# CFD modelling of dispersion in neutrally and stably-stratified atmospheric boundary layers : results for Prairie Grass and Thorney Island

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**Abstract:** It is a known problem that CFD models using the standard $k - \varepsilon$ turbulence model do not maintain the correct atmospheric boundary layer (ABL) profiles along a flat, unobstructed domain. The present work examines the impact of these errors in the ABL profiles on dispersion model predictions for three field-scale experiments from the Prairie Grass and Thorney Island datasets. The modified ABL profiles produced by the CFD model in the Prairie Grass experiments result in differences in the predicted concentrations of up to a factor of two, as compared to a reference model. For the Thorney Island experiment, the results for the standard $k - \varepsilon$ turbulence model are sensitive to the ground surface roughness and problems are identified in relation to the grid resolution near the ground. Industrial risk assessments involving atmospheric dispersion of toxic or flammable substances using CFD models should take into account these limitations of the $k - \varepsilon$ turbulence model.

**Keywords:** CFD; atmospheric boundary layers; ABLs; passive gas; dense gas; dispersion; Prairie Grass; Thorney Island.

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Simon Gant has a Master's in Mechanical Engineering from the Leeds University and a Doctorate in Computational Fluid Dynamics from the Manchester University. He is currently a Principal Scientist at the UK HSE's Laboratory, Buxton, where he is worked for the last 11 years on fluid flow analysis, incident investigations, support work on new guidance and standards, government-funded research and consultancy. His recent research topics have included: flammable mists, area classification, carbon capture and storage and atmospheric dispersion model validation.

Jean-Marc Lacome is a Research Engineer working at the INERIS since 2002. He has previously worked on air quality modelling at the Research Center of EDF and at the Aria Technologies Company. He has a PhD in the Atmospheric Chemistry and Physics from the University of Toulouse in 1994. His research interests mainly concern atmospheric physics and chemistry and the processes involving toxic material in confined and free atmosphere. He contributed to the definition of practices for atmospheric modelling within the context of risk assessment.

Benjamin Truchot is an Engineer specialising in fluid mechanics and thermochemistry with a PhD in Energy and Reactive Flows. He worked in risk modelling, mainly for tunnels and petrochemical installations, before joining INERIS. Between 2006 and 2011, he was an Engineer in the Accidental Risk Division of INERIS in the field of fire and ventilation. Since 2011, he has led the Fire and Dispersion unit at INERIS. He uses experimental approaches and numerical simulation. Recently, he coordinated the French national working group on atmospheric dispersion with 3D models. Finally, he is an INERIS emergency team Engineer.

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## 1 Introduction

There is a growing interest in the use of CFD to assess the risks posed by atmospheric releases of toxic and flammable gases from industrial sites, such as chemical plants and refineries (e.g., Pontiggia et al., 2009; Hansen et al., 2010). However, there are a number of challenges to be overcome in modelling these flows with CFD. The focus of the present work is on assessing the capabilities and limitations of the standard $k - \varepsilon$ turbulence model that is widely used in CFD codes for industrial risk assessments. One of the known problems with this model is that it is unable to preserve the correct atmospheric boundary layer (ABL) profiles throughout the length of the flow domain. Although the correct ABL profiles may be imposed at the inlet to the computational domain, they are progressively modified by the CFD model as the flow develops downwind of the inlet. The calculated ABL profiles eventually reach an equilibrium at some downwind distance, but they may not represent the required stability class and/or wind speed. The modification to the velocity and temperature profiles are not the only issue; the turbulence profiles (turbulent kinetic energy, $k$ and dissipation rate, $\varepsilon$) are also important, since they can have a significant impact on mixing and dilution. Stably-stratified ABLs are of primary interest, since turbulent mixing is reduced as compared to the levels seen in neutral boundary layers and they often produce the largest hazard distances in industrial risk assessments.

The standard constants for the $k - \varepsilon$ turbulence model were originally chosen to produce good predictions for a range of classical shear flows found in engineering, such as flows in ducts, boundary layers with imposed pressure gradients and flows over a spinning disc (Jones and Launder, 1974). As noted by Pope (2000), the constants used by the standard model represent a compromise and for any particular flow it is possible to obtain more accurate predictions by adjusting their values. The standard model constants were not designed for preserving the correct profiles in ABLs and various researchers have therefore proposed modifications specifically aimed at improving ABL predictions. Some have applied modifications by changing the $k - \varepsilon$ model constants (e.g., Duynkerke, 1988; Richards and Hoxey, 1993; Alinot and Masson, 2005; Vendel, 2011) whilst others have introduced additional source terms (e.g., Pontiggia et al., 2009; Parente et al., 2011). An important common feature of all these approaches is that they present complete models in which the inlet profiles, boundary conditions and turbulence model modifications are not treated independently but are designed to be consistent with each other. Despite this, Hargreaves and Wright (2007) noted that this important point was often disregarded in practice.

Perhaps one of the main reasons why self-consistent modelling approaches for ABLs are rarely used is due to the difficulty faced in coding these approaches, especially in general-purpose commercial CFD software. Complicated user-coding is almost a prerequisite of achieving a consistent ABL model as Hargreaves and Wright (2007) themselves demonstrated for the neutral ABL. The recent study by Batt et al. (2016) demonstrated that stably-stratified ABL profiles were more accurately maintained using the Alinot and Masson (2005) model as compared to the standard $k - \varepsilon$ model in the ANSYS-CFX CFD software, but that the ABL profiles still changed along the length of a 2 km long domain. The cause of the remaining differences was attributed to a lack of consistency in the boundary conditions (primarily, the wall functions). However, there were limited options available to modify these boundary conditions in ANSYS-CFX.

