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THE INCORPORATION OF WIND SHEAR EFFECTS INTO BOX MODELS OF HEAVY GAS DISPERSION

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SUMMARY The box model is an important type of model used to predict and assess the hazards that may arise following the accidental release of a large mass of toxic or flammable gas. There are many existing box models, but none include explicitly the effects of the degree of shear in the vertical profile of the mean wind. The present paper summarizes some of the results of an investigation, undertaken for the U.K. Health and Safety Executive, into whether, and how, such effects ought to be included within the box model structure.

1 EXISTING BOX MODELS

1.1 The Purpose And Philosophy Of Box Models

The recent increase in interest, worldwide, into the dispersion of heavy gases in the atmosphere has been primarily motivated by the need for reliable assessment of the hazards consequent upon the accidental release of dangerous materials which, when released, are (or rapidly become) heavier-than-air gases. The U.K. Health and Safety Executive (HSE) is organizing an extensive research programme, involving both experimental and theoretical investigations, and sponsored by organizations from many countries (McQuaid 1979, 1982). One major aspect of HSE's research programme is the development, and validation, of mathematical models of heavy gas dispersion. Recent summaries of models in current use are given by Blackmore, Herman and Woodward (1982) and Havens (1982). The work described in this paper was performed for HSE and deals with one class of models, known as box models.

Before describing the structure of box models, it is important to understand that they have a simple, but important, aim, which is to predict, to adequate accuracy for practical purposes, the position of the gas cloud and the average (over the cloud) of the gas concentration. They do not attempt to describe the detailed spatial structures of the gas velocity and concentration. The first box model was proposed by van Ulden (1974), using a general approach reminiscent of work, now classical and well verified experimentally, by Morton, Taylor and Turner (1956) on turbulent convection.

1.2 The Basic Structure Of Existing Box Models

For reasons of space the following account attempts to emphasize the common features of box models for the simplest situation which they all consider, namely the instantaneous release at $t=0$ of a finite volume v_0 of heavy gas, of uniform initial density ρ_0. The dispersion process is assumed to be isothermal and the ambient atmosphere to be neutrally stratified. It should be noted however that many existing box models do incorporate modifications to deal with practically important complications like thermodynamic processes arising through phase or temperature differences. A comprehensive summary of box models, with full details, is given by Webber (1983).

The basic premise of all box models is, as shown in Figure 1, that predictions of adequate accuracy for practical purposes can be obtained by assuming that the dispersing gas cloud has, for all time t, the shape of a vertical circular cylinder of radius, height and volume r, h and v respectively, where $v=\pi r^2 h$. The density of the gas at time t will be denoted by ρ and the density of the air by ρ_a. Initial values of all variables will be denoted by a zero subscript (e.g. ρ_0). The (assumed uniform) ensemble mean concentration C of the heavy gas is given, in arbitrary units, by

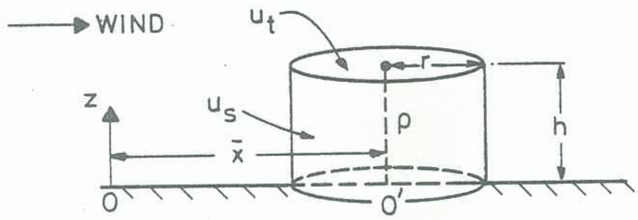

Figure 1 Sketch for discussion of box models

$$C = C_0(v_0/v), \tag{1}$$

and one prime aim of all box models is to predict $v = v(t)$. Under the assumed isothermal conditions the total negative buoyancy of the cloud is conserved, so that

$$vg' = \pi r^2 h g' = \pi b_0 \quad \text{where } g' = g(\rho-\rho_a)/\rho_a, \tag{2}$$

and b_0 is a basic constant of the dispersion process. Equation (2) is known (Webber 1983) to be a good approximation in many practical situations where conditions are not isothermal.

