for example flow inside pipes or mixers) or for external aerodynamic simulations (such as lift and drag wing forces). As a consequence, no models for the closure of the RANS approach
specific for the atmospheric boundary layer analysis are available as standard tools that could be used for engineering purposes.

A few theoretical works have been carried out to investigate the possibility of including atmospheric turbulence effects in CFD simulations. Riddle et. al. [10] demonstrated that the k-ε model can not maintain the boundary conditions established accordingly to Monin-Obukhov profiles even in open field simulations: without any external influence, velocity, temperature, turbulent kinetic energy (k) and turbulent dissipation rate (ε) change over the domain. A seven-equations closure model is also provided in order to achieve consistency between CFD simulations and Monin-Obukhov theory, but it requires heavy computational resources not suitable for engineering computations. To ensure the consistency between Monin-Obukhov theory and CFD predictions, Hargraves and Wright [11] and Blocken et al. [12] developed a wall-law modification for representing the wall roughness effect in the k-ε model for neutral atmospheric stratification. This solution enhances the previous results but still does not provide stable profiles over a flat terrain.

Other works focused on the turbulence generated by obstacles within the domain, but paid almost no attention to atmospheric stability consistency [13], [14] since they eventually provide initial profiles that are substantially changed by the geometrical features, [15], [16].

Finally, some works developed new atmospheric-specific closure models [17] or change k-ε constants to achieve better agreement with atmospheric profiles [18], [19]. Even if they leads to reasonable predictions for atmospheric turbulence in open field, these models are not validated for other kinds of turbulence, such as that arising from the interaction with obstacles.
In this study a new methodology for including the effects of atmospheric stratification on dense gas dispersion CFD simulations has been developed. Heavy gases have been considered since they represent the worse case scenario when dealing with safety problems. Moreover neutral and stable stratification (D and F stability classes), which are commonly used in risk assessment when dealing with hazardous gas dispersion, have been considered. New boundary conditions have been proposed for both inlet and ground surface to include atmospheric turbulence effects and k-\(\varepsilon\) turbulence model has been improved to achieve profiles-consistency with the similarity theory. The proposed model is simple, not CPU demanding and stable enough to be used for engineering computations.

2 Theoretical Background

CFD codes solve numerically continuity (1) and Navier-Stokes (2) equations, through the partition of the domain and the realization of a computational grid, called mesh. This allows reducing the partial derivative equations system to an algebraic equations system, which is solved through various numerical methods. The Finite Volume method [20] stores the results in the centre of each element of the mesh; the continuous solutions is obtained through the interpolation of the discrete stored data.

Along with Navier-Stokes equations, CFD codes solve specific model equations, such as energy balance (3), species diffusion, turbulence, etc..

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (1)
\]

\[
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla \cdot \left( \tau \right) + \rho \vec{g} \quad (2)
\]
\[
\frac{\partial}{\partial t}\left( \rho c_v T \right) + \nabla \cdot \left( \rho \nu c_p T \right) = \nabla \cdot (k_r \nabla T) \quad (3)
\]

In the equation above \( \rho \) is the density, \( t \) the time, \( v \) the velocity, \( p \) the pressure, \( \tau \) the shear stress, \( g \) the gravity acceleration, \( c_v \) and \( c_p \) the specific heats, \( T \) the temperature and \( k_r \) the thermal conductivity.

In this work the k-\( \varepsilon \) model has been used for representing the effects of the turbulence. This model introduces two additional transport equations for turbulent kinetic energy \( k \) (4) and turbulent kinetic energy dissipation rate \( \varepsilon \) (5), respectively [21]:

\[
\frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M \quad (4)
\]

\[
\frac{\partial}{\partial t} (\rho \varepsilon) + \frac{\partial}{\partial x_i} (\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{\mu} \frac{\varepsilon}{k} (G_k + C_{g_k} G_b) - C_{\varepsilon} \rho \frac{\varepsilon^2}{k} \quad (5)
\]

where \( u_i \) is the velocity component along \( x \) direction, \( \mu \) the viscosity, \( \mu_t \) the turbulent viscosity, \( G_k \) the shear stress-related turbulent kinetic energy production, \( G_b \) the buoyancy-related turbulent kinetic energy production, \( Y_m \) the compressibility-related kinetic energy production. \( C_{\mu}, C_{\varepsilon}, C_{g_k}, \sigma_k, \sigma_\varepsilon \), and \( C_\mu \) are empirical constants. Jones and Launder [21] values have been used for all the k-\( \varepsilon \) model constants (Table 1)