Another important consideration is that the modifications to the standard $k - \varepsilon$ model aimed at improving predictions of ABLs may adversely affect the prediction of more complex cases, for example involving flow around obstacles. To overcome this problem, models have recently been proposed that take a zonal approach, where the turbulence model modifications are deactivated near obstructions (e.g., Balogh et al., 2012). The good practice guide published by the French Working Group (2015) on atmospheric dispersion modelling recommends that the standard constants are used with the $k - \varepsilon$ model for simulating the flow around obstacles.

The present work examines the effect of errors in the ABL profiles on passive and dense-gas dispersion using the general-purpose CFD software, ANSYS-CFX. Simulations are performed of two Prairie Grass experiments that involved releases of passive (neutrally-buoyant) tracer gas in neutral and stably-stratified conditions: Prairie Grass trials 33 and 36 (henceforth, referred to as PG33 and PG36). Simulations are also performed for one of the Thorney Island experiments (TI47), which involved a release of dense gas in a stably-stratified atmosphere. All three experiments involved continuous releases of gas in essentially flat, unobstructed terrain. Further details of the experiments can be found in the works of Barad (1958) and McQuaid and Roebuck (1985).

The aim of the present work is not to comprehensively evaluate the CFD model. To do so would require simulations of many more experiments and a statistical assessment of the model's performance (see, for example, Ivings et al., 2007). Nor is the aim to develop a validated model. Instead, the purpose of the present work is to investigate how changes in the ABL profiles affect the dispersion results.

The paper proceeds by briefly reviewing the boundary conditions used by CFD models to simulate atmospheric dispersion. This is followed by a description of the CFD model configuration for the Prairie Grass and Thorney Island experiments, then the results in terms of the ABL profiles and concentrations for the three test cases and finally a summary of conclusions.

## 2 Review of boundary conditions for CFD models of atmospheric dispersion

### *2.1 Inlet boundary*

For the $k - \varepsilon$ turbulence model, the ABL is usually prescribed at the inlet boundary in terms of profiles for the mean streamwise velocity, $U$, mean temperature, $T$ (for the stably-stratified ABL) and turbulence quantities, $k$ and $\varepsilon$. For a neutral ABL, probably the most common set of profiles used for modelling atmospheric dispersion in industrial risk assessments are those of Richards and Hoxey (1993), which involve a log-law velocity profile. Models of a stably-stratified boundary layer are less frequently used in practice. When stable ABLs are modelled, they are usually based on profiles that use the Monin-Obhukov similarity theory modifications to the neutral case (e.g., Alinot and Masson, 2005). The assumption of constant shear stress means that the log-law-based wind profiles are only strictly valid within the surface layer, which is less than 100 m deep in stably-stratified ABLs. For some industrial risk assessments, particularly those involving terrain or obstacles, gas dispersion may not be restricted to the surface layer and it may be necessary to use a higher domain and a model that is also appropriate above the surface layer. Different approaches have been proposed to extend ABL profiles above the surface layer, often by extensions to the Monin-Obukhov similarity theory or by profile matching. Several of these options are discussed by Optis et al. (2014).

## *2.2 Ground boundary*

The wall functions employed in ANSYS-CFX for the $k - \varepsilon$ model (which are similar to those present in many commercial CFD codes) are based on an assumed log-law profile for the mean velocity profile, with the surface roughness incorporated in terms of an equivalent sand grain roughness length, $k_s$. The value of $k_s$ can be approximated as about 30 times the aerodynamic roughness length, $z_0$, i.e., $k_s \approx 30\ z_0$. There is a limit on the maximum roughness length in ANSYS-CFX requiring that $k_s$ must be less than half the height of the near-wall grid cell. Effectively, this restriction means that it is not possible to use a fine grid with a rough wall.

For example, to model the flow over low crops and occasional large obstacles, a surface roughness length of $z_0 = 0.1$ m should be used (Uijt de Haag and Ale, 2005). This equates to a sand-grain roughness length of $k_s = 3$ m and a minimum cell height in ANSYS-CFX of 6 m. If the purpose of the simulation is to model dense-gas dispersion, it will be unacceptable to use such a coarse mesh, since the depth of the gas cloud may be resolved by only one cell.

Various methods to overcome this problem are discussed by Blocken et al. (2007). One option is to use a wall function that uses $z_0$ directly, rather than $k_s$ (see, for example, Richards and Hoxey, 1993). This approach allows for the use of a much smaller near-wall cell. However, $z_0$-based wall functions cannot be easily implemented in commercial CFD codes such as ANSYS-CFX. It is also unclear how to interpret the flow predictions near the wall when this approach is used. The aerodynamic roughness length, $z_0$, represents the height at which the mean velocity, when extrapolated towards the ground, falls to zero. It does not represent the physical size of the unresolved obstacles, which are typically around ten times the height of $z_0$. The CFD model with a $z_0$-based wall function may capture the overall effect of the rough wall on the ABL, but it will still not resolve the localised variations in velocity or concentration through the unresolved roughness elements, which may be important in the context of dense-gas dispersion of flammable or toxic substances.

## *2.3 Top boundary*

Different approaches have been proposed for the top boundary condition in CFD models (i.e., the sky). These include expressions for the shear stress (e.g., Hargreaves and Wright, 2007; Parente et al., 2011), an inlet condition (e.g., Alinot and Masson, 2005; Blocken et al., 2007; Pontiggia et al., 2009), symmetry (e.g., Franke et al., 2007), flux (e.g., Vendel, 2011) or pressure (e.g., Montavon, 1998). It is generally accepted that the top boundary of the computational domain should be as far away from the flow field of interest as possible in order to minimise its effects. Franke et al. (2007) recommended that the domain height should be at least five times the height of the largest obstacle whilst Pontiggia et al. (2009) recommended that in dispersion simulations it should be at least double the maximum gas cloud height.

