# COMPARISON OF THORNEY ISLAND DATA WITH PREDICTIONS OF HEGABOX/HEGADAS

#### J.S. PUTTOCK

Shell Research Ltd., Thornton Research Centre, P.O. Box 1, Chester, CH1 3SH (Great Britain) (Received October 20, 1986; accepted March 6, 1987)

#### Summary

The box model HEGABOX has been developed to simulate gravity-dominated dispersion behaviour soon after a sudden release of dense gas. It is used as a front-end to the HEGADAS dense gas dispersion model, and there is a smooth transition from the gravity-dominated phase to the region in which ambient turbulence has greater influence. Comparisons have been made between the model predictions and data from the instantaneous gas releases performed at Thorney Island. Various features of the data have been compared to give confidence in the applicability of the models; these include the time-development of the cloud-averaged concentration, peak concentration as a function of distance, and cloud speed. Far downwind, a slow rise to the peak concentration is predicted, as observed. The effective roughness length at the Thorney Island site is dependent on upwind terrain and therefore on wind direction. For low concentrations, the best predictions are obtained when this is taken into account.

### 1. Introduction

Although accidental releases of significant quantities of hazardous gases are rare, users of flammable or toxic gases need to understand what might happen if such a release occurred. A variety of mathematical models have therefore been developed to quantify the dispersion of dense gases in the atmosphere [1]. Data from field experiments involving spills of liquefied gases have been available for some time, and have been used in the validation of models [2,3]. In the Thorney Island experiments the release conditions were very different: the material was released as gas in an initially high cloud. They thus provide data for releases in which slumping with its associated mixing and time-dependence are important effects. Such conditions may be obtained in accidental releases – in low wind speeds, for example, or with a sudden release of a large quantity of gas.

The Thorney Island experiments each involved the release of about 2000  $m^3$  of gas with density normally about twice that of air [4]. The gas was initially contained in a 'tent' of 14 m diameter and 14 m high, whose sides dropped suddenly at the start of the experiment. The dispersion was monitored by an

extensive array of gas sensors and meterological instrumentation. The fifteen Phase I tests were performed on flat ground without obstructions.

A front-end model (HEGABOX) has recently been developed to describe the gravity-dominated stage of dense gas dispersion. A smooth transition is made to the HEGADAS model which continues the calculations into the region where ambient turbulence is important.

This paper concerns the comparison of predictions of the models with the Thorney Island data. A variety of observations from the trials have been used in order to provide as full a test of the models as possible.

In addition, the effect is studied of assuming a constant surface roughness parameter instead of the wind-direction-dependent values obtained from meteorological analysis. The dependence on wind direction is due to gross variations in the terrain upwind of the release site.

## 2. The model

### 2.1. The front-end: HEGABOX

The model used for the simulations was HEGABOX with HEGADAS. The dense gas dispersion model HEGADAS [5,6] has been used principally for the simulation of dispersion from spills of liquefied gases, and it can handle the time-dependent vapour evolution from an evaporating pool of liquefied gas. The gravity-driven lateral spreading of the dense gas is modelled explicitly. In very low winds, or for a sudden release of gas, however, there is also strong gravity-spreading along the wind direction, which HEGADAS cannot handle. To simulate the early stages of such spills the front-end model HEGABOX has been developed.

HEGABOX is a box model which treats the cloud as a cylinder of uniform gas concentration, and is thus similar to a number of published box models [7-9]. A brief summary of the formulation is given below. Its derivation, and the determination of parameter values from laboratory experiments, are given by Puttock [10].

The cylindrical cloud is affected by gravity-driven slumping which causes the radius, R, to increase according to

$$\frac{\mathrm{d}R}{\mathrm{d}t} \equiv U_{\mathrm{f}} = 1.15\sqrt{g'H} \tag{1}$$

where  $g' = g (\rho - \rho_a) / \rho_a$  is the reduced gravity,  $\rho$  and  $\rho_a$  are densities of cloud and air, respectively. *H* is the cloud height which initially decreases but eventually increases owing to entrainment of air into the cloud. There is air entrainment associated with the slumping of the cloud, principally at the head (edge), and further entrainment through the top.

