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CFD MODELLING OF DISPERSION IN NEUTRAL AND STABLE ATMOSPHERIC BOUNDARY LAYERS: RESULTS FOR PRAIRIE GRASS AND THORNEY ISLAND

Rachel Batt[1]*, Simon Gant*[1]*, Jean-Marc Lacome*[2]*, Benjamin Truchot*[2] *and Harvey Tucker*[1]

[1]Health and Safety Executive, Buxton, UK
[2]INERIS, Verneuil-en-Halatte, France

Abstract: The purpose of this paper is to assess the impact on dispersion model predictions of errors introduced by Computational Fluid Dynamic (CFD) models of Atmospheric Boundary Layers (ABLs). It is a known problem that CFD models using the standard *k*-*ε* turbulence model struggle to maintain the correct ABL profiles along the length of a flat, unobstructed computational domain. Appropriate ABL profiles may be imposed at the inlet but they are often progressively modified downwind by the CFD model until they no longer represent the specified stability class and/or wind speed. Various solutions have been proposed in the literature to address this issue, although many of them are complex and difficult to implement in commercial CFD software. Also, little is known about the impact of the ABL profiles on dispersion model predictions.

To examine this issue, CFD simulations are presented for two sets of field scale experiments: Prairie Grass and Thorney Island. The Prairie Grass cases considered involve continuous releases of a passive tracer in both neutral and stable ABLs. One of the reasons for studying these experiments is to compare dispersion predictions from a standard CFD solution to results obtained from fixing the ABL with prescribed profiles throughout the flow domain. This approach is only possible for passive releases, where the flow field is unaffected by the presence of the tracer gas. Simulations are then presented for a Thorney Island experiment which involved a continuous release of dense gas in a stable ABL.

The results show that the modified ABL profiles produced by the CFD models affect the predicted concentrations in most cases. The maximum differences range from 50% to a factor-of-two in the two Prairie Grass cases, although the differences are minimised in the neutral ABL by using a short upwind fetch in the CFD model. For the Thorney Island case, attempts were made to use a modified *k*-*ε* turbulence model to maintain the correct stable ABL profiles but the solution was numerically unstable and it failed to produce results. Results are presented for the standard *k*-*ε* turbulence model with two different roughness lengths, which produce different results. The inherent difficulties in resolving dense-gas flows over rough surfaces using CFD models are discussed.

Key words: *CFD, atmospheric boundary layers, passive gas, dense gas, dispersion, Prairie Grass, Thorney Island*

INTRODUCTION

There is growing interest in the use of CFD to assess the risks posed by atmospheric releases of toxic and flammable gases from industrial sites. However, there are a number of challenges to overcome in modelling these flows. A central problem is that CFD models with the standard *k*-*ε* turbulence model are unable to preserve the correct ABL profiles throughout the flow domain. The problem is particularly acute in modelling stable ABLs, which are of primary interest to industrial risk assessments, since they often produce the largest hazard distances.

A companion paper by Batt *et al*. (2016) explores different treatments for CFD boundary conditions and adjustments to the standard *k*-*ε* turbulence model to overcome the problems in sustaining the correct ABL profiles throughout the domain. The work shows that improvements can be obtained by using the modified *k*-*ε* turbulence model of Alinot and Masson (2005) with consistent boundary conditions, but the ABL profiles still change along the length of a 2 km long domain. The Batt *et al*. (2016) work focuses solely on the ABL profiles themselves and does not consider gas dispersion. The present work extends that work to consider passive and dense-gas dispersion. Two Prairie Grass experiments (Barad, 1958) in neutral (PG33) and stable (PG36) conditions and one Thorney Island trial (TI47, McQuaid and Roebuck, 1985) in stable conditions are simulated. These three cases do not provide a full picture of the CFD model's abilities: to do so would require simulations of many more experiments and a statistical assessment of the model's performance. The aim therefore is not to develop a validated model but to illustrate how changes in the ABL profiles affect dispersion results, with the experimental data providing a useful comparison measure.