### 2.4 Outlet boundary

At the ABL outlet boundary, CFD models commonly apply a constant-pressure condition. For the special case of neutral ABL with a CFD model that adopts a Boussinesq treatment for buoyancy effects (where density differences are accounted for solely in a buoyancy force), the relative pressure can be set to zero at the outlet, since the air density is constant. For all other cases, it is necessary to apply a pressure profile to avoid unphysical flow behaviour. This includes cases where the atmosphere is neutral but the air is treated as an ideal gas (since the density varies with height). For stably-stratified ABLs, the pressure profile requires integration of the temperature or density profile (see Vendel, 2011). All other variables on the outlet are usually assigned a zero-gradient condition across the outlet boundary.

Further information on boundary conditions can be found in the good practice guidelines published by the (French Working Group, 2015) and the COST Action 732 (Franke et al., 2007).

## 3 CFD model configuration

The CFD simulations presented here were all performed using ANSYS-CFX version 15. The configuration of the CFD model for the three test cases are summarised in Table 1. In all of the simulations, the wind speed and direction were modelled as constant, i.e., wind-meandering was not taken into account.

**Table 1** Conditions for the three test cases

| *Trial* | *PG33* | *PG36* | *TI47* |
|---|---|---|---|
| Atmos. stability (Pasquill class) | Neutral (D) | Stable (F) | Stable (F) |
| Source temperature (K) | 302.15 | 293.15 | 287.45 |
| Source elevation (m) | 0.45 | 0.45 | 0 |
| Source diameter (m) | - | - | 2 |
| Spill rate ($kgs^{-1}$) | 0.0947 | 0.04 | 10.22 |
| Wind speed ($ms^{-1}$) | 8.5 | 1.9 | 1.5 |
| Wind reference height (m) | 2 | 2 | 10 |
| Roughness length, $z_0$ (m) – ABL | 0.006 | 0.006 | 0.01 |
| Roughness length, $z_0$ (m) – wall | 0.006 | 0.006 | 0.0008 and smooth |
| Friction velocity ($ms^{-1}$) | 0.585 | 0.107 | 0.0378 |
| Domain size (m × m × m) | 2,000 × 100 × 30 | 2,000 × 100 × 30 | 1,000 × 800 × 10 |
| Total grid nodes (millions) | 1.6 | 1.6 | 2.9 |
| Near-wall cell height (m) | 0.4 | 0.4 | 0.05 |
| Turbulence model | Standard $k – \varepsilon$ | Standard $k – \varepsilon$ | Standard $k – \varepsilon$ and A-M |

Notes: Standard $k – \varepsilon$ = default ANSYS-CFX version of $k – \varepsilon$ using coefficients from Jones and Launder (1974)
A-M = Alinot and Masson (2005)

The CFD boundary conditions are summarised in Table 2. The ABL profiles proposed by Lacome and Truchot (2013) were applied at the inlet. These incorporate the velocity profile of Gryning et al. (2007) and $k$ and $\varepsilon$ profiles that are modified so that the friction velocity depends on height. The friction velocities given in Table 1 are not the experimental values but are instead the values calculated from the Gryning et al. (2007) velocity profile using the reference wind speed values. For the stably-stratified cases (PG36 and TI47), the temperature profile at the inlet was specified using the approach taken by Alinot and Masson (2005).

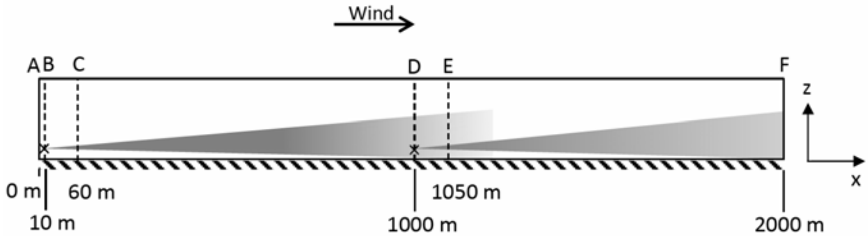
**Table 2** Boundary condition summary

| *Boundary* | *Condition* |
|---|---|
| ABL inlet | Profiles for $u$, $k$, $\varepsilon$ (PG33) and $T$ (PG36, TI47), $z_0$ as calculated in experiments |
| ABL outlet | Height dependent relative pressure. Zero gradient other variables |
| Top | Inlet boundary for $u$, $k$, $\varepsilon$ (PG33) and $T$ (PG36, TI47) |
| Sides | Symmetry |
| Ground | Rough wall $k_s$ value, dependent on nearwall cell height |

For the top boundary of the flow domain, an inlet boundary condition was used with values of $U$, $k$, $\varepsilon$ and $T$ prescribed from the ABL inlet profiles. A height-dependent pressure profile was imposed on the outlet boundary which was calculated by integrating the temperature profile following the approach taken by Vendel (2011). On the bottom boundary, two values are shown in Table 1 for the roughness length, $z_0$. The first is for the ABL inlet profiles and the other is for the ground surface boundary condition within the CFD model. For the two Prairie Grass cases, these two values were identical because the size of the smallest near-wall cell was acceptable. However, for the Thorney Island test case, the $z_0$ value of 0.01 m would have required a near-wall cell size of 0.6 m in ANSYS-CFX, which was unacceptable, since the height of the dense gas cloud in the experiments was only approximately 1 m. Therefore, a fine grid was used with a near-wall cell height of 0.05 m, which necessitated a smoother wall in the CFD model, with $z_0$ = 0.0008 m. To assess the effect of this choice of roughness length on the dispersion results, the Thorney Island case was also simulated with a perfectly smooth wall (i.e., a roughness length of zero).