Most box models suppose that the rate of spreading of the cloud about its axis, namely dr/dt, is proportional to the excess hydrostatic pressure at the base of the cloud. A relationship adopted in many box models is therefore

$$\frac{dr}{dt} = \alpha(g'h)^{1/2}, \tag{3}$$

which is in agreement with a wide range of experiments when $\alpha \approx 1$. A consequence of (2) and (3) is (Picknett 1978)

$$r^2 = r_0^2\{1+(t/t_0)\} \quad \text{where } t_0 = r_0^2/2\alpha b_0^{1/2}. \tag{4}$$

The time t_0 is characteristic of that taken for the cloud to spread under its excess weight. For the Porton trials (Picknett 1978), conducted for HSE during 1976-1978, t_0 was of order $0.5s$, which is also likely to be a reasonable estimate for the Thorney Island trials, currently being undertaken for the HSE consortium (but with detailed results not yet available).

The next step in box models is the entrainment equation, representing the mixing by turbulence of heavy gas and air. As shown schematically in Figure 1, entrainment is assumed to occur uniformly over the top of the cloud with speed u_t and uniformly over the side of the cloud with speed u_s. This leads to the entrainment equation

$$\frac{dv}{dt} = \pi r^2 u_t + 2\pi r h u_s. \qquad (5)$$

Models differ greatly in their prescriptions of u_t and u_s. As a generalization, a formula like

$$u_t = \beta u_* / Ri \quad \text{where } Ri = g'h/u_*^2, \qquad (6)$$

and β is a numerical constant, is used in many models and represents the tendency of the stable interface at the top of the cloud to inhibit vertical mixing. Typical values of Ri_o, the release Richardson number, for both the Porton and Thorney Island trials are in the range $10^2 - 10^3$. In (6), u_* is the shear velocity for the mean wind. The side entrainment speed is usually taken to be proportional to dr/dt in (3); thus

$$u_s = \gamma (g'h)^{1/2}, \qquad (7)$$

where γ is a further constant.

The prescriptions above in (3), (6) and (7) cannot be valid for all time since $Ri \to 0$ as $t \to \infty$, and there must therefore be a passive dispersion phase. Many box models describe this phase using a Gaussian model (Pasquill 1974) into which the box model described above is assumed to evolve abruptly when one or more transition criteria are met. A typical transition criterion is

$$(Ri)^{1/2} = \text{constant}, \qquad (8)$$

(van Ulden 1974, Picknett 1978). The abrupt transition is clearly unphysical and a more satisfactory procedure would be to devise a box model that evolves gradually from the behaviour given above for $Ri \gg 1$ to appropriate behaviour when $Ri \ll 1$, which (on dimensional grounds) must have (3), (6) and (7) replaced by

$$\frac{dr}{dt} = \alpha_1 u_*, \quad u_t = \beta_1 u_*, \quad u_s = \gamma_1 u_*, \qquad (9)$$

where $\alpha_1, \beta_1, \gamma_1$ are further numerical constants. The consequences of (9) are consistent with Lagrangian similarity (Batchelor 1964) when $t \gg r_o/u_*$ (Chatwin 1983, 1984). The value of r_o/u_* is of order $10-20s$ for the Porton trials.

2 WIND SHEAR AND BOX MODELS

2.1 Introduction

It will be evident from the summary above that no explicit account is taken of wind shear in the modelling of spreading and entrainment. However wind shear does, of course, cause the observed tilt of heavy gas clouds in the early stages of dispersion (Picknett 1978; Hall, Hollis and Ishaq 1982); furthermore all observations, albeit mainly qualitative until the detailed results from the Thorney Island trials become available, strongly suggest that the mixing of heavy gas and air is much more vigorous in the period immediately after release than is predicted by the standard box model. The work described in this paper was performed for HSE to examine

(a) whether the neglect of ambient wind shear was justified, and
(b) whether wind shear could be incorporated into box models to explain observations like those reported above.