The entrainment is given by

$$\frac{\mathrm{d}V}{\mathrm{d}t} = 2\pi R H U_{\mathrm{E}} + \pi R^2 U_{\mathrm{T}} \tag{2}$$

The head entrainment velocity is taken to be proportional to the gravity-spread velocity

$$U_{\rm E} = \alpha_{\rm E} U_{\rm f} \tag{3}$$

and a constant value for  $\alpha_E$  of 0.85 gives a good fit to the largest-scale still-air laboratory data of Spicer and Havens [11] for area-averaged ground-level concentration. An initial time delay is needed to model the build-up to full entrainment. For still air, from Spicer and Havens, the delay should be by a dimensionless time\*  $t^*=3.6$ . For releases of the Thorney Island type in a wind, however, the early mixing is dominated by the shear layer which is initially present on the surface of the cloud [12]. The Thorney Island data show that in this case the initial dimensionless time delay should be 0.83 [10], and so this value was used in the simulations.

Mixing through the top of the cloud is described by an entrainment velocity  $U_{\rm T}$ . This is inhibited by the density difference between the cloud and the air, whose effect can be quantified by a Richardson number. Thus we take

$$U_{\rm T} = k_{\rm v} u_{*{\rm I}} \phi^{-1}$$

$$\phi = (1 + 0.8 R i_{*{\rm I}})^{\frac{1}{2}}$$

$$R i_{*{\rm I}} = \frac{g' H}{u_{*{\rm I}}^2}$$
(4)

 $u_{*I}$  is an internal velocity scale chosen to be consistent with the uniform density assumed through the height of the cloud, and a bulk velocity of  $U_{\rm B}$  (to be derived below):

$$u_{*I} = \frac{k_{v} U_{B}}{\ln (H/z_{r}) - 1}$$
(5)

where  $k_{\rm v}$  is the von Karmann constant (0.41) and  $z_{\rm r}$  the surface roughness length.

In addition, heat transfer and convective entrainment are included as in HEGADAS [6].

A simple approach to modelling the cloud's velocity  $U_{\rm B}$  is obtained by assum-

$$t^* = \left(\frac{g_0'}{V_0^{1/3}}\right)^t t \text{ and } g_0' = g\frac{\rho_0 - \rho_a}{\rho_a}$$

where  $\rho_{a}$  is the density of air.

<sup>\*</sup>We define a dimensionless time in terms of the initial volume  $V_0$  and density  $\rho_0$  of the cloud by:

ing that its momentum is entirely due to the air entrained, and that the effective velocity of the air is a constant factor times the average, over the cloud height H, of the external wind velocity. A value of 0.8 for this factor gives a good fit to the observations (see Section 3.2). In laboratory experiments by Simpson and Britter [13], an ambient flow changed the speed of advance of a gravity current by an amount equal to 0.62 times the ambient velocity.

As the gas becomes very dilute, it must eventually accelerate to match the ambient flow, so the factor of 0.8 must then be modified. This is satisfied by taking the apparent ambient wind speed to be

$$U_{\rm A} = \left(0.8 + \frac{0.2}{1 + Ri_*}\right) \frac{1}{H} \int_0^H U(z) \, \mathrm{d}z \tag{6}$$

using  $Ri_*$ , which is based on the ambient  $u_*$ 

$$Ri_* = \frac{g'H}{u_*^2} \tag{7}$$

# 2.2 The link between HEGABOX and HEGADAS

The HEGADAS model [5] exists in steady-state and time-dependent versions. The steady-state model takes an initially uniform crosswind concentration profile, but as dispersion progresses a Gaussian profile imposed at the edges increases in width. Gravity-spreading contributes to the increase of width of the cloud. The effects of density gradients on vertical mixing are quantified by a Richardson number expression. This formulation is also consistent with passive dispersion in a neutral, stable or unstable atmosphere, so that the model can be used for calculating dispersion to very low concentrations if required.