### 3 Boundary conditions and source terms for representing different atmospheric stability classes

In order to validate the proposed methodology, Prairie Grass experiments [22] have been used. These involve continuous releases of small amount of Sulphur dioxide at or near ground level over a flat terrain. The experiments were carried out during both day and night giving rise to a wide range of atmospheric stability conditions (table 2).
Concentration values of sulphur dioxide were measured from an array of sensors located at downwind distances of 50, 100, 200, 400 and 800 [m]. Among all the experiments, in this work only those involving neutral and stable stratifications have been considered since these atmospheric conditions are the most used when assessing the consequences of industrial accidents. Unstable conditions raise the atmospheric turbulence and, therefore, the dilution of the released gas, reducing the zone interested by hazardous gas concentration and leading to less severe consequences.

When performing CFD simulations of these experiments with constant profiles for wind velocity, air temperature, turbulent kinetic energy and turbulent dissipation rate as inlet boundary conditions for the wind inlet, it can be easily verified that, even in open field, the profiles change drastically, due to two opposing effect: a progressive rise of turbulence intensity near the ground produced by the terrain roughness, and a quick disappearance of turbulent intensity away from ground the level due to the lack of shear stress in the flat-profile air flow. These changes in the profiles mean that the air flow is not fully developed. This is a problem since when performing atmospheric open field steady-state simulations wind is expected to behave as a fully developed flow.

Moreover the profiles of temperature, velocity and turbulence must be representative of the atmospheric physics, in order to describe carefully the gas dispersion.

In order to describe the atmospheric flow over uniform flat terrain, the turbulent viscosity can be expressed as a function of the mixing length relation through the Monin-Obukhov similarity theory [23]:

\[
\mu_{\tau_0}(z) = \frac{\rho K u_z z}{\Phi_m \left( \frac{z}{L} \right)}
\]  

(6)
where $K = 0.42$ is the von Karman constant, $u^*$ the turbulent friction velocity, $z$ the vertical coordinate ($z=0$ at ground), $\Phi_m$ a function that depends on $z$ and $L$, the Monin-Obukhov length. For neutral and stable stratification $\Phi_m = \left(1 + 5\frac{z}{L}\right)$.

The Monin-Obukhov length is an estimate of the height where the turbulent dissipation due to the buoyancy is comparable with the shear stress production of turbulence; it can be expressed by the following relation [23]:

$$L = \frac{u^2_w T_w}{K g T_\infty}$$

(7)

The turbulent friction velocity, $u^*$, and temperature, $T^*$, are defined as:

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}}$$

(8)

$$T^* = \frac{-q_w}{\rho c_p u_\tau}$$

(9)

where $\tau_w$ is the surface shear stress, $T_w$ the surface temperature, $q_w$ the surface heat flux, and $g$ the gravitational acceleration module.

Assuming the shear stress and heat flux constant over the lower part of the atmospheric boundary layer, modified logarithmic velocity and temperature profiles for stable stratification can be obtained [23]:

$$u = \frac{u^*_\tau}{K} \left[ \ln \left( \frac{z}{z_0} \right) + \Phi_m \left( \frac{z}{L} \right) - 1 \right]$$

(10)

$$T(z) - T_w = \frac{T^*_\tau}{K} \left[ \ln \left( \frac{z}{z_0} \right) + \Phi_m \left( \frac{z}{L} \right) - 1 \right] - \frac{g}{c_p} \left( z - z_0 \right)$$

(11)

where $z_0$ is the roughness length of the site. Measuring $u$, $T$ at a known quote $z$, $T_w$ and $z_0$, it is possible, trough equations 10 and 11, to evaluate $u^*$ and $T^*$. 
In CFD simulation the approximation of incompressible gas is usually retained for air; therefore it is not possible to balance the adiabatic profile of temperature (11) varying the pressure along z-direction. As a consequence 1 reduced temperature has been implemented as boundary conditions at the wind inlet:

$$\theta = T(z) + \frac{\rho}{c_p}(T_w - T_{z_0}) = T_w + \frac{T_*}{K} \left[ \ln \left( \frac{z}{z_0} \right) + \Phi_m \left( \frac{z}{L} \right) - 1 \right]$$  \hspace{1cm} (12)

While velocity and temperature profiles can be directly imposed as boundary conditions, turbulent viscosity is evaluated by the k-ε model as a function of turbulent kinetic energy and turbulent dissipation rate; so proper profiles for turbulent quantities must be obtained in order to have consistency between CFD computed values of μt and the values provided by the Monin-Obhukov similarity (equation 6). The consistency between Monin-Obhukov profiles and k-ε model predictions is necessary to assure constant (that is, fully developed) profiles in open field simulations.