CFD MODEL CONFIGURATION

The simulations were all performed using the ANSYS-CFX v15 commercial CFD code with grids constructed from prism-shaped cells and grid-refinement near the ground. Conditions for each of the simulations 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 modelled. Two values are shown in Table 1 for the roughness length, z_0: one for the ABL inlet profiles and one for the ground surface boundary condition within the CFD model. The reason these two values are different in the Thorney Island case is that the wall functions employed in ANSYS-CFX for the k-ε model (which are similar to those present in most CFD codes) have a limit on the maximum roughness length: the equivalent sand-grain roughness (which is approximately 30 times the value of z_0), must be less than half the height of the near-wall grid cell. For fine grids it is therefore necessary to use a smoother wall than is present in reality. In the Thorney Island case, the dense gas cloud was less than 1 m deep and 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 a z_0 of 0.0008 m, as compared to the experimental value of 0.01 m.

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)	2000 × 100 × 30	2000 × 100 × 30	1000 × 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-ε	Standard k-ε	Standard k-ε and A-M

Standard k-ε = default ANSYS-CFX version of k-ε using coefficients from Jones and Launder (1974)
A-M = Alinot and Masson (2005)
* The standard k-ε model used either $z_0 = 0.0008$ m or $z_0 = 0$ m and the Alinot and Masson (2005) used $z_0 = 0.0008$ m.

The ABL inlet profiles for the mean velocity and turbulence parameters (U, k and ε) were specified using the French Working Group profiles (Lacome and Truchot, 2013) and for the stable cases (PG36 and TI47) the temperature (T) profile was given by Alinot and Masson (2005).

An additional test was performed for TI47 with the inlet ABL profiles for U, k, ε and T all taken from Alinot and Masson (2005) with their modified k-ε model. The reason for this extra case was that previous work (Batt *et al*., 2016) showed that the model worked best with consistent inlet profiles. Other boundary conditions at the top, sides and outlet to the flow domain are the same as those used by Batt *et al*. (2016).

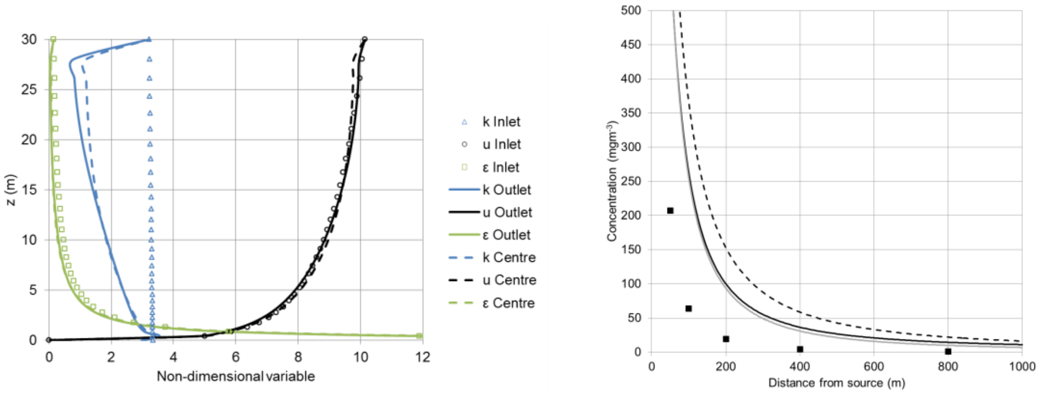
For the two Prairie Grass cases, the sulphur dioxide tracer gas was modelled as a passive scalar, i.e. the presence of the gas had no influence on the calculated flow field. To investigate the influence of the developing ABL profile on the results, two sets of simulations were performed: one denoted “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, ε and T, only the passive scalar) and another where the CFD model calculated the U, k, ε and T profiles (by solving the transport equations for U, k, ε, 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 injected at different locations in the CFD domain: one at 10 m downstream from the inlet boundary and another at 1000 m downstream. The results from these two scalars at 10 m and 1000 m are denoted “Full G1” and “Full G2”, respectively

In the Thorney Island simulations, the source of dense gas composed of 32% freon and 68% nitrogen, (with a density of about twice that of air) was released at a downstream distance of 250 m through a disc-shaped opening 2 m in diameter with a 2 m diameter capping disc 0.5 m above the opening. Simulations were also performed with no dense gas to assess how the ABL profiles changed along the length of the domain.

