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3-DIMENSIONAL MODEL PREDICTIONS FOR THE UPWIND BUILDING TRIAL OF THORNEY ISLAND PHASE II

D.M. DEAVES

Atkins Research & Development, Epsom, Surrey (Great Britain)

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Summary

This short contribution is concerned with three dimensional computer predictions of dense gas dispersion in obstructed flows. A brief review is given of the current status of 3D computer modelling, with special reference to the inclusion of turbulence effects. There follows a description of the computer program HEAVYGAS which was used to produce the predictions which form the main part of the paper. After some discussion of the results and comparison with data provided at one point near the building, the paper concludes with recommendations for future improvements in 3D hydrodynamic heavy gas computer codes.

1. Introduction

The objective of the second phase of the Thorney Island trials was to obtain data for the dispersion of heavy gas clouds around obstacles for comparison with and calibration of wind tunnel tests [1]. The modesty of this aim compared with that of Phase I — to validate mathematical models — reflects the general lack of faith in these models for such complex flows. Indeed, there is still considerable uncertainty even in the prediction of passive dispersion in the presence of obstructions [2] , without the added complications of density effects.

Evidently, the simple "box models", which describe unobstructed dense gas dispersion well, and can relatively easily be calibrated to full-scale data, cannot correctly model the physics of complex gas/obstacle interactions, and therefore cannot be expected to produce useful predictions. The best that can be done is to apply empirical corrections [3] obtained from full- or model-scale data for a particular class of problems.

Computer prediction of complex heavy gas flow therefore necessitates the use of full 3D hydrodynamic models [4] which solve a suitably modelled form of the Navier—Stokes equations. This paper briefly reviews some of the background to these methods, and presents results from one such computer model.

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2. Turbulence modelling for heavy gas dispersion

The downwind dispersion of a heavy gas cloud in a steady wind is generally characterised by a region in which the negative density gradient suppresses turbulent mixing, and this stratification not only affects the dispersion of the cloud, but also tends to modify the structure of the atmospheric turbulence. It is evident that, when a heavy gas cloud interacts with buildings, obstructions or complex terrain, the physical situation will include both turbulence enhancement e.g. in wakes of buildings, and turbulence suppression as noted above. The K-theory models [4] which are in use at present are unable to model this situation satisfactorily in any general formulation of the problem, since K has to be related to the local flow characteristics in an empirical way to account for all the complex interactions. An improvement on K-theory is the κ—ϵ turbulence model [5], in which transport equations (which implicitly incorporate the various interactive effects) are solved for both turbulence energy (κ) and dissipation (ϵ). The eddy diffusivity, K, is then obtained from the locally derived values of κ and ϵ.

Although κ—ϵ models are superior to standard K-theory, they still utilise the gradient diffusion relationship (concentration flux proportional to concentration gradient) in a region where diffusivities are very low, and therefore difficult to specify accurately. The algebraic stress model (ASM) [6] replaces this relationship with fundamentally derived algebraic expressions relating the various stresses and fluxes to all the velocity and concentration (or density) gradients. In principle, this model provides a more realistic representation of the physics. However, the modelling and solution techniques for ASM are not yet well enough advanced to facilitate its use in practical computer models.

3. The computer program HEAVYGAS

Atkins R & D have recently been developing a computer code incorporatint the κ—ϵ turbulence model for use in the prediction of heavy gas dispersion [5]. The program HEAVYGAS allows for the suppression (or enhancement) of turbulence due to density effects, and has been used in a range of situations, from internal ventilating flow [5] to the enhancement of dispersion by water spray barrier [7].

The main features of the program are:

(a) Computation of full flow field, allowing the presence of the gas and of obstacles to affect the air flow.
(b) Inclusion of turbulence suppression effects.
(c) 2D or 3D versions available.
(d) Steady-state or transient solution possible.