### 3.1 Neutral stratification

For neutral stratification, the heat flux from the ground is equal to zero; therefore the Monin-Obukhov length is infinite and $\Phi_m$ tends to 1; the friction temperature $T_*$ tends to zero and temperature is constant with z. Assuming flat profile for the kinetic energy [23] and rearranging the transport equations of turbulent kinetic energy (4) in steady-state conditions with equations (6) and (10), over flat terrain (i.e., with no gradients along x and y direction) we can find:

$$\varepsilon(z) = \frac{u_z^3}{Kz}$$  \hspace{1cm} (13)
Equations (13) and (14) are mathematically consistent with $k$ transport equation; in order to assure the consistency also with turbulent dissipation rate equation, Alinot and Masson [19] suggested to alter the $k$-$\varepsilon$ model constants. This solution, however, while leading to good performances for the evaluation of atmospheric profiles over flat terrains, has not been validated for turbulence arising from other sources, such as obstacles. Consequently, the addition of a $z$-dependent source term, $S_\varepsilon$, to the $\varepsilon$ transport equation should be preferred. This term can be obtained through the substitution of the profiles (13) and (14) in equation (5):

$$S_\varepsilon(z) = \frac{\rho u_i^4}{z^2} \left[ \frac{(C_{2z} - C_{1z}) \sqrt{C_\mu}}{K^2} - \frac{1}{\sigma_\varepsilon} \right] - \mu \frac{u_3^3}{2Kz^3} \tag{15}$$

Depending on the elevation ($z$), this source term can represent both a reduction ($S_\varepsilon < 0$) or an increment ($S_\varepsilon > 0$) of the turbulent dissipation rate, and, therefore, an increment or a reduction of the turbulence due to some atmospheric features that the $k$-$\varepsilon$ standard model can not reproduce. Moreover, since this term is added to all the other turbulence source contribution (e.g., gas expansion, jet propagation, interaction with obstacles, ...) the resulting equation:

$$\frac{\partial}{\partial t}(\rho \varepsilon) + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_f}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] + C_{1z} \frac{\varepsilon}{k} \left( (1 - C_{3z}) \frac{\varepsilon}{k} - C_{2z} \rho \frac{\varepsilon^2}{k} \right) + S_\varepsilon(z) \tag{16}$$

is expected to be able to represent the simultaneous effect of all these contributions.

It should be noted that $S_\varepsilon$ is composed by two terms: the fist one contains all the dependences on $k$-$\varepsilon$ model constants, while the second one depends on molecular
viscosity. Neglecting this second term, it is possible to obtain the relations used by Alinot and Masson [19] for the evaluation of their new constants.

### 3.2 Stable stratification

In stable stratification $\Phi_m$ does not tend to 1 and temperature is not constant; therefore the mathematics becomes more complex. Considering again flat k-profile (that is, neglecting the diffusion terms in equation 4) and rearranging the same equations as done before, turbulent profiles are obtained for both $k$ and $\varepsilon$:

\[
\varepsilon = \frac{u^2}{Kz} \Phi_\varepsilon \tag{17}
\]

\[
k = \frac{u^2}{\sqrt{C\mu}} \Phi_k \left( \frac{z}{L} \right) \tag{18}
\]

where $\Phi_\varepsilon$ is a function similar to $\Phi_m$, equal to that proposed by Panofsky and Dutton (1984):

\[
\Phi_\varepsilon = \left( 1 + 4 \frac{z}{L} \right) \tag{19}
\]

Turbulent kinetic energy (18) depends on $z$ and consequently, in this case, it is not possible to neglect the diffusion term without introducing an identical but opposite source term in the $k$ equation (4):

\[
S_k = -\frac{\partial}{\partial z} \left[ \left( \frac{\mu + \mu_\varepsilon}{\sigma_k} \right) \frac{\partial k}{\partial z} \right] \tag{20}
\]

However, it can be noted from equation (18) that the $k$ dependence on $z$ is quite negligible since $k$ tend rapidly to a constant value. Consequently, its derivative in
equation (20) is close to zero and the $S_k$ term can be safely neglected. Without any significant loss of accuracy as verified through proper simulations, including $S_k$ term increases computational efforts without any significant profile improvements.