RESULTS

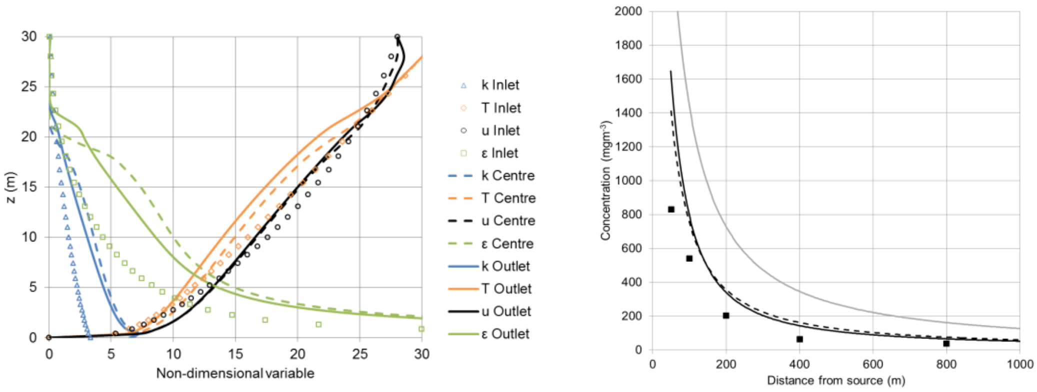
Prairie Grass

The results for the neutral Prairie Grass PG33 case, presented in Figure 1, show that the ABL profiles are well maintained, except for the turbulence kinetic energy which decreases downwind from the inlet. The predicted concentrations from the scalar released near the inlet (Full G1) are practically identical to those produced using the fixed ABL profiles. However, the results from the scalar released 1000 m downstream of the inlet are up to 50% higher, which demonstrates that minor changes in the ABL profiles along the length of the domain have an impact on the dispersion behaviour. All of the results predict concentrations between 3 and 30 times larger than the experiments, which suggest that mixing is globally underestimated.



(a) (b)

Figure 1 Predicted results for Prairie Grass PG33 (a) Dimensionless ABL profiles at the inlet, centre and outlet of the domain (b) Concentrations downwind of the source along the centreline at a height of 1.5 m



(a) (b)

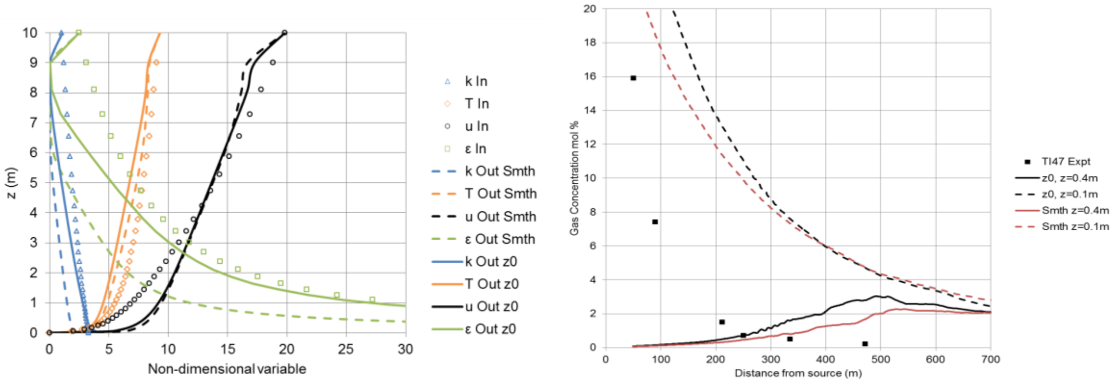
Figure 2 Predicted results for Prairie Grass PG36 (a) Dimensionless ABL profiles at the inlet, centre and outlet of the domain (b) Concentrations downwind of the source along the centreline at a height of 1.5 m