For the two Prairie Grass cases, the source was modelled as a point source located on the centreline of the domain at a height of $z$ = 0.45 m. The sulphur dioxide tracer gas was modelled as a passive scalar, i.e., the presence of the gas had no influence on the calculated velocity, turbulence or temperature fields. To investigate the influence of the developing ABL profile on the results, two sets of simulations were performed: one denoted ‘fixed’ where the ABL profiles were fixed throughout the domain to be the correct inlet profiles (i.e., the CFD model did not solve for $U$, $k$, $\varepsilon$ and $T$, only the passive scalar) and another where the CFD model calculated the $U$, $k$, $\varepsilon$ and $T$ profiles (by solving the transport equations for $U$, $k$, $\varepsilon$, $T$ and the passive scalar). In the latter simulations, to investigate how the distance upstream of the source influenced the results, two separate passive scalars were released at different locations in the CFD domain: one at a location 10 m downwind from the inlet boundary and another at 1,000 m downwind. This setup is shown in Figure 1 with the sources at 10 m and 1,000 m indicated as locations B and D, respectively. Also shown in Figure 1, to facilitate later discussion of the Prairie Grass results are the following locations: the inlet boundary, A, the outlet, F and measurement locations at 60 m, C and at 1,050 m, E.

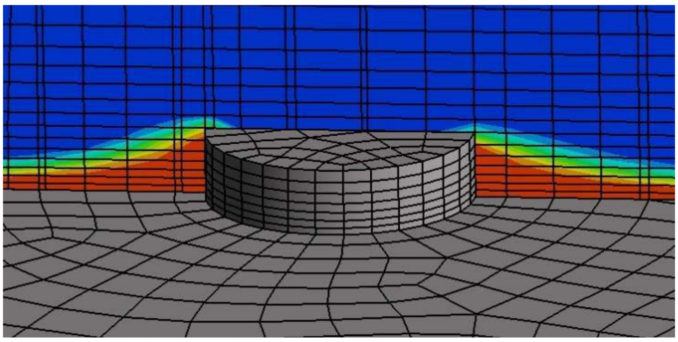
**Figure 1** Diagram of the *z*-*x* centre plane of the computational domain used in the Prairie Grass simulations showing domain inlet and outlet (A and F), two passive scalar point sources at 10 m and 1,000 m (B and D) and two measurement locations at 60 m and 1,050 m (C and E), 50 m downwind of each source




Note: Not to scale.

In the Thorney Island experiments, a mixture of 32% Freon and 68% nitrogen (with a density of about twice that of air) was released through a disc-shaped opening 2 m in diameter with a 2 m diameter capping disc 0.5 m above the opening. The capping disc was supported using radial fins parallel to the gas flow. In the CFD model, the source was resolved in the geometry and modelled as a mass flow inlet on the vertical walls of a cylinder of diameter 2 m and height 0.5 m as shown in Figure 2. Simulations were performed both with and without the presence of the dense gas, to assess how the ABL profiles changed along the length of the flow domain, due to the presence of the dense gas.

**Figure 2** Enlarged image with dimensions of the source geometry and computational mesh used in the Thorney Island simulations (see online version for colours)



The mesh for the Prairie Grass simulations was composed of hexahedral cells aligned with the wind direction. The near-wall cell height was 0.4 m and cell heights increased gradually in the vertical direction with a growth rate of approximately 6%. The length of the domain meant that the cells were stretched horizontally but the aspect ratio was less than or equal to ten in the regions of interest. For the Thorney Island test case, the mesh consisted of a mixture of hexahedral and prism-shaped cells. The mesh was refined in the horizontal directions near the source and there were seven cells spanning the height of the inlet face. The smallest near-wall cell height was 0.05 m, which was necessary in order to resolve the dense gas cloud and the vertical growth rate in cell height was approximately 10%. The small cell height near the ground meant that the aspect ratio of the cells was very large. To try to reduce the aspect ratio of the cells without producing a very large mesh, the length of the computational domain was reduced to 1 km, but nevertheless the cell aspect ratios were still very large (up to 100) and in excess of the factor of ten recommended in the French Working Group (2015) good practice guidelines.

The standard unmodified $k - \varepsilon$ turbulence model was used in all cases. For the two Prairie Grass cases, a second-order accurate numerical scheme was used for $U$, $k$, $\varepsilon$, $T$ and the passive scalar, in all simulations, as recommended by the good practice guidelines. For the Thorney Island test case, satisfactory numerical convergence could not be achieved with a second-order accurate numerical scheme throughout and so a first-order order numerical scheme was used for $k$ and $\varepsilon$. The convergence issues were likely to have resulted from the use of high-aspect ratio cells and it may have resulted in some artificial (numerical) diffusion.

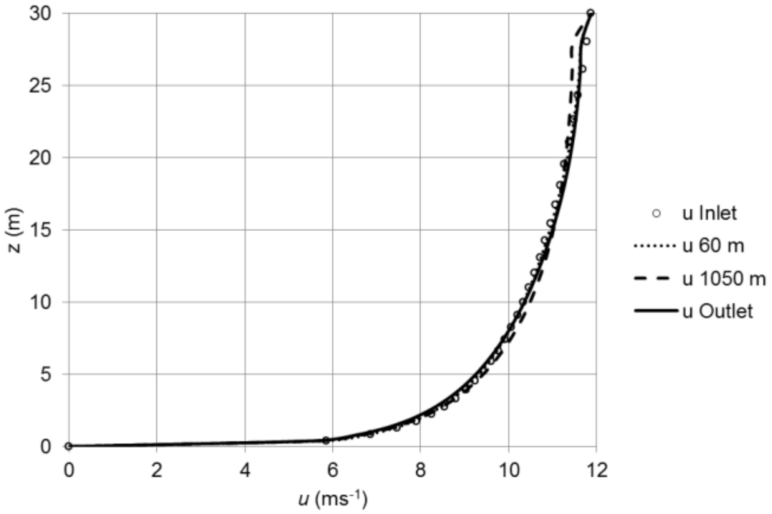
## 4 Predicted ABL profiles

The results for the neutral Prairie Grass PG33 case presented in Figure 3 show that the ABL profiles were well maintained along the length of the 2 km long computational domain with the exception of the turbulence kinetic energy. The profiles are shown at the inlet and outlet (locations A and F in Figure 1) and also at distances of 60 m (location C) and 1,050 m (location E). Figure 3(b) shows that the turbulence kinetic energy profile changed significantly during the first 1,000 m. The value of $k$ increased very near to the ground but decreased at higher elevations. This trend is similar to that shown by Hargreaves and Wright (2007) for a neutral ABL, but they did not observe such a large decrease in $k$ with height.