Along the same line discussed for neutral stratification, an equation for $S_\varepsilon$ has to be obtained in order to assure $k-\varepsilon$ model consistency with the Monin-Obhukov similarity theory, leading to the following relation:

$$
S_\varepsilon(z) = \frac{u^4 \rho}{z^2} \left[ \frac{(C_{2_\varepsilon} - C_{1_\varepsilon})}{K^2} \sqrt{C_\mu} \Phi_\varepsilon^2 \left( \sqrt{\frac{\Phi_\varepsilon}{\Phi_m}} - \frac{1}{\sigma_\varepsilon} \left( \frac{2}{\Phi_m} - \frac{1}{\Phi_m^2} + \frac{T_1}{KT} \right) \right) - \mu \frac{2u^3}{Kz^3} \right] \tag{21}
$$

Also in this case $S_\varepsilon$ is composed by two terms; the molecular viscosity-dependent term remains unchanged, while the first one becomes much more complex.

### 3.3 Wall treatment

The shear stress turbulence production is particularly important near the ground; CFD codes usually model the laminar region near walls using a logarithmic velocity profile:

$$
\frac{uu_*}{\tau_w/\rho} = \frac{1}{K} \ln \left( \frac{E \rho u_* x_j}{\mu} \right) - \Delta B \tag{22}
$$

where $\tau_w$ is the shear stress, $E$ an empirical constant ($E = 9.793$), $\mu$ the molecular viscosity, $\Delta B$ a roughness-dependent correction. Varying the roughness effects on fluid motion, it is possible to define three different regions, which provide different equations for the velocity profile correction term [21]:
$K^+ \leq 2.25 \rightarrow \Delta B = 0$

$\begin{align*}
2.25 \leq K^+ \leq 90 \rightarrow \Delta B &= \frac{1}{K} \ln \left( \frac{K^+ - 2.25}{87.75} + C_S K^+ \right)^{\sin \left(0.425\ln (K^+ - 0.811)\right)} \\
K^+ > 90 \rightarrow \Delta B &= \frac{1}{K} \ln \left(1 + C_S K^+\right)
\end{align*}$

(23)

with $K^+ = \frac{\rho K u_\tau}{\mu}$ and $K_S$ roughness height, $C_S$ a constant that depends on roughness type. While $K_S$ should be directly measured, $C_S$ is hardly interpreted: it is 0.5 for fully uniform surface roughness, and tends to 1 for inhomogeneous surface patterns.

Low value of $K^+$ ($K^+ < 2.25$) means that viscosity rules over turbulent effects and, therefore, $\Delta B$ can be neglected. When $K^+$ is large ($K^+ > 90$), roughness effects become prominent and $\Delta B$ equation is provided. In atmospheric flows $K^+$ values are generally high and fully turbulent situation are considered. Anyway, both fully turbulent and intermediate behaviours can be rewritten as:

$$\Delta B = \frac{1}{K} \ln f(K_S, C_S)$$

(24)

which, replaced in equation 22 leads to the following velocity profile:

$$u = \frac{u_\tau}{K} \ln \left( \frac{E \rho u_\tau x_j}{\mu f(K_S, C_S)} \right)$$

(25)

Near the wall shear stress prevails over buoyancy, and neutral stratification profile should be considered for velocity. By equaling equations (25) and (10), $C_S$ can be implicitly obtained as:

$$\frac{E \rho u_\tau}{\mu f(K_S, C_S)} = \frac{1}{z_0}$$

(26)

$C_S$ values have been calculated for all the simulated tests obtaining a constant value of 0.979, that can be considered a suitable value for wall treatment in atmospheric gas
dispersion problems. As stated before, a value of $C_s$ close to 1 means inhomogeneous surface and it is well suited to describe terrain roughness.

4 Profiles tuning through periodic simulations

Validation of the proposal approach requires at first to verify that CFD fully developed profiles correctly compare with those arising from the Monin-Obhukov similarity theory. When using CFD codes for simulating atmospheric gas dispersion, usually a long domain upwind the gas release location is required to allow the vertical profiles of all the relevant variables (that is, velocity, temperature, turbulence intensity and dissipation rate) to became fully developed (that is, in agreement with both the BCs and the equations used for the particular situation) starting form the (arbitrary) profiles set as boundary conditions at the wind inlet boundary. This means that a large part of the computational domain is wasted (since it is required only to develop the atmospheric profiles) leading to a unnecessary increase of the CPU time. A simpler approach able to easily compute the correct profiles to be set as boundary conditions on the wind inlet boundary has been developed and it is discussed in the following.