Although it is felt that the modelling used in HEAVYGAS is an improvement over standard K-theory, it is recognised that further development of the model is necessary in order to improve the accuracy of the predictions in complex flows. Possible future development is discussed in Section 5.

4. Predictions for Thorney Island Trial 29

In Trial 29, the mobile building (nominally 10 m cube, but actually 9 m cube in the trials) was located some 27 m upwind of the spill "point" i.e. the centre of the cylindrical gas tent. This configuration is shown in Fig.1., where the separation between the *edges* of building and gas tent is 20 m.

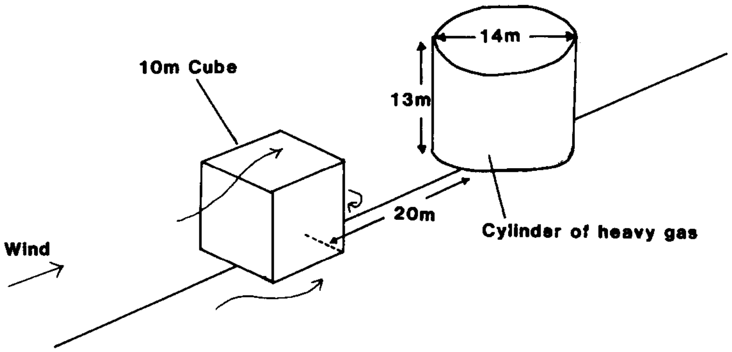

Fig.1. Layout of Thorney Island Phase II Trial 29.

The flow field was assumed to be symmetrical about the centre-line, thus requiring only half the region considered to be covered with grid nodes. There was a total of about 6,500 grid nodes, allowing a resolution of about 0.5 m close to the ground, and to any buildings. Although this grid resolved the gross features of the flow, it was not expected to predict, for example, the recirculation length behind the cube very accurately.

The computations were undertaken firstly for a steady-state wind field with a rigid cylinder in place. This was then used as the initial condition for a series of transient computations, with the gas released at time $t = 0$. The time-step was initially set at 1 s, but this was gradually increased as the transient effects became slower, thus saving computational effort.

Results are plotted in Fig.2 in the form of peak concentration (% by weight) vs. distance from the source for a number of different heights above the ground. There are two particular features to notice from this plot:

(a) The small increase in concentration as the building is approached. This only occurs for non-zero heights, and indicates the effects of gas being drawn into the building wake.

(b) The rapid decrease of concentration with height at any given downwind location. Detailed examination of the full computational results indicated that a suppression of turbulence was predicted at early stages of the transient close to the edge of the gas cloud. This suppresses vertical mixing, and ensures that most of the gas "slumps" under gravity, and remains close to the ground.

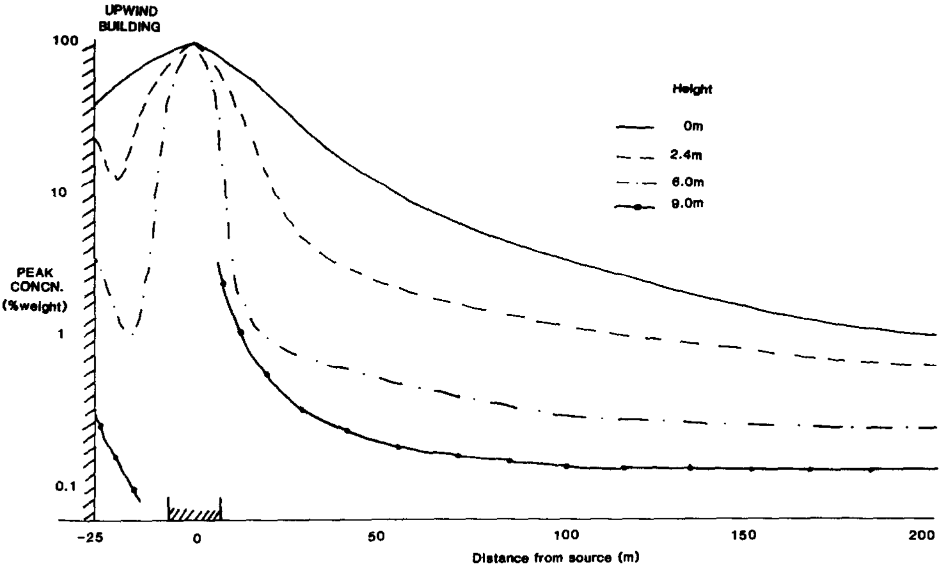

Fig.2. Computer prediction of peak concentration for Trial 29.