For a time-dependent gas source, as from an evaporating liquid pool, a number of "observers" travelling with the wind are imagined to pass over the source. These observe the rate of take-up of gas from the pool as they pass over, and the dispersion of this gas is then calculated using the steady-state model. Finally, for any given time, the state of the gas cloud can be compiled from the observations of all the observers at that time. Allowance is then made for longitudinal diffusion, and, if required, the effects of gravity-spreading can be redistributed between the crosswind and downwind directions.

If the box model is used to calculate the early stages of dispersion, the transition from the cylindrical box formulation to a standard HEGADAS calculation occurs when  $Ri_{*1}$  drops to the transitional value of 10. At this time, a number of HEGADAS observers are placed along the length of the circular cloud. Each observer then starts with the uniform mid-part 'b' equal to the cloud width at that distance.  $S_y$ , the width of the Gaussian edge, is initially zero. The ground level concentration  $C_A$  in HEGADAS is set equal to the uniform cloud concentration C from the box model. There is thus a discontinuity in the concentration predicted at any height above the ground, since the assumed form of the concentration profile changes from "top hat" to  $\exp(-(Z/S_z)^{1+\alpha})$ . The entrainment relations in HEGA-BOX and HEGADAS have been formulated principally to predict ground level concentration and a measure of cloud height  $(H \text{ or } S_z)$ ; prediction of the detailed shape of the vertical concentration profile has been regarded as less important. It would be possible to assume a nominal profile which changes smoothly between the two shapes, but it seems that this would serve little practical purpose. A small change in cloud speed, due to the profile change, also has little effect.

### 2.3. Air temperature

An alteration to the model which was made after initial examination of the data concerns the temperature of the entrained air. This temperature had been taken as the temperature of the air at the surface. Taking the unstable Trial 15 as an example, with an air temperature at 10 m of  $10.3^{\circ}$ C, this leads to all the entrained air having a temperature of  $20^{\circ}$ C. By contrast, the air even at 1 m is only at  $11.8^{\circ}$ C. When the gas concentration reaches a low level a very buoyant cloud is then predicted. This assumption is clearly inappropriate, and a change was made so that the temperature of the entrained air is taken as the ambient temperature at half the cloud height. Results are not very sensitive to the height taken, as long as it is not very close to the surface.

### 3. Comparison with Thorney Island data

The comparison between predictions and data has been made for as many of the Thorney Island Phase I (unobstructed) trials as possible. Thus, Trials 9 and 12 have been included despite the existence of considerable vertical nonuniformity and rapidly changing conditions in these trials [14]. (Such conditions often occur in a strongly stable atmosphere.) However, Trial 10 produced very little data owing to a wind direction more than 90° from the experimental axis, and in Trial 5 problems with the gas-bag mechanism caused a two-stage release. The remaining trials are represented in the tables below.

The surface roughness  $z_r$  used has been taken, as a function of wind direction, from a smooth line through the data of Fig. 12 of Puttock [14]. It is assumed that the scatter of the points on that figure is due mainly to the need to average over even more sensors or time for more accurate estimation of  $z_r$ . The values of  $z_r$  used are listed in Table 2. The effect of surface roughness is discussed further in Section 4 below. The Monin-Obukhov length L, determining atmospheric stability, has also been taken from Ref. [14]. The wind speeds given by the data books [15] have been used for trials where the wind was steady. In other cases, an average from nearby sensors, restricted to the period when the gas was dispersing, has been obtained.



Fig. 1. Observations of cloud area-average concentration obtained by Wheatley et al. [16] for Thorney Island Trial 8. The solid line shows the predictions of HEGABOX up to the transition point of  $Ri_* = 10$ . The dashed line shows the result of running the model beyond this point.

Since the range of spill conditions at Thorney Island was limited, confidence in the model can only be generated by successful comparison with a number of features of the data. Correct prediction of, for instance, distance to a given peak concentration could be provided fortuitously by a model which is not simulating other aspects of the spills well. Use of such a model to extrapolate to other conditions could provide erroneous predictions.