Knowing the right profiles (that is, those corresponding to fully developed profiles for a given atmospheric stability class) allows to avoid the empty domain upwind the gas release location, thus strongly reducing the cell number and consequently CPU time.

The procedure for computing the fully developed profiles involves 2D periodic simulations over flat terrains. Periodic simulations use conditions obtained at the outlet boundary as an input for the inlet boundary and are provided as standard tools in CFD codes. This approach mimes, using a very short domain, a virtually infinite domain thus
providing fully developed profiles. Moreover 2D simulations are much faster than 3D ones and consequently this approach is definitely no time consuming.

Figure 1 and 2 show the results of this analysis with a comparison between the profiles required by the Monin-Obhukov similarity theory and those predicted CFD computations for the atmospheric conditions of two Prairie Grass experimental tests, PG 13 and PG 17 (see table 2). These tests are characterized either by neutral or very stable stratification. From the profiles predicted by the Monin-Obhukov similarity theory reported in Fig. 1 and 2 it is possible to observe the effect of atmospheric stability: neutral conditions mean larger effect of turbulence, which, in the RANS approach is resumed by the turbulent viscosity value. In neutral conditions, turbulent viscosity should increase with a linear profile along z accordingly with equation (6), reaching about 4 [Pa s] at the top of the domain. In stable conditions the $\mu_T$ profile is altered by the $\Phi_m$ contribution, and its maximum value is about 0.8 [Pa s]. This means that, as expected, stable stratification reduces atmospheric turbulence. Wind speed profiles reflect turbulent viscosity profiles: higher viscosity means more uniform wind speed, while low viscosity means larger velocity gradient.

We can see from Fig. 1 and 2 that there is a good agreement between the profiles required by the Monin-Obhukov similarity theory and those predicted by CFD computations implementing the modified k-$\varepsilon$ model. However, we can also see that increasing the height above ground, the effect of the upper boundary (that have been set as velocity inlet, with the air velocity tangential to the boundary surface itself) actually interferes in turbulent viscosity determination since, while assuring the right velocity value, this boundary bring to zero the flux of turbulent kinetic energy and turbulent dissipation rate. This problem can be easily faced by setting, as used, a domain high
enough to avoid this interference in the cloud region. For instance, in the investigated
gas releases, the SO$_2$ clouds height never exceed 5 [m] above ground, where turbulence
previsions are still acceptable.

As a rule of thumbs, a domain height at least double then the maximum cloud height
should be used in practical CFD computations.

We can also see that in neutral stratification the wall-boundary condition of infinite
derivative set by the CFD code at wall-type boundary conditions is well absorbed close
to the ground, and the whole profile can be considered reasonably flat. Moreover, the
good agreement found also in stable stratification conditions means that the
approximation of neglecting the $S_k$ term do not interfere heavily in profiles
determination, leading, instead, to a considerable improvement of the solution stability.

Finally, Figures 1 and 2 also report the results of the same CFD computations
performed using the standard k-$\varepsilon$ model. The large improvement obtained using the
developed approach is quite evident.

The k, $\varepsilon$ and $\nu$ profiles obtained from 2D periodic simulations have been imported in
fully 3D simulations over a flat retain. It has been found that these fully developed
profiles remain unchanged in the whole domain. This demonstrates that the proposed
approach allows for avoiding, in 3D CFD computations the simulation of an adjusting
zone upwind the gas release region, which is usually required for k, $\varepsilon$ and $\nu$ profiles
development. This allows to reduce domain dimensions and, therefore, computational
efforts.
5 Comparison with experimental data

Simulations of the SO$_2$ releases summarized in table 1 have been performed and the results are compared with the available experimental data, that is gas concentration at 1.5 [m] above ground at the plume centre, for several distances downwind. Since SO$_2$ was released in open field, the scenario has a symmetry plane. This allows imposing symmetry boundary conditions on this plane (which means null orthogonal derivatives) in order to simulate only half the domain with a lower computational efforts. The computational domain is about 800 [m] long, 30 [m] high and 50 [m] wide and the first attempt mesh counts about 700000 elements. After some preliminary simulations, the mesh has been adapted for case-by-case with a selective mesh refinement: only a cluster of grid elements covering the cloud region selected and refined. This approach saves a large number of elements in comparison with the refinement of the whole domain. Meshes with about 900000 – 10000000 elements have been obtained in this way and the results have been proved grid-independent. The boundary conditions used in all this simulations are summarized in table 3.