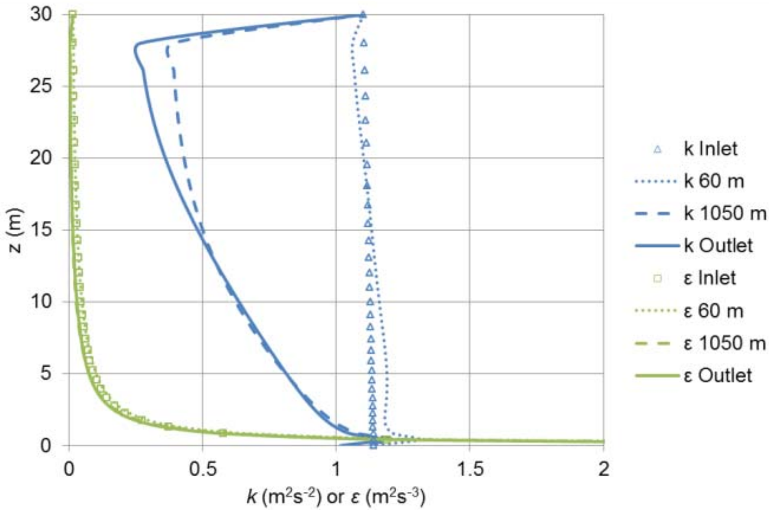
For the stably-stratified Prairie Grass PG36 case, Figure 4 shows that all of the profiles change with distance downwind of the inlet. The velocity and temperature profiles [Figure 4(a)] both increase near the ground and decrease above a height of around 5 m. The turbulence profiles [Figure 4(b)] generally increase below about 20 m and decrease above this height. At a downwind distance of 60 m (location C in Figure 1), the velocity and temperature profiles are similar to those at the inlet. However, the $k$ and $\varepsilon$ profiles are different from the inlet profiles at this point [Figure 4(b)]. The turbulence profiles change more quickly with distance downwind in the stably-stratified case than in the neutral case.

The CFD results are presented for the Thorney Island TI47 case in Figure 5 using the standard $k - \varepsilon$ model and two different roughness lengths ($z_0$ = 0.0008 m and smooth). The results show that the ABL profiles are not maintained along the length of the 1 km long domain in either the rough or the smooth case. The turbulence levels are higher for the rough wall case [Figure 5(b)], as expected.

**Figure 3** CFD results for Prairie Grass (PG33) with a neutral ABL, profiles are shown at the inlet (A), 60 m (C), 1,050 m (E) and at outlet (F) of the domain for (a) velocity, *u* and (b) turbulence kinetic energy, *k* and turbulence dissipation rate, *ε* (see online version for colours)

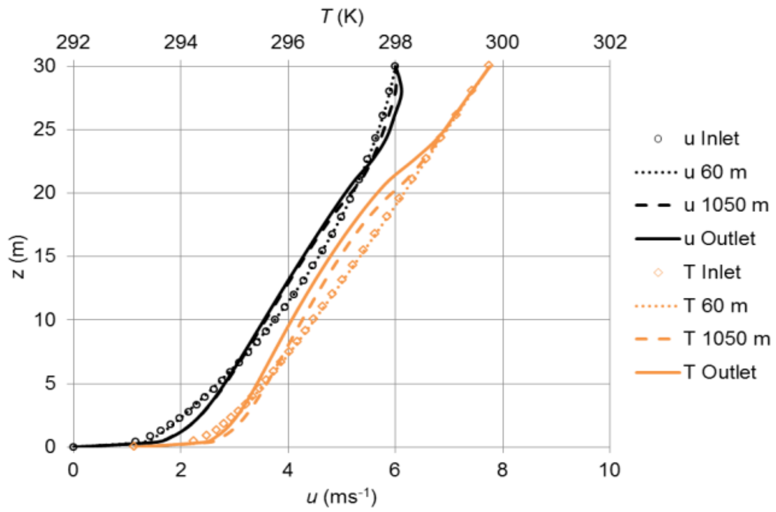



(a)

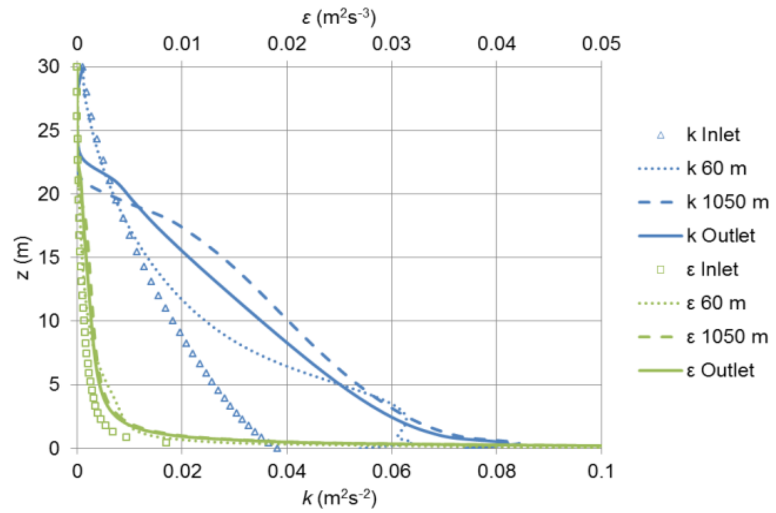



(b)

**Figure 4** CFD results for Prairie Grass (PG36) with a stably-stratified ABL, profiles are shown at the inlet (A), 60 m (C), 1,050 m (E) and at outlet (F) of the domain for (a) velocity, $u$ and (b) turbulence kinetic energy, $k$ and turbulence dissipation rate, $\varepsilon$ (see online version for colours)