#### 3.1. Area-averaged concentrtion versus time

The dilution of the cloud due to the slumping in the early part of the dispersion is independent of the motion of the cloud. Thus the development of the concentration with time early on is of interest. Also the model ought to be predicting the area-averaged ground-level concentration correctly, even if there is initially significant inhomogeneity in the cloud. Wheatley et al. [16] have evaluated the concentration of gas, averaged over all the lowest-level sensors in the cloud, as a function of time for the Phase I trials. Examples of the data are shown in Figs. 1 and 2 for two trials: Trial 8 at low windspeed and Trial 13 at higher windspeed.

Also plotted on Figs. 1 and 2 are the predictions of the HEGABOX model both before, and continued beyond, the point of transition to HEGADAS. The agreement between observations and predictions is good both before and after



Fig. 2. As Fig. 1, for Trial 13.

transition, showing that in this respect the choice of transition point is not critical.

Figures 1 and 2 are typical of the results for the majority of the Phase I trials. However, for Trials 9, 12 and 17 the predicted concentration starts to drop quite sharply below that observed at about  $t^*=60$ . Trials 9 and 12 each had the cloud contained within a shallow strongly-stable layer bounded by an inversion, and the wind in this layer was almost decoupled from the external flow, in a way not modelled by the constant-flux assumptions of the model. The predicted dilution is thus due to top entrainment driven by a higher cloud velocity than that obtaining in reality. Note that, owing to the lower than expected velocity, the prediction of rapid dilution in time does not translate to a marked underpediction of concentration as a function of distance (Section 3.3). Trial 17 is discussed in Section 3.3.

### 3.2 Bulk cloud speed

The predictions of cloud speed and observations derived by Prince et al. [17] are listed in Table 1<sup>\*</sup>. Trial 10 is included here since the necessary photographic data are available. Trials 9 and 12 are omitted owing to the extreme

<sup>\*</sup>A surface roughness length of 8 mm was used for these model runs. See the discussion in Section 4 below.

#### TABLE 1

| Trial  | <b>Relative</b><br>density | Wind<br>speed,<br>m/s | Approximate<br>time after release,<br>s | Cloud speed      | ł                 | Ratio              |
|--------|----------------------------|-----------------------|---|------------------|-------------------|--------------------|
| number |                            |                       |   | Observed,<br>m/s | Predicted,<br>m/s | predicted/observed |
| 7      | 1.73                       | 3.2                   | 12-24                                   | 1.39             | 1.27              | 0.91               |
| 8      | 1.63                       | 2.4                   | 20-40                                   | 1.49             | 1.20              | 0.81               |
| 10     | 1.80                       | 2.4                   | 16-40                                   | 1.06             | 1.18              | 1.11               |
| 11     | 1.96                       | 5.1                   | 12-28                                   | 1.57             | 2.22              | 1.41               |
| 13     | 2.00                       | 6.2                   | 8-16                                    | 2.89             | 2.62              | 0.91               |
| 14     | 1.76                       | 6.0                   | 12-24                                   | 2.49             | 2.84              | 1.14               |
| 15     | 1.41                       | 5.4                   | 8-16                                    | 2.36             | 2.32              | 0.98               |
| 16     | 1.68                       | 4.6                   | 8-16                                    | 1.80             | 1.84              | 1.02               |
| 19     | 2.12                       | 5.0                   | 8-12                                    | 2.18             | 1.85              | 0.85               |
|        |                            |                       |   |                  | Mean              | 1.02               |
|        |                            |                       |   | Standard d       | eviation          | 0.18               |

Comparison of predictions with observations of cloud speed in Thorney Island trials

departure from constant-flux conditions already discussed. In Trial 17, a large part of the cloud was not visible over the white runway, making photographic determination of the centre of gravity inaccurate.

The relatively simple approach for cloud momentum represented by eqn. (6) appears to work reasonably well, once the entrainment of air into the cloud is modelled correctly. The mean ratio of predicted/observed speed is 1.02, which is close to one since this dataset was used to establish the factor of 0.8 in eqn. (6) (Section 2.1 above). The standard deviation is 0.18.

