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THE SUITABILITY OF DENSE-CONTAMINANT MODELS FOR EMERGENCY PREPAREDNESS SYSTEMS

Richard M. Eckman

Air Resources Laboratory
Silver Spring, MD
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Richard M. Eckman
Atmospheric Turbulence and Diffusion Division
Oak Ridge, Tennessee

Air Resources Laboratory
Silver Spring, MD
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LIST OF SYMBOLS

a_c	acceleration of a contaminant cloud
c	proportionality constant for the rate of spread of dense fluid
c_1	proportionality constant for vertical entrainment
F_a	reaction force resulting from the acceleration of ambient fluid
F_d	dynamic pressure force
F_s	static pressure force
F_v	non-hydrostatic pressure force
g	gravitational acceleration
h	depth of dense-contaminant cloud behind the head region
H	depth of dense-contaminant cloud at the head
I_E	internal energy
k_a	von Kármán constant
K_y	eddy diffusivity for horizontal diffusion
K_z	eddy diffusivity for vertical diffusion
K_E	kinetic energy of a dense cloud's radial motion
L	length scale of a contaminant cloud in downwind direction
M_r	radial momentum of a dense-contaminant cloud
n	constant used for power law
P_E	potential energy of a dense cloud
Q	buoyancy flux
R	radius of a cylindrical cloud
Ri, Ri_b, Ri_*	Richardson numbers
s	downslope distance
t	time

t_c	time required for a contaminant cloud to accelerate to ambient wind speed
T_E	turbulent kinetic energy
u_e	entrainment velocity for the side of a cylindrical cloud
u_*	friction velocity
U	ambient wind speed
U_c	bulk speed of a dense cloud down an incline
U_f	speed of the leading edge of a dense cloud
V	volume of a dense cloud
w_e	entrainment velocity for the top of a cylindrical cloud
z	height above ground
θ	angle between inclined surface and the horizontal
π	3.14159...
ρ_a	density of ambient fluid
ρ_c	density of contaminant cloud
ϕ	empirical function of Richardson number

THE SUITABILITY OF DENSE-CONTAMINANT MODELS FOR EMERGENCY PREPAREDNESS SYSTEMS

Richard M. Eckman

ABSTRACT. Many hazardous atmospheric contaminants are denser than air, so an emergency preparedness system should be able to simulate the transport and diffusion of such contaminants. Over the past two decades a number of modeling techniques have been developed to estimate the transport and diffusion of dense contaminants. In this report the suitability of these modeling techniques for an emergency preparedness system is examined. None of the currently available models is entirely suitable for emergency preparedness, because the models are either too complex to run in real time or are too restricted in their applicability to different atmospheric conditions and terrain features. It is recommended that a puff model be used in an emergency preparedness system to simulate the transport and diffusion of both passive and dense contaminants. But when the contaminant is dense, the puffs should initially be cylindrical, and a similarity model for cylindrical dense puffs should be used to simulate the initial diffusion.

1. INTRODUCTION

The meteorological community has developed a large number of modeling techniques for simulating the transport and diffusion of atmospheric contaminants. Eckman and Dobosy (1989) evaluated the suitability of a number of these techniques for an emergency preparedness system. They recommended that a puff model combined with an interpolated wind field would be most suitable for a "Class A" dispersion model, which must provide real-time estimates of transport and diffusion during an accidental release. For a "Class B" model, which is slower than a Class A model but simulates a release in more detail, they recommended a puff model combined with a wind field that at least fulfills the continuity equation, and possibly also obeys a simple form of the momentum equation.

Eckman and Dobosy's (1989) evaluation dealt only with modeling techniques for passive contaminants. However, many of the hazardous atmospheric contaminants that an emergency preparedness system must handle are denser than air, and the diffusion and transport characteristics of these dense contaminants are significantly different from those of passive contaminants. Numerous modeling techniques have been developed to simulate the diffusion of dense-contaminant clouds over flat, unobstructed terrain, but only the most complex models are able to simulate dense-contaminant diffusion and transport in complex terrain.

This report evaluates the suitability of various dense-contaminant modeling techniques for an emergency preparedness system. The recommendations that stem from this evaluation are based not only on the techniques' physical completeness, but also on their ability to remain within the time and input-data constraints that are imposed on an emergency preparedness system. Additionally, a dense-contaminant technique has an advantage if it can be easily combined with one of the techniques recommended for passive contaminants by Eckman and Dobosy (1989). Such a combination avoids the problem of running two separate models for passive and dense contaminants and makes the eventual transition of a dense cloud to a passive cloud easier to accomplish.

2. GENERAL FEATURES OF DENSE-CONTAMINANT TRANSPORT AND DIFFUSION

2.1. Transport

For both passive and dense contaminants, the force exerted by the ambient mean wind has a major influence on the contaminant's transport. Acting alone, this force tends to accelerate the contaminant cloud to the ambient wind speed U. (Since the ambient wind speed varies with height in the surface layer, U can be interpreted as an average ambient speed over the depth of the cloud.) Most dispersion models assume that this acceleration occurs instantaneously, so the cloud moves with the ambient wind speed at all times after release.

A rough estimate of the time t_c it takes for a cloud initially at rest to accelerate to U can be obtained by assuming that the ambient flow, with density ρ_a, applies a dynamic pressure $0.5\rho_a U^2$ to the cloud's cross-sectional area perpendicular to the wind. If the cloud has a density ρ_c and a length scale L in the downwind direction, the dynamic pressure must accelerate a mass per unit cross-sectional area of $\rho_c L$. Relating the dynamic pressure to the cloud's change in momentum therefore gives

$$\frac{1}{2}\rho_a U^2 \approx \rho_c a_c L \, , \tag{1}$$

where a_c is the cloud's acceleration. Assuming that $a_c t_c \approx U$, Eq. (1) predicts that

$$t_c \sim 2\frac{\rho_c}{\rho_a}\frac{L}{U}. \tag{2}$$

This equation is similar to that used by Hunt *et al.* (1984) when $\rho_c/\rho_a = 1$. A similar equation can also be derived from Rottman *et al.*'s (1987) potential-flow theory.