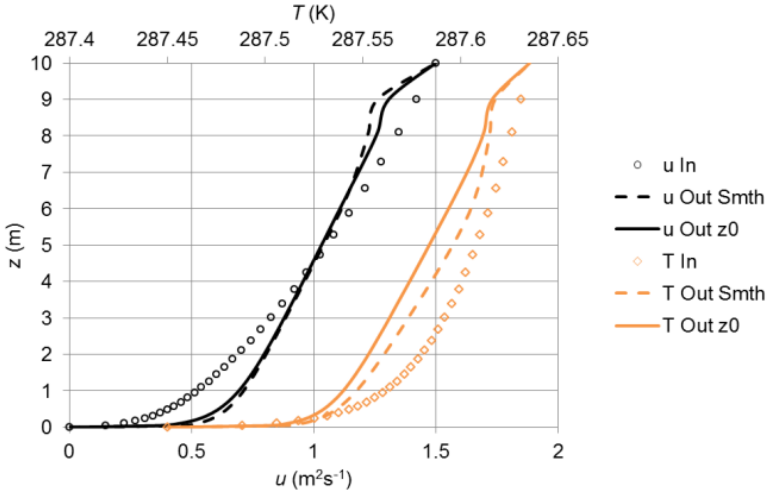



(a)

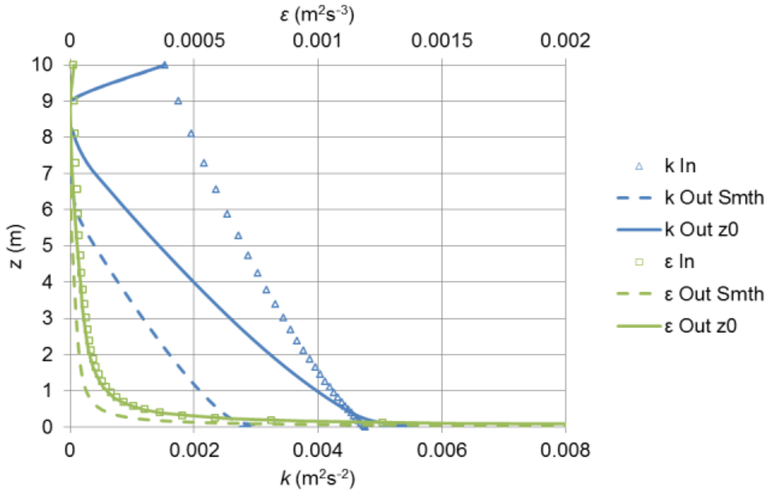



(b)

**Figure 5** CFD results for Thorney Island TI47 ABL profiles at the inlet of the domain and at the outlet using standard $k - \varepsilon$ with a rough wall (z0) and a smooth wall (Smth) (a) velocity $u$ and temperature $t$ and (b) turbulence kinetic energy $k$ and turbulence dissipation rate $\varepsilon$ (see online version for colours)




(a)

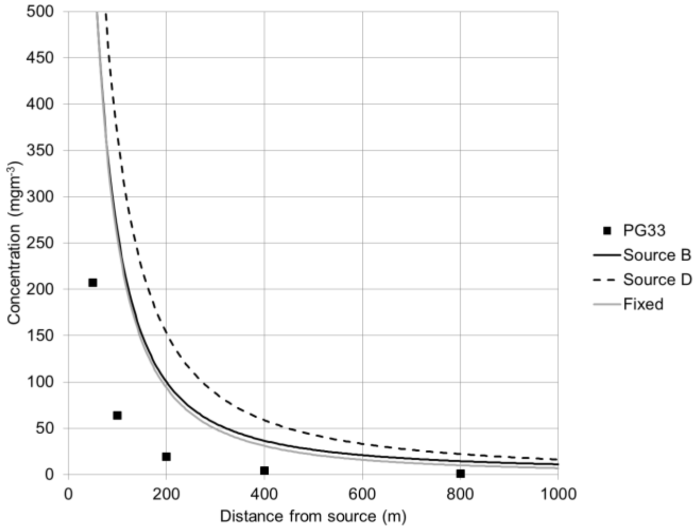



(b)

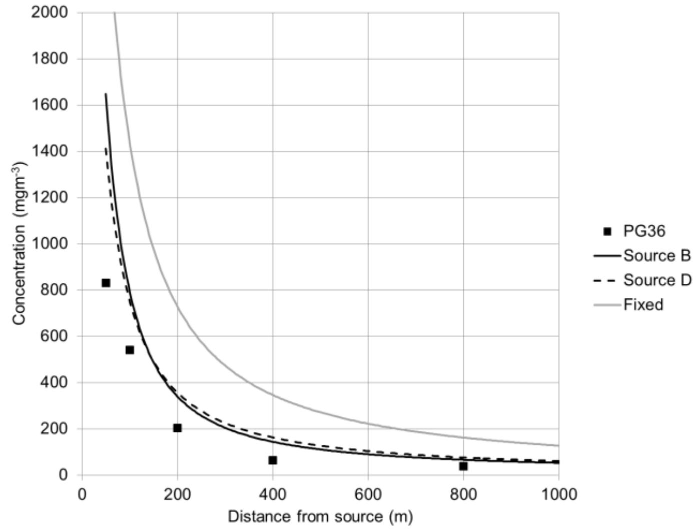
## 5 Predicted concentrations

The predicted centreline concentrations for the two Prairie Grass cases are given in Figure 6. These concentrations were output from the model at a height of 1.5 m, which is the same height as the measurements. For the neutral case (PG33), Figure 6(a) shows that predicted concentrations from the scalar released at source B, near the inlet, are practically identical to those produced using the fixed ABL profiles. However, the results from the scalar released at source D, 1,000 m downstream of the inlet, are up to 50% higher. This behaviour is consistent with the trends shown in the turbulence profiles [Figure 3(b)] and it demonstrates that changes in the ABL profiles along the length of the domain have an impact on the dispersion behaviour. In comparison to the experimental data, the predicted concentrations are between 3 and 30 times larger than the measurements in the neutral case, which suggests that mixing is underestimated.