### 3.3 The decrease of concentration with distance from the release spill

If the time decay of concentration and the cloud speed are successfully simulated, then one might expect the decrease of concentration with distance also to be correct. However, the plots against time used above were of average cloud concentration; because of its practical significance, we have analysed the decay of *peak* concentration with distance.

Figures 3 and 4 show the peak concentrations measured at various distances from the spill point for Trials 12 and 15. Data from the lowest gas sensor, at 0.4 m height, have been used. The predictions of ground level peak concentration from HEGABOX/HEGADAS are superimposed. These fit the observations well.

To provide a fuller picture of the performance of the model in this important respect, results from all the trials analysed are listed in Table 2. The distances required for the observed peak concentration to decay to 5%,  $2\frac{1}{2}$ % and 1% are given, together with model predictions. The observations were derived from



Fig. 3. Peak concentrations observed at the lowest gas sensors (0.4 m height) as a function of distance from the source, for Trial 12. The HEGABOX and HEGADAS prediction of centreline peak ground-level concentrations is plotted for comparison.

plots such as Figs. 3 and 4. The results are very satisfactory. At 1% the mean ratio of predicted to observed distance is 1.10 with a standard deviation of 0.19.

Two trials stand out as having worse predictions than the others and hence making the main contribution to the standard deviation. These are Trials 17 and 18. Trial 17 was the only Phase I trial performed with pure freon, giving a release with the very high density of 4.2 times that of air. This slumped to form a very low cloud. From the detailed examination of the concentration it appears that the low aspect ratio of the cloud resulted in considerably more non-uniformity than for the other trials. In particular, sensors at the leading edge of the cloud recorded sometimes much lower concentrations than were present at the same time further upwind. So in this case the model's assumption of a uniform cloud was less appropriate.

Trial 18 had the highest wind speed: 7.4 m/s. In such a wind, the effect of



Fig. 4. As Fig. 3, for Trial 15.

the wake formed behind the gas bag before release, and of the vortex sheet around the gas cloud at the moment of release, could be considerable. This may explain the overprediction of dispersion distances in this case.

With the exclusion of these two trials, the mean ratio of predicted/observed distance to 1% is 1.04 with standard deviation 0.13.

# 3.4 Time-series of concentration

A further test of the realism of the simulation provided by the model is to compare with the time history of concentration from individual gas sensors at various distances downwind. Simple box models have been criticised for predicting sharp changes of concentration at the edges of the cloud whereas the data several hundred metres from the source at Thorney Island show a relatively slow increase to the maximum concentration. HEGADAS should be better able to predict this behaviour since it allows for diffuse edges to the cloud.

Figures 5a and 5b show the gas concentration measurements obtained on

**TABLE** 2

Observed and predicted distances for peak concentrations to decay to  $5\%, 2\frac{1}{2}\%$  and 1%