In (b), any modifications proposed should not materially alter the simplicity of box models which is one of their greatest advantages. Furthermore, in order to avoid any abrupt transition, the attempt is made to incorporate shear effects into a box model describing all phases of dispersion, thereby extending an idea introduced in the models of Eidsvik (1980) and Fay and Ranck (1981).

2.2 Spreading

Observations (including those from one of the Thorney Island trials) suggest that (3) is reasonably accurate when r is interpreted as the visible radius or, more satisfactorily, when r^2 is taken to be proportional to the visible plan area. Thus, although dispersing heavy gas clouds in the early stages after release appear to have asymmetric and annular rather than symmetric and circular plans (Picknett 1978), the wind shear appears to affect only the assumed circular shape, and not the effective value of r. During passive dispersion, the effect of wind shear can be incorporated into box models by adopting the result for dr/dt in (9), with the understanding that r is to be interpreted in terms of the plan area of the cloud. A simple formula that reduces to (3) when $Ri \gg 1$, and to (9) when $Ri \ll 1$ is

$$\frac{dr}{dt} = \alpha (g'h)^{\frac{1}{2}} \{1 + (\alpha_1/\alpha)(Ri)^{-\frac{1}{2}}\}. \qquad (10)$$

The merit of (10) over other formulae having the same limiting properties is its simplicity and the convenient fact that it can be integrated exactly with the result

$$\delta_*(r - r_o) - r_o \ln\left\{\frac{[1 + \delta_*(r/r_o)]}{[1 + \delta_*]}\right\} = \frac{1}{2} r_o \delta_*^2 \left(\frac{t}{t_o}\right), \qquad (11)$$

where

$$\delta_* = 2\alpha_1 (u_* t_o / r_o). \qquad (12)$$

Values of δ_* for both the Porton and the Thorney Island trials are typically very small (0.01 to 0.05). Further discussion of (11) is given in Chatwin (1983).

2.3 Direct And Shear Dispersion

In the gravity-dominated stage of dispersion, the spreading is caused by the slumping of the cloud under gravity, and would occur whether or not there was simultaneous transverse mixing. In the passive stage, conversely, spreading and side entrainment are different terms for what is essentially the same phenomenon, namely the result of stirring by the turbulent eddies with characteristic speed u_*. It is appropriate to consider the processes of spreading and side entrainment in a little more detail.

One mechanism causing spreading and side entrainment is direct horizontal turbulent diffusion, shown in Figure 2 (i). However, there is a second mechanism, first

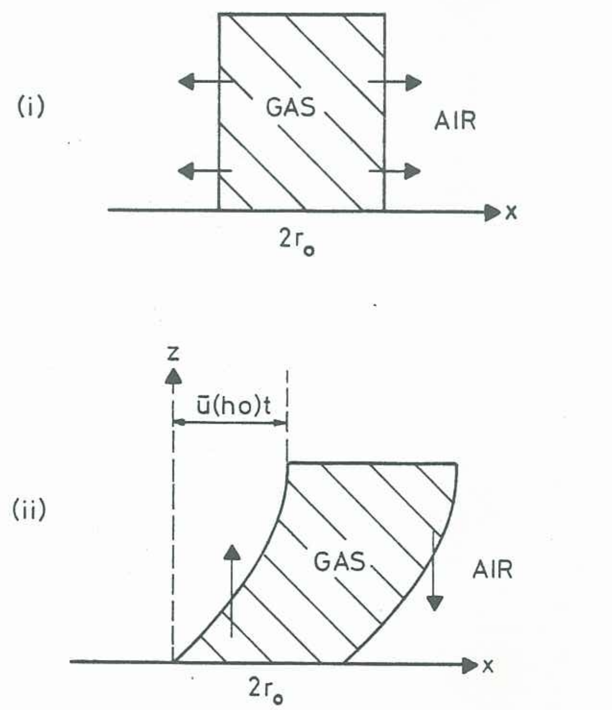

Figure 2 Mechanisms causing horizontal entrainment:
(i) direct horizontal dispersion;
(ii) shear dispersion.