Figures 3 to 5 show the comparison between experimental data and predicted concentration profiles at 1.5 [m] above ground for each field test. As summarized in table 2, the experimental data refer to very different weather conditions, with wind speed raging from 1[m s$^{-1}$] to about 10 [m s$^{-1}$], and neutral, stable and very stable stratification. Despite this wide range of atmospheric conditions, there is a good agreement between model predictions and experimental data, even where only long distance (1000 [m]) and, therefore, low concentration (10 [ppm]), data are available. This means that the proposed approach is able to reproduce correctly the atmospheric stability class influence on gas dispersion. It should be stressed that the
results summarized in Figures 3 to 5 are true predictions, that is, no model parameters have been tuned against these experimental data. Moreover, since fully developed profiles have been used as boundary conditions at the wind inlet boundary (in other words, such profiles are not altered in open field) using the proposed approach, based on 2D periodic simulations, it has been possible to place the source term near the inlet boundary, avoiding the simulation of an initial adjusting zone usually required to allow the $k$, $\varepsilon$, $T$ and $v$ vertical profiles to fully develop and consequently reducing the computational time. This is especially useful when geometrical complexity rises grid dimension, and a reduction of the number of elements is especially appreciated.

From the results shown in Figures 3 to 5 it can be noted that at 1 [m] downwind from the release point, in neutral stratification SO$_2$ concentration has already reached a value of $10^{-4}$ [% mol], while in stable stratification this concentration is reached at about at 1.3 [m] downwind and in very stable stratification at 1.7 [m]. This is due to the lateral spreading of the SO$_2$ jet, that is influenced by atmospheric turbulence: a more turbulent stability class (D) means larger air entrainment and consequently a faster lateral spreading of the jet. Also this features is well predicted by the proposed model, as shown in figure 6, where iso-concentration profiles of SO$_2$ on the vertical symmetry plane for three different stability class, are reported. The faster the lateral spreading is, the sooner the iso-concentration profile reach an elevation on the ground of 1.5 [m], from 1 [m] to 1.7 [m] as discussed before from constant elevation concentration profiles.

The improvement of the proposed approach can be fully appreciated from figure 8, where CFD predictions obtained using the standard $k$-$\varepsilon$ model are also reported.
All the obtained results are summarized in figure 7, where a plot of CFD previsions versus experimental data is reported.

We can see that the proposed CFD model is able to predict experimental measurement within a factor of 2.

6 Conclusion

In this work a new approach for the consequences analysis of gas releases in neutral and stable atmospheric stratification through CFD modelling has been proposed. It provides ground wall-type boundary characterization and inlet boundary profiles in agreement with Monin-Obhukov similarity theory through the following steps:

1) a new source term is added to the $\varepsilon$ balance equation (5) depending on the stability class as:

$$S_\varepsilon(z) = \frac{\rho u_*^4}{z^2} \left[ \frac{(C_{z\varepsilon} - C_{1\varepsilon})}{K^2} \sqrt{C_\mu} - \frac{1}{\sigma_\varepsilon} \right] - \mu \frac{u_*^3}{2Kz^3} \quad \text{(neutral stratification)}$$

$$S_\varepsilon(z) = \frac{u_*^4 \rho}{z^2} \left[ \frac{(C_{z\varepsilon} - C_{1\varepsilon})}{K^2} \sqrt{C_\mu} \Phi^2 \frac{\Phi_\varepsilon}{\Phi_m} - \frac{1}{\sigma_\varepsilon} \left( \frac{2}{\Phi_m} - \frac{1}{\Phi_m^2} + \frac{T_r}{K T} \right) \right] - \mu \frac{2u_*^3}{Kz^3} \quad \text{(stable stratification)}$$

2) a new value of $C_S=0.979$ is used in the wall functions used for the wall boundary conditions.

Moreover, a new procedure has been proposed to compute $k$, $\varepsilon$, $T$ and $v$ vertical profiles at the wind inlet boundary. This requires periodic 2D simulations and allows to obtain fully developed profiles therefore avoiding the simulation of a large empty domain upwind the release point. The proposed approach has been successfully validated
through the comparison with several different field test of Prairie Grass series, involving neutral, stable and very stable stratification conditions.