| le, Relative<br>density | Wind<br>speed,  | ${1/L, m^{-1}}$   | Pasquill<br>stability                                 | Roughness<br>length,                                  | Max. dista<br>m   | nce to 5%,  | Max. dista<br>2½%, m   | nce to  | Max. dista<br>m  | nce to 1%,  |
|-------------------------|---|---|---|---|---|---|--|---|--|---|
|                         | m/s   |   | class   |   | Observed  | Predicted   | Observed   | Predicted   | Observed   | Predicted   |
| 1.60                    | 2.5   | 0.000   | D   | 18  | 100   | 121   | 150  | 185   | 240  | 297   |
| 1.73                    | 3.2   | 0.011   | D/E   | 18  | 125   | 123   | 190  | 193   | <b>≃</b> 350   | 317   |
| 1.63                    | 2.4   | -0.110  | В   | 12  | 125   | 127   | <b>≥</b> 220   | 202   | ≃370   | 336   |
| 1.60                    | 1.7   | 0.650   | Ę۲  | 80  | 125   | 103   | 195  | 171   | <b>≃</b> 360   | 306   |
| 1.96                    | 5.1   | 0.004   | D   | 18  | 110   | 134   | 175  | 208   | <b>≥</b> 290   | 335   |
| 2.37                    | 2.6   | 0.100   | ĿТ  | 18  | 115   | 100   | 175  | 161   | 290  | 277   |
| 2.00                    | 6.2   | -0.011  | D   | 10  | 130   | 147   | 215  | 222   | 370  | 370   |
| 1.76                    | 6.0   | -0.029  | C/D   | 2   | 130   | 173   | 215  | 276   | <b>≃</b> 400   | 459   |
| 1.41                    | 5.4   | -0.080  | B/C   | 2   | 180   | 194   | 275  | 300   | 455  | 460   |
| 1.68                    | 4.6   | -0.030  | C/D   | 2.5   | 120   | 157   | 205  | 243   | 370  | 380   |
| 4.20                    | 4.5   | -0.005  | D   | 18  | 20  | 112   | 110  | 178   | 185  | 293   |
| 1.87                    | 7.4   | -0.023  | c/D   | 5   | <b>0</b> 6  | 145   | 150  | 237   | 275  | 335   |
| 2.12                    | 5.0   | 0.003   | D   | 10  | 100   | 136   | 160  | 217   | $\simeq 275$   | 350   |
| 1                       | 1.60<br>1.60<br>1.63<br>1.63<br>1.63<br>1.63<br>1.63<br>1.63<br>1.64<br>1.41<br>1.68<br>1.68<br>1.68<br>1.68<br>1.68<br>1.68<br>1.68<br>1.6 | 1.60 2.5 m/s m/s m/s m/s m/s m/s m/s 2.4 m/s 2.4 1.63 2.4 1.7 1.96 5.1 2.6 5.1 2.37 2.6 5.1 2.37 2.6 5.1 1.41 5.4 1.68 4.6 1.41 5.4 1.68 4.6 1.45 1.45 1.68 4.5 2.12 5.0 2.12 5.0 5.0 | $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | $\begin{array}{c ccccccccccccccccccccccccccccccccccc$ | 1.60       2.5       0.000       D       18         1.73       3.2       0.011 $D/E$ 18         1.73       3.2       0.011 $D/E$ 18         1.73       3.2       0.011 $D/E$ 18         1.66       1.7 $0.650$ $F$ 8         1.60       1.7 $0.650$ $F$ 8         1.96       5.1 $0.004$ $D$ 18         2.37       2.6 $0.100$ $F$ 8         1.96       5.1 $0.004$ $D$ 18         2.37       2.6 $0.100$ $F$ 18         2.37       2.6 $0.100$ $F$ 18         2.00       6.2 $-0.011$ $D$ 10         1.76       6.0 $-0.029$ $C/D$ 2         1.41       5.4 $-0.030$ $C/D$ 2         1.43       7.4 $-0.023$ $C/D$ 5         2.12       5.0 $0.003$ $D$ 10 | Implementation         Implem | Implying         Class         mm         class         class         mm         mm <thm< th="">         mm         mm</thm<> | Imply         Description         Description <thdescrit< th=""> <thdescrit< th="">         Descrit&lt;</thdescrit<></thdescrit<> | m/sclassmmclassmmclassmm1.602.50.000D181001211501851.733.20.011D/E181251231901931.601.70.650F8125127 $\simeq 220$ 2021.661.70.650F81251001752081.661.70.650F81251001752081.661.70.650F181101341752081.965.10.004D181101341752082.372.60.100F181101341752082.372.60.0011D101301472152222.006.2 $-0.011$ D101301732152761.766.0 $-0.029$ C/D2.51301732152761.415.4 $-0.030$ C/D2.51942753001.877.4 $-0.023$ C/D2.51001672052432.125.00.003D18701121101782.137.4 $-0.023$ C/D2.5901452052432.125.00.003D18701121101782.137.4 $-0.023$ C/D | monodim         < |



Fig. 5a. Time series of concentration obtained at 0.4 m height on the cloud centreline for Trial 15 at 50 m and 200 m from the release point. The predicted ground-level concentrations at the same locations are plotted as heavy lines.

the cloud centreline in Trial 15, at four distances from the release point. The development can be seen from a sharp front, causing a rapid initial rise in concentration, to a more diffuse cloud edge further downwind. The model predictions superimposed on the figures show generally very good agreement. The gas arrives at the first sensor three seconds later than predicted. Part of this discrepancy could be due to uncertainty about the release time in this trial, in the absence of a release marker in the data.