identified by Taylor (1953) and known as shear (or longitudinal) dispersion, and illustrated in Figure 2(ii). As the result of the mean shear, the cloud is itself sheared in the mean wind direction. Acting by itself this would cause the cloud to spread at a rate proportional to $\overline{u}(h_0)$. However vertical gradients of C are then greatly enhanced, and so therefore is vertical turbulent diffusion. The net effect of the wind shear and the vertical diffusion on the horizontal distribution of gas is shear dispersion. The first discussion of shear dispersion was for flow along a pipe (Taylor 1953), when the net effect of shear dispersion on the axial distribution of gas is as if the material is being diffused in this direction by an effective longitudinal dispersion coefficient. This result has led many workers to model shear dispersion in different situations also by means of a longitudinal dispersion coefficient. However (Saffman 1962, Chatwin 1968) such a model is known to be incorrect for atmospheric dispersion, essentially because the region available for dispersion is not bounded vertically. In fact, for passive dispersion in neutrally stable atmospheres, the effects of direct horizontal diffusion and shear dispersion have the same dependence on t , and this dependence is that given by Lagrangian similarity which, for box models, is ensured by adopting (9) for the passive stage. In the gravity-dominated stage, on the other hand, the rate of spreading $\overline{u}(h_0)$ due to wind shear is much less than that due to slumping, which is of order $(g'h_0)^{1/2}$ and is already incorporated in (10).

The conclusion is that, at least for high and low values of Ri , no further account need be taken of shear dispersion in modelling spreading. It is however necessary to examine the change in side entrainment caused by the tilting of the cloud (which wind shear alone induces). Consistent with the approach of box models, it is natural, as shown in Figure 3, to represent the mixing

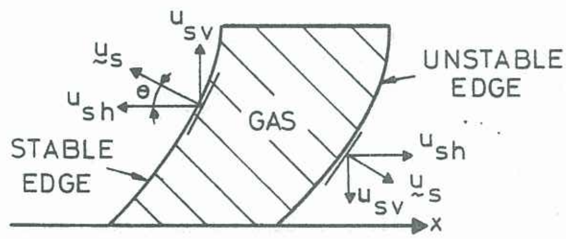

Figure 3 Side entrainment for sheared heavy gas clouds.

across a point on the side of a tilted cloud by an entrainment velocity $\underset{\sim}{u}_s$, with horizontal and vertical components u_{sh} and u_{sv} respectively. Across a surface element δA inclined at an angle θ to the horizontal, the entrainment rate is therefore

$$|\underset{\sim}{u}_s|\,\delta A = (u_{sh}\cos\theta + u_{sv}\sin\theta)\,\delta A. \tag{13}$$

Consider the upstream edge of the cloud where the interface is developing stable stratification. For high values of Ri , the values of u_{sh} and u_{sv} there seem likely to be given by expressions given earlier for u_s and u_v , namely (7) and (6) respectively. Note that (6) leads to a value of u_{sv} much less than u_{sh} for the high values of Ri currently being considered. As a consequence (13) becomes, on the upstream edge,

$$|\underset{\sim}{u}_s|\,\delta A = (g'h)^{\frac{1}{2}}\left\{\gamma'''\cos\theta + \frac{\gamma'\sin\theta}{(Ri)^{3/2}}\right\}\delta A, \tag{14U}$$

where γ' and γ''' are of order unity. Conversely, on the downstream edge, the unstable stratification induces vigorous vertical mixing when $Ri \gg 1$. However the value of u_{sv} there can hardly be of greater order than $(g'h)^{1/2}$, the speed of free fall from the top of the cloud. Thus u_{sh} and u_{sv} will both be of the same order, and (13) becomes, on the downstream edge,