For the stable Prairie Grass PG36 case, Figure 2 shows that the velocity and temperature profiles change along the domain: both of them increasing near the ground and decreasing above a height of around 6 m. The concentrations from the two tracer releases near the inlet and 1000 m downstream are practically identical (Cases Full G1 and Full G2) but both are around a factor of two lower than the result obtained with the fixed ABL profiles. Again, all of the model predictions are higher than the measurements, which may be due to several factors, such as the assumed constant wind speed and direction.

Sensitivity tests were performed with finer meshes and lower roughness lengths for the two Prairie Grass cases (not presented here) which showed that the results were insensitive to the grid resolution but they were affected by the roughness value (a 7 - 15% increase in concentration along the plume centreline for a release from 1000 m when the roughness was reduced from 0.006 m to 0.003 m).

Thorney Island

Attempts were made to model the Thorney Island TI47 case using the Alinot and Masson (2005) turbulence 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 Alinot and Masson (2005) model's use of tuning factors that produce unrealistically large source terms in the *k* and *ε* transport equations in the regions of the flow where the dense gas produces strong density gradients. The model was developed for stable ABLs without the presence of any dense gas. Future work could consider modifying the model equations or using a zonal approach.



(a) (b)

Figure 3 Predicted results for Thorney Island TI47 (a) Dimensionless ABL profiles at the inlet of the domain and at the outlet, using standard *k*-*ε* with a rough wall and a smooth wall (b) 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). The experimental measurements (TI47 Expt) were at height $z = 0.4$ m

Results are presented for Thorney Island TI47 in Figure 3 using the standard k-ε model and two different roughness lengths (see Table 1 for details). Figure 3 (a) shows that the profiles are not maintained along the domain in either the rough or the smooth case with the smooth case showing significantly reduced turbulence levels, as might be expected. The predicted concentrations are shown in Figure 3 (b) at 0.4 m, the height at which the concentrations were measured in the experiments, and the arbitrary height of 0.1 m to show the strong vertical gradient in concentration. The results show that the roughness length has a modest effect on the predicted concentrations, with a maximum difference of a factor of two. In both cases, the predicted concentrations at 0.4 m are considerably lower than the measurements in the near-field, up to a distance of around 250 m downwind from the source, and further downwind the models significantly over-predict the measurements. The predicted plume is very shallow in the near-field with insufficient vertical mixing, which may be responsible for concentrations being over-predicted further downstream. 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 the wall-function limits), which would not have resolved such a shallow layer of dense gas. A further complication of the relatively fine grid used was that the length-to-height ratio of the grid cells near the wall was large (up to a hundred). These high aspect ratio cells may be partly responsible for the small undulations shown in the concentration profiles in Figure 3 (b).

CONCLUSIONS

The results presented here have demonstrated that CFD simulations using the standard k-ε turbulence model produce changes to the ABL profiles along the length of a CFD domain which affect the predicted gas concentrations. In the neutral Prairie Grass PG33 case, these changes were minimal if the gas was released near to the inlet to 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 “correct” ABL profiles. In the stable 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 orifice or further downwind.

The Thorney Island test case showed that CFD models face several challenges in modelling dense-gas dispersion over long distances in the atmosphere. It was not possible to produce a reference case with correct ABL profiles since the Alinot and Masson (2005) model was found to be numerically unstable and failed to produce results. CFD results from the standard k-ε 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 roughness value from the experiments due to the limitations of the CFD wall functions and the need to use a fine near-wall grid. Future work could examine the use of a porosity/distributed resistance model to overcome this problem.

The results are in line with previous studies which pointed towards inherent limitations of CFD models based on k-ε turbulence models for modelling atmospheric dispersion of passive and dense gases. It is important that risk assessments using CFD results take into account the uncertainties introduced by the limitations of the k-ε turbulence model and issues relating to surface roughness and grid resolution.

DISCLAIMER

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