**Figure 6** Predicted results for Prairie Grass concentrations downwind of the source along the centreline at a height of 1.5 m for (a) neutral ABL (PG33) and (b) stably-stratified ABL (PG36)




(a)

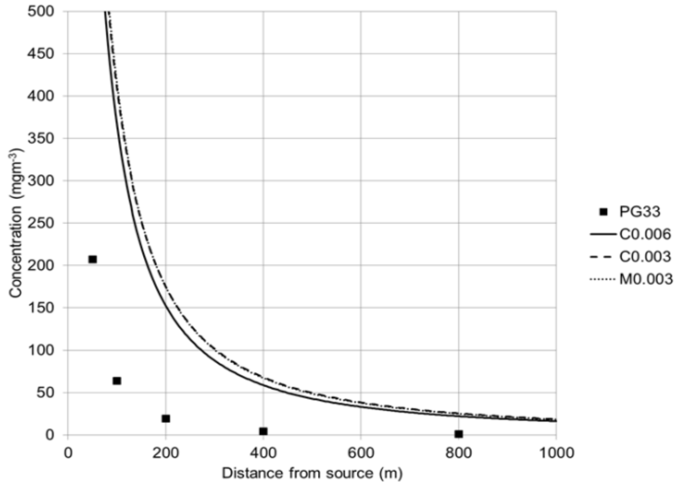



(b)

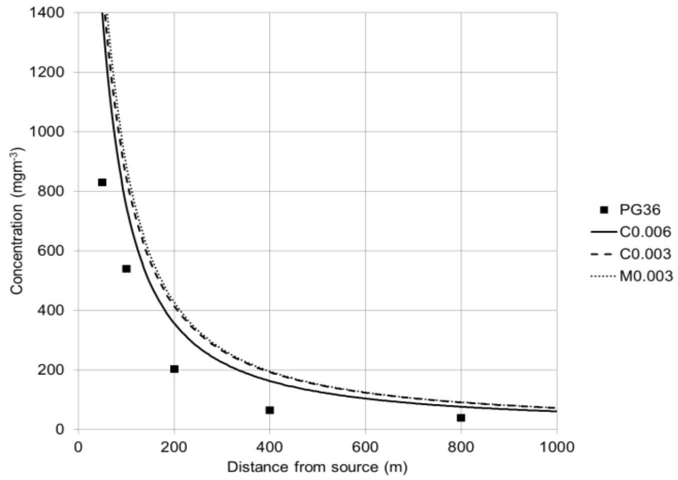
Note: Source B is at 10 m and source D is at 1,000 m.

For the stably-stratified Prairie Grass PG36 case, Figure 6(b) shows that concentrations from the scalar released at source B and source D are practically identical, but that both concentrations are around a factor of two lower than the concentrations obtained with the fixed ABL profiles. Again, this is consistent with the turbulence profiles shown in Figure 4(b). In comparison to the experimental data, the predicted concentrations are in closer agreement with the measurements when the $U$, $k$, $\varepsilon$ and $T$ equations are solved rather than when the nominally 'correct' fixed ABL profiles are used. There are several possible reasons for this behaviour, such as the absence of wind meandering effects in the model. The source B and D results in Figure 6(b) may be an example of a model appearing to be 'right for the wrong reasons'.

**Figure 7** Prairie Grass concentrations downwind of source D along the centreline at a height of 1.5 m for coarse mesh with correct roughness length (C0.006) and coarse and medium mesh with smaller roughness length (C0.003 and M0.003) for (a) neutral ABL (PG33) and (b) stably-stratified ABL (PG36)