At all distances there is a tendency for the observed concentration to drop to a low level a little sooner than predicted.

The development from sharp edges to smoother concentration profiles is well modelled. In similar plots for Trial 7, there was some indication of the cloud edges becoming slightly diffuse before the transition from HEGABOX and HEGADAS allowed the model to do the same [7]. This suggests that the transition could usefully take place earlier. However, the gain in doing this



Fig. 5b. As Fig. 5a, at 300 m and 500 m from the release point.

could be outweighed by the loss of downwind gravity-spreading after transition. On balance, the transition value of 10 for  $Ri_{*1}$  appears good.

#### 4. Which surface roughness should be used?

In the analysis described so far in this paper, the values of the surface roughness length used in the model runs have been those derived by Puttock [14]. These were obtained from analysis of atmospheric turbulence measurements at up to ten locations. These values vary by about an order of magnitude. The explanation for this is that for most of the trials the atmospheric boundary layer was in the late stages of transition at the experimental area. For wind directions near the array axis, this was a smooth-to-rough transition, with the wind coming off the sea. For winds well off the axis, there were trees several hundred metres upwind, giving a rough-to-smooth transition. It seems that a longer fetch over a grass surface as at the site would have given a roughness length between the extremes of 2 mm and 18 mm, probably about 8 mm.

In these circumstances the question arises: which surface roughness should be used in modelling dense gas dispersion, that derived from turbulence measurements, or that appropriate to the local surface? In the early stages of dispersion of a dense cloud, the internal flow would tend to be isolated from the ambient turbulence by the strong density gradient at the cloud top. Indeed, the assumption in the box model of entirely inward entrainment implies that the relevant turbulence is that within the cloud, presumably generated largely at the local surface. (The mixing box experiments of Turner [18] show how the entrainment in each direction across the interface is related to the turbulence in the entraining layer.)

On the other hand, the strong stratification only lasts for a limited time and dispersion of the cloud eventually approaches a neutral limit, which one would expect to be related to the ambient turbulence.

The Thorney Island trials clearly provide an opportunity to investigate this question. The practical effects of taking the measured  $z_r$  values or a constant value in the model can be tried and the results compared. If one approach reduces the scatter of model predictions compared with data, then that choice would appear to be better.

The results of performing this comparison are shown in Table 3. The trials used are those for which there is roughly a factor of two (or more) difference between the value used in Section 3 and 8 mm. The observed and predicted maximum distances to 5% and 1% concentration are repeated from Table 2, and predictions for  $z_r=8$  mm are added. The mean and standard deviation of the ratio of predicted to observed distance has been calculated in each case.

At the 5% level, the results show negligible difference between the two approaches. Even with the exclusion of Trials 17 and 18, whose values dominate the standard deviation  $\sigma_r$ , the values of  $\sigma_r$  are similar: 0.14 for  $z_r = 8$  mm, 0.16 otherwise. The results at the  $2\frac{1}{2}\%$  level (not listed in Table 3) give the same conclusions.

For distances to 1%, however, there are differences. By this stage, use of the wind-direction-dependent surface roughnesses gives noticeably less scatter than the fixed value (Table 3). With the exclusion of Trials 17 and 18 again, the effect is more marked, with  $\sigma_r = 0.18$  for  $z_r = 0.08$  mm, but 0.11 taking the direction-dependent roughness.

Thus it appears that using the local surface roughness in the model does not give significant benefits for the early stages of dispersion. The model results are not very sensitive to  $z_r$  in this region anyway. But a little further on, the effect of upstream terrain, which modifies the ambient turbulence, is indeed felt by the cloud.