$$|\underset{\sim}{u}_s|\,\delta A = (g'h)^{\frac{1}{2}}\{\gamma^{iv}\cos\theta + \gamma''\sin\theta\}\,\delta A, \tag{14D}$$

with γ'' and γ^{iv} again of order unity. Since (14U) and (14D) represent the two extremes, the rate of entrainment when $Ri \gg 1$ can be taken everywhere on the side of the cloud as

$$|\underset{\sim}{u}_s|\,\delta A = \gamma\,(g'h)^{\frac{1}{2}}\,\delta A, \tag{14}$$

i.e. by equation (7). Therefore, when $Ri \gg 1$, no additional parameters need to be included in box models to estimate the effect of wind shear on the local rate of side entrainment. It has already been noted that the same conclusion holds when $Ri \ll 1$, with (14) replaced by

$$|\underset{\sim}{u}_s|\,\delta A = \gamma_1 u_* \,\delta A. \tag{15}$$

2.4 The Effect Of Increasing Side Surface Area

However, although the local rate of entrainment needs no new parameterization, there is one other effect of wind shear that needs separate treatment, namely its tendency to increase the total side surface area of the cloud, and therefore the total contribution of side entrainment to dv/dt. This effect seems certain to be most important in the early stages of dispersion, before the vigorous mixing on the downstream edge of the cloud combines with the rapid slumping both to reduce the asymmetry shown schematically in Figure 3, and also to reduce the side surface area as a fraction of the total surface area of the cloud. Nevertheless, since observations suggest that box models seriously underestimate the intensity of the total mixing in the early stages of dispersion, it seems worthwhile to try to model empirically the effect of increasing side surface area.

The simplest method seems to be that illustrated schematically in Figure 4. At time t after release, the

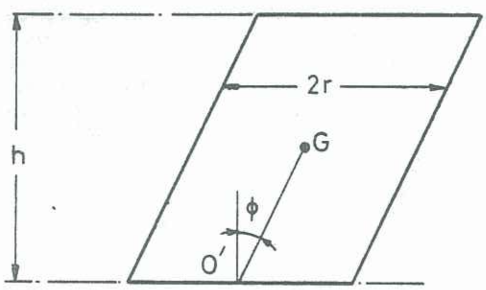

Figure 4 The tilted cylinder box model.

gas cloud is assumed to have the shape of an oblique cylinder of vertical height h and of circular cross-section of radius r , and with the axis of the cylinder inclined at an angle $\phi = \phi(t)$ to the vertical. The side surface area of this cylinder is $4rh\sec\phi\, E(\sin\phi)$ where E is the complete elliptic integral of the second kind. Tables (Abramowitz and Stegun 1965, Chapter 17) suggest that, to acceptable accuracy for practical purposes, $E(\sin\phi)$ can be replaced by $E(0) = \pi/2$ (Chatwin 1983). This proposal has the effect of replacing u_s by $u_s\sec\phi$ in (5). It remains to develop an equation for ϕ in terms of t , which will depend on the velocity at the top of the cloud. Calculations in Chatwin (1983,1984), supported by some isolated experimental results in Hall, Hollis and Ishaq (1982), suggest that an appropriate formula for times of interest (when $Ri \gg 1$) is

$$\tan\phi = \delta\,(u_* t/h)\,\ln\left(\frac{h}{e z_0}\right) \tag{16}$$

where δ is a constant to be determined from experiments and likely to be of order 5 .

Further discussion of the effects of these proposals is given in Chatwin (1983), where it is shown that significantly increased entrainment (up to a factor of 4.5 in one case) is predicted at values of t/t_0 equal to 8 . Qualitatively, such large increases are as observed, but the experimental data presently available does not unfortunately allow quantitative comparisons. Furthermore, equation (16) for ϕ together with the proposed replacement of u_s by $u_s \sec\phi$ can only be a reasonable proposal for small values of t/t_o (high values of Ri), when values of ϕ predicted by (16) remain moderate.