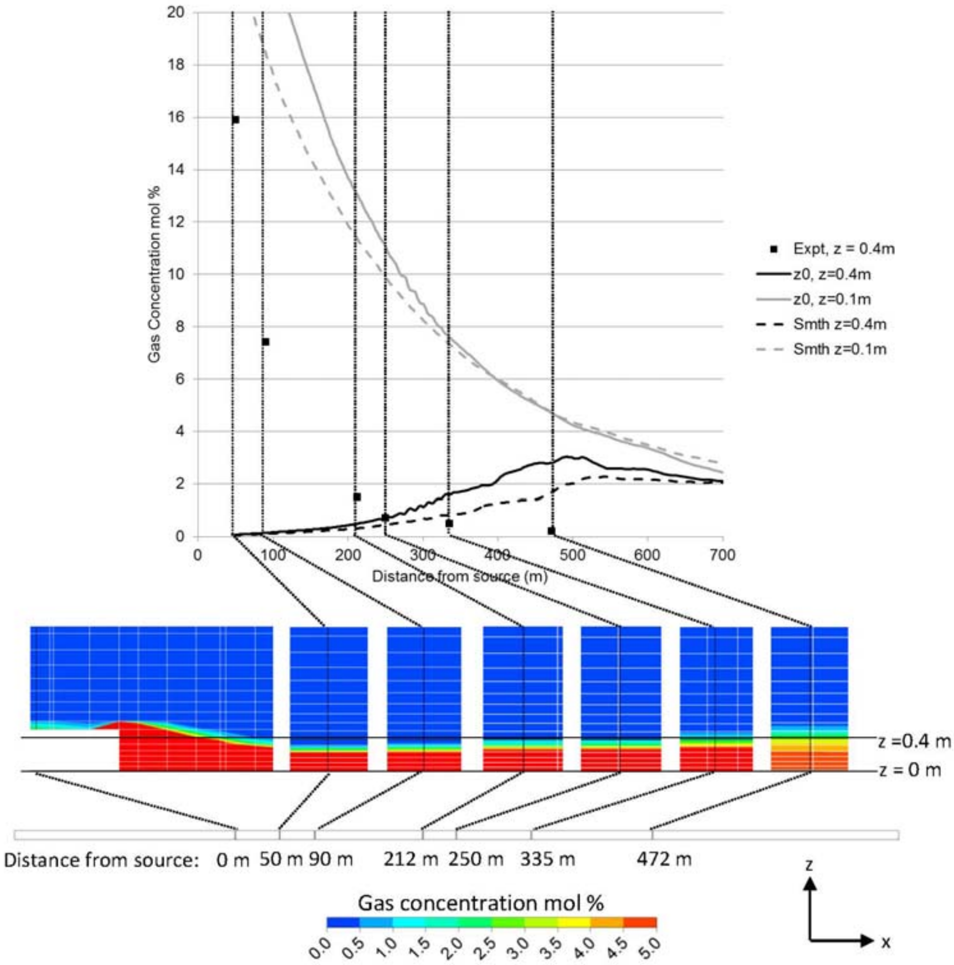

(a)




(b)

Sensitivity tests were performed with a finer mesh and lower roughness length for the two Prairie Grass cases and these are summarised in Table 3 and Figure 7. In both the neutral and stably-stratified cases, the concentration was insensitive to the grid resolution but it was somewhat affected by the choice of surface roughness. There was a 7% to 15% increase in concentration along the plume centreline when the roughness length was reduced from 0.006 m to 0.003 m.

**Figure 8** Predicted results for Thorney Island TI47 concentration (mol %) downwind of the source along the centreline at $z = 0.4$ m and $z = 0.1$ m for the model with roughness (z0) and with a smooth wall (Smth) (see online version for colours)




Notes: The experimental measurements (Expt) were at height $z = 0.4$ m. Also shown are contours of predicted concentration on vertical slices at various downwind locations. The outline of the grid cells are shown on these contours in white.

The predicted concentrations for the Thorney Island test case are shown in Figure 8. The concentrations were output from the CFD model at two heights: a height of 0.4 m, which corresponded to the height where the concentrations were measured in the experiments, and a lower height of 0.1 m. The purpose of showing the concentrations at the lower height was to help show the strong vertical gradient in concentration. Figure 8 also shows concentration contours on a vertical slice through the simulation on the centreline plane, at various different downwind locations.

The graph in Figure 8 shows that the choice of roughness length affected the predicted concentrations with a maximum difference of a factor of two between the rough and smooth CFD model results. In both cases, the predicted concentrations were considerably lower than the measurements near the release point. Beyond a distance of around 250 m downwind from the source, the CFD models significantly over-predicted the measurements. The concentration contours show that the predicted plume was very shallow in the near-field, with insufficient vertical mixing. This behaviour may be due to the model using a roughness length that was lower than the experimental value. However, the correct roughness length could not be used in the CFD model, since to do so would have required grid cells to be at least 0.6 m high (due to limitations of the wall-function), which would have meant that the shallow layer of dense gas was not adequately resolved. A further complication of the relatively fine grid was the high aspect ratio of the grid cells near the wall. These high aspect ratio cells may have resulted in numerical instabilities that produced the small undulations shown in the concentration profiles in Figure 8.

**Table 3** Mesh and roughness sensitivity tests undertaken for PG33 and PG36

| *Sensitivity test name* | *C0.006 (original)* | *C0.003* | *M0.003* |
|---|---|---|---|
| Roughness length, $z_0$ (m) – ABL | 0.006 | 0.006 | 0.006 |
| Roughness length, $z_0$ (m) – wall | 0.006 | 0.003 | 0.003 |
| Total grid nodes (millions) | 1.6 | 1.6 | 5.9 |
| Near-wall cell height (m) | 0.4 | 0.4 | 0.2 |

Attempts were made to model the Thorney Island TI47 case using the Alinot and Masson (2005) model in order to maintain the correct ABL profiles along the length of the domain. However, the solution was numerically unstable and it did not produce results. This was probably due to the fact that the tuning functions in the Alinot and Masson (2005) model produced unrealistically large source terms in the $k$ and $\varepsilon$ transport equations in the regions of the flow where the dense gas produced strong density gradients. The Alinot and Masson (2005) model was developed for stably-stratified ABLs without the presence of any dense gas. Future work could consider modifying the model equations or using a zonal approach. A mesh sensitivity test was also attempted, but increasing the number of nodes in the vertical direction led to increased problems with numerical stability.

## 6 Conclusions

The results presented here have demonstrated that CFD simulations using the standard $k - \varepsilon$ turbulence model produce changes to the ABL profiles along the length of a 1 km or 2 km long CFD domain which affect predicted gas concentrations. In the neutral Prairie Grass PG33 case, these changes were minimal if the gas was released near to the inlet of the domain. However, if the gas was released further downstream, the predicted concentrations differed by up to 50% as compared to the reference case with the 'correct' ABL profiles. In the stably-stratified PG36 Prairie Grass experiment, the predicted concentrations differed by up to a factor-of-two from the reference case, irrespective of whether the gas was released close to the inlet or further downwind.

The Thorney Island test case showed that CFD models face several challenges in modelling dense-gas dispersion over long distances. It was not possible to produce a reference case with correct ABL profiles, since the presence of the dense gas affected the flow behaviour. The CFD results from the standard $k - \varepsilon$ turbulence model were in poor agreement with the measurements. This may have been due to the model using a smoother ground surface than was present in the experiments. Tests showed that the roughness length affected the predicted concentrations, but it was not possible to use the correct surface roughness value from the experiments, due to the limitations of the CFD wall functions and the need to use a fine near-wall grid.

The results presented here are consistent with previous studies that identified inherent limitations of CFD models based on $k - \varepsilon$ turbulence models for simulating ABLs. It is important that risk assessments using CFD results take into account the uncertainties introduced by the limitations of the $k - \varepsilon$ turbulence model and issues relating to surface roughness and grid resolution.

## Disclaimer

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