### **5.** Conclusions

The model HEGABOX has been developed as a front-end to HEGADAS for use when gravity spreading in all directions is important in the early stages of dispersion.

Predictions from HEGABOX/HEGADAS have been compared with Thorney Island gas releases. All the Phase I trials were used, except two which were limited by experimental problems. The comparison involved a variety of observations from the trials. These include the decrease of cloud average concentration with time, bulk motion of the cloud, decrease of peak concentration with distance, and individual gas sensor signals.

**TABLE 3** 

| Trial | Roughness                     | Maximum    | distance to 5% | %, <b>m</b>         |                                       |                     | Maximum (     | listance to 19 | %, m                |                                    |                     |
|-------|-------------------------------|------------|----------------|---------------------|---------------------------------------|---------------------|---------------|----------------|---------------------|------------------------------------|---------------------|
|       | lengto z <sub>r</sub> ,<br>mm | Observed   | Predicted      | Ratio<br>pred./obs. | Predicted for<br>z <sub>r</sub> =8 mm | Ratio<br>pred./obs. | Observed      | Predicted      | Ratio<br>pred./obs. | Predicted for $z_r = 8 \text{ mm}$ | Ratio<br>pred./obs. |
| 9     | 18                            | 100        | 121            | 1.21                | 127                                   | 1.27                | 240           | 297            | 1.24                | 326                                | 1.36                |
| 7     | 18                            | 125        | 123            | 0.98                | 128                                   | 1.02                | <b>≃</b> 350  | 317            | 0.91                | 347                                | 66.0                |
| 11    | 18                            | 110        | 134            | 1.22                | 141                                   | 1.28                | <b>~ 290</b>  | 335            | 1.16                | 365                                | 1.26                |
| 12    | 18                            | 115        | 100            | 0.87                | 103                                   | 06.0                | 290           | 277            | 0.96                | 296                                | 1.02                |
| 14    | 2                             | 130        | 173            | 1.33                | 158                                   | 1.22                | ≃ <b>4</b> 00 | 459            | 1.15                | 398                                | 1.00                |
| 15    | 2                             | 180        | 194            | 1.08                | 175                                   | 0.97                | 455           | 460            | 1.01                | 375                                | 0.82                |
| 16    | 2.5                           | 120        | 157            | 1.31                | 145                                   | 1.21                | 370           | 380            | 1.03                | 328                                | 0.89                |
| 17    | 18                            | 70         | 112            | 1.60                | 116                                   | 1.66                | 185           | 293            | 1.58                | 319                                | 1.72                |
| 18    | 5                             | 90         | 145            | 1.61                | 153                                   | 1.70                | 275           | 335            | 1.22                | 320                                | 1.16                |
|       |                               | Mean       |                | 1.25                |                                       | 1.25                | Mean          |                | 1.14                |                                    | 1.14                |
|       |                               | Standard d | eviation       | 0.24                |                                       | 0.26                | Standard de   | eviation       | 0.19                |                                    | 0.26                |

Comparison of predictions using the wind-direction-dependent surface roughness values, and using a constant value

Agreement between model and data was generally very good. However, dispersion distances were overpredicted for the one trial with very high gas density (4.2), where the release produced a very low, less homogeneous cloud, and for the trial with the highest wind speed. The discrepancy in the latter case is probably due to the fact that the initial flow around the stationary gas bag is not explicitly modelled. Excluding these two cases, the mean ratio of predicted/observed distance to 1% concentration was 1.04, with standard deviation 0.13.

At the lower concentrations, the rise and fall in concentration measured at a fixed point becomes gradual, in contrast to the sudden changes predicted by simple box models. This aspect is successfully modelled by HEGADAS.

The atmospheric turbulence at the Thorney Island site was to some extent dependent on the upwind terrain, giving a larger effective surface roughness for off-axis wind directions. Predictions at 1% concentration are improved by taking this into account. At 5% concentration, however, equally good results are obtained using a constant surface roughness.

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