**References**


Table 1: k-ε model constants [18].

<table>
<thead>
<tr>
<th>$C_{\varepsilon 1}$</th>
<th>$C_{\varepsilon 2}$</th>
<th>$C_{\varepsilon 3}$</th>
<th>$\sigma_k$</th>
<th>$\sigma_{\varepsilon}$</th>
<th>$C_{\mu}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.44</td>
<td>1.92</td>
<td>1.0</td>
<td>1.0</td>
<td>1.3</td>
<td>0.09</td>
</tr>
</tbody>
</table>
Table 2: Experimental set up for Prairie Grass test [19].

<table>
<thead>
<tr>
<th></th>
<th>PG 13</th>
<th>PG 17</th>
<th>PG 34</th>
<th>PG 41</th>
<th>PG 58</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Release rate</strong></td>
<td>[kg s(^{-1})]</td>
<td>0.0611</td>
<td>0.0565</td>
<td>0.0974</td>
<td>0.0399</td>
</tr>
<tr>
<td><strong>Release velocity</strong></td>
<td>[m s(^{-1})]</td>
<td>11.1</td>
<td>10.5</td>
<td>18.4</td>
<td>7.3</td>
</tr>
<tr>
<td><strong>Stability class</strong></td>
<td></td>
<td>F</td>
<td>D</td>
<td>D</td>
<td>E</td>
</tr>
<tr>
<td><strong>Wind speed (z = 2 [m])</strong></td>
<td>[m s(^{-1})]</td>
<td>1.3</td>
<td>3.3</td>
<td>9</td>
<td>4</td>
</tr>
<tr>
<td><strong>Ambient temperature</strong></td>
<td>[K]</td>
<td>293.15</td>
<td>300.15</td>
<td>304.15</td>
<td>294.15</td>
</tr>
<tr>
<td><strong>Monin-Obhukov length</strong></td>
<td>[m]</td>
<td>9</td>
<td>∞</td>
<td>∞</td>
<td>21</td>
</tr>
</tbody>
</table>
Table 3: Boundary conditions definition.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Type</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wind Inlet boundary</td>
<td>velocity inlet</td>
<td>wind velocity, temperature and turbulence values for the wind inlet flux</td>
</tr>
<tr>
<td>Wind Outlet boundary</td>
<td>pressure outlet</td>
<td>constant pressure outlet surface</td>
</tr>
<tr>
<td>Top boundary</td>
<td>velocity inlet</td>
<td>wind velocity, tangential to the surface</td>
</tr>
<tr>
<td>Symmetry boundary</td>
<td>symmetry</td>
<td>zero derivative value for all the variables</td>
</tr>
<tr>
<td>Lateral boundary</td>
<td>velocity inlet</td>
<td>wind velocity, tangential to the surface</td>
</tr>
<tr>
<td>Ground boundary</td>
<td>wall</td>
<td>no slip boundary, roughness specification, fixed temperature</td>
</tr>
<tr>
<td>Gas inlet boundary</td>
<td>mass flow inlet</td>
<td>mass flow, temperature and turbulence values for the gas inlet flux</td>
</tr>
</tbody>
</table>
Figure 1: 2D periodic simulation results for PG-17 test with neutral stratification.
Figure 2: 2D periodic simulation results for PG-13 test with stable stratification.
Figure 3: Comparison between field tests experiments (•) and CFD model predictions with the modified k-ε model (-); stability class D, neutral stratification.
Figure 4: Comparison between field tests experiments (•) and CFD model predictions with the modified k-ε model (-); stability class E, stable stratification.
Figure 5: Comparison between field tests experiments (●) and CFD model predictions with the modified k-ε model (-); stability class F, very stable stratification.
Figure 6: Iso-concentration ($10^{-4}$ [% mol]) curves on the vertical symmetry plane for three different stability classes.
Figure 7: Parity plot of the modified CFD model predictions VS experimental data. Dashed lines delimitate the region where the error is lower a factor of 2, that is $C_{exp}/2 < C_{CFD} < 2 C_{exp}$. 
Figure 3: Comparison between field tests experiments, CFD model predictions with the modified k-\(\varepsilon\) model and CFD model prediction with the standard k-\(\varepsilon\) model; stability class D, neutral stratification.