Consider now the development of a model for side entrainment that is valid for all stages of dispersion. According to the discussion above, this requires that $u_s \approx \gamma (g'h)^{1/2} \sec\phi$ for $Ri \gg 1$, where use has been made of (14), and that $u_s \approx \gamma_1 u_*$ for $Ri \ll 1$, where use has been made of (15). There are many possible formulae which satisfy both of these conditions, of which one of the simplest is

$$u_s = \frac{\{\gamma(Ri) + \gamma_1 u_*\}}{\{\cos\phi\,(Ri) + \gamma_*(Ri)^{1/2}\}}(g'h)^{1/2}, \tag{17}$$

where ϕ is to be determined from (16), and γ_* is a new constant whose role is to determine when transition from gravity-dominated to passive behaviour occurs. Thus (17) gives gravity-dominated behaviour, or passive behaviour, according as $(Ri)^{1/2}$ is much greater, or much less, than $\gamma_* \sec\phi$. But note that, unlike the transition in many existing models, determined by the criterion (8), the transition inherent in equation (17) is gradual and not abrupt.

2.5 Top Entrainment

There seems no reason why wind shear should cause changes in the modelling of top entrainment by the top entrainment velocity u_t in equation (5). Although the experimental evidence (e.g. Turner 1979, p.298) is not altogether clear, it is normal in existing box models to adopt (6) when $Ri \gg 1$, i.e. $u_t = \beta u_*/Ri$. For $Ri \ll 1$, u_t must be given by (9), i.e. $u_t = \beta_1 u_*$. Formulae for u_t designed to apply for all values of Ri have been proposed by Eidsvik (1980) and Fay and Ranck (1981). The two formulae will have very similar effects, but that in Eidsvik's model, namely

$$u_t = \frac{\beta \beta_1 u_*}{\{\beta + \beta_1 (Ri)\}}, \tag{18}$$

is marginally simpler and is recommended here.

2.6 Advection Of The Cloud

In order to predict distances downstream from the site of an accidental release at which hazardous conditions cease to exist, all box models must include a prescription for the rate of advection of the cloud as a whole, i.e. $d\bar{x}/dt$, where $\bar{x}$ is shown in Figure 1. Existing models either prescribe this to be a constant fraction of the mean wind (Eidsvik 1980), or by a formula of the type (van Ulden 1974, Fryer and Kaiser 1979, Fay and Ranck 1981)

$$\frac{d\bar{x}}{dt} = \bar{u}(\epsilon h), \tag{19}$$

where ϵ is a constant. The latter alternative seems more appropriate since it takes account naturally of the effect of the large changes in h that occur during the dispersion period as a whole. Fay and Ranck (1981) showed that (19) was in good agreement with experimental results when $\epsilon = 0.4$; however these results did not include substantial data from the passive phase, and Chatwin (1983,1984) suggests that satisfactory agreement for the whole dispersion may require taking a value of ϵ of about 0.32. Further discussion of this important matter is contained in these papers.

3 CONCLUSIONS

Equations (2), (5), (10), (16), (17) and (18) constitute a closed system of equations that determine the volume of the cloud for all t. Together with (19), they form a new box model that (a) attempts to incorporate those effects of wind shear that seem likely to be most important, and (b) is simple but evolves gradually from release through the different stages of dispersion. This model must be tested against experimental data, like all other proposed models. However, as already implied earlier in this paper, the situation regarding available and suitable data is not altogether satisfactory at present, although there will be a marked improvement when the results of the Thorney Island trials are released, probably in 1984. The task of testing any model against data in this field requires careful planning, and some discussion of relevant points is given by Chatwin (1983). Some conclusions of that discussion are: (i) allowance for the effect of initial conditions must be made; (ii) the simpler models should be tested before more complicated models (like that introduced in the present paper); (iii) in using data, it is necessary to state precisely how quantities like U are to be determined from the experimental results.

4 ACKNOWLEDGMENTS

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