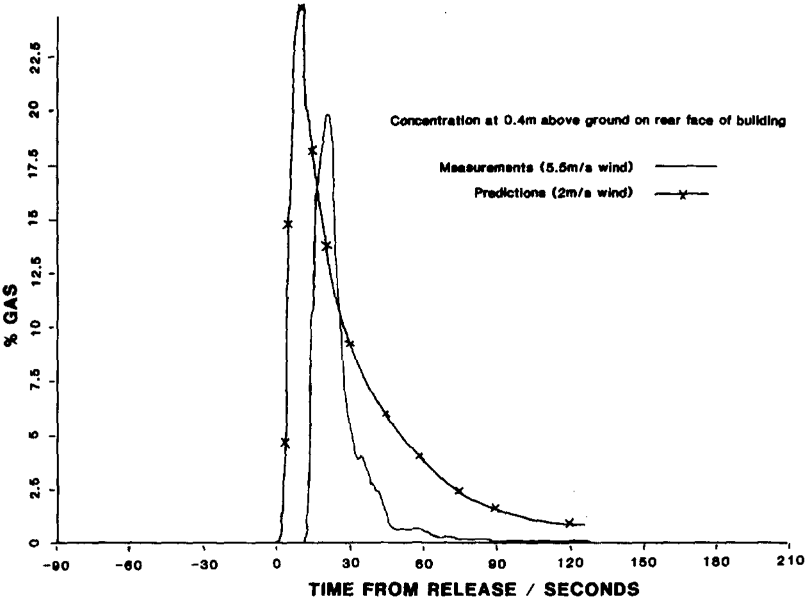

Fig.3. Comparison of HEAVYGAS predictions with hard copy data for Trial 29.

Since these computations were genuine predictions, undertaken some months before Trial 29 was completed, an assumed windspeed from the quoted range (2—5 m/s) was used. This was chosen as 2 m/s, since density effects are greatest at low windspeed, whereas the trial was performed in a 5.5 m/s wind. Although the results are therefore not strictly comparable, a sample comparison is given in Fig.3, which is a reproduction of a hard copy plot of the time history of concentration at the base of the rear of the building.

The predicted arrival time is much sooner, and the peak concentration higher, as is to be expected in a lower windspeed. The width of the peak, which is a measure of the residence time of the gas at the measurement point, is also rather greater in the predictions. For example, taking the "c % residence time", t_c, as (time at which concentration drops below c) – (time at which concentration rises above c), $t_{2.5}$ and t_5 are over-predicted by almost exactly the ratio of the windspeeds.

Thus, as far as they can be compared, the predictions show encouraging agreement with the full scale results.

5. Conclusions

The computer program HEAVYGAS has been used to predict the dispersion of a heavy gas in the vicinity of an obstruction. It has been demonstrated that the program incorporates such features as the suppression of turbulence, and correct modelling of building wakes, and is therefore capable of giving at least qualitatively correct predictions of complex heavy gas dispersion.

In order to improve the modelling to provide quantitatively accurate predictions, it is anticipated that further development is necessary. Development of the turbulence modelling, along the lines indicated in Section 2, will be necessary so that the physics should be more realistically modelled. Additionally, it is anticipated that numerical techniques will have to be improved both to deal with the new turbulence modelling formulation, and also to ensure that accurate and economical solutions are possible.

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