For $U = 5\,\mathrm{m\,s^{-1}}$, $L = 10\,\mathrm{m}$, and $\rho_c/\rho_a = 2$, Eq. (2) produces $t_c \sim 8\,\mathrm{s}$. Hence, the acceleration time t_c will in practice only be significant when the cloud is large and the wind speed is small. The field experiments described by Koopman *et al.* (1982) tend to confirm this assertion; of the nine releases of liquefied natural gas they discuss, only the lowest wind-speed release with $U = 1.8\,\mathrm{m\,s^{-1}}$ resulted in a significant acceleration time for the dense cloud.

Buoyancy forces can affect the bulk transport of a dense cloud that is on an inclined surface or is well above a surface. In either situation the retardant effects of turbulent entrainment and surface drag partially offset the buoyancy forces. Most accidental releases of dense contaminant occur at or near the surface, so the transport of a dense cloud on an inclined surface is of more importance to emergency preparedness than the descent of an elevated cloud.

The motion of a dense-contaminant cloud on a terrain slope has rarely been systematically measured in the field. However, a number of water-tank experiments and one-dimensional models for gravity currents are relevant to this problem. Ellison and Turner (1959) proposed a one-dimensional model for the development of a buoyant plume on an incline. Their model indicates that downstream of the source the plume rapidly adjusts to a configuration for which the bulk Richardson number

$$Ri_b = g\frac{\rho_c - \rho_a}{\rho_a}\frac{h}{(U_c - U)^2}\cos\theta \qquad (3)$$

is constant with downstream distance s. In this expression, g is the gravitational acceleration, h is the plume's depth perpendicular to the incline, U_c is the bulk plume speed, U is the ambient wind speed, and θ is the angle the incline makes with the horizontal. The constant value of Ri_b is maintained in the model by having a constant value of U_c along the slope, a linear increase of h with s, and a compensating decrease of ρ_c with s. Ellison and Turner used water-tank experiments involving plumes of brine to empirically estimate the entrainment of ambient fluid into the plume. The ambient water was at rest in these experiments, although the general form of Ellison and Turner's model included an ambient speed U.

Manins and Sawford (1979) and Fitzjarrald (1984), who were interested in modeling katabatic winds, extended Ellison and Turner's (1959) model by including a stable ambient stratification and radiational cooling along the slope. The model in the former paper assumed a calm environment, while Fitzjarrald included an ambient wind. For dense-contaminant transport the effects of radiational cooling are not important, but the ambient stratification could affect the dense plume's transport in some situations. Although the models developed by Ellison and Turner (1959) and Fitzjarrald (1984) are one-dimensional, they could still be useful for estimating the transport of a dense cloud in the presence of an ambient wind.

A number of recent water-tank experiments are also relevant to dense-contaminant transport. Britter and Linden (1980) conducted water-tank experiments similar to those discussed by Ellison and Turner (1959). But they were primarily interested in the head at the leading edge of the dense plume (Fig. 1). The depth H of this head

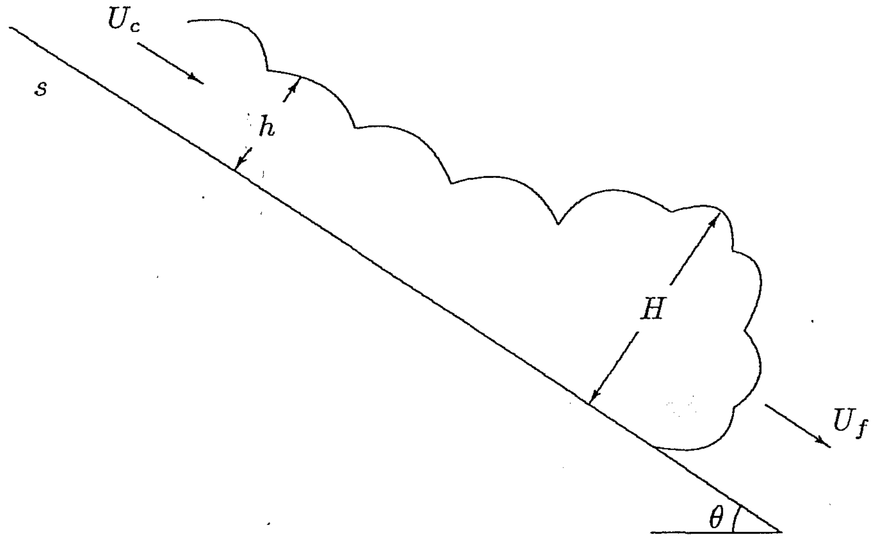

Figure 1. Schematic illustration of a dense plume moving down an incline with slope θ.

is significantly larger than that of the following flow, and the speed U_f of its front is not necessarily the same as the following flow's speed U_c. Britter and Linden found experimentally that if the constant buoyancy flux Q of the steady-state plume behind the head is defined as

$$Q = g\frac{\rho_c - \rho_a}{\rho_a}hU_c\,, \tag{4}$$

then the dimensionless ratio $U_f/Q^{1/3}$ was essentially independent of slope angle θ, downslope distance s, and surface roughness for $\theta \geq 5°$. The front speed is constant with θ because the buoyancy force and the drag due to entrainment increase at about the same rate as θ increases. For values of θ between 0.5° and 5°, Britter and Linden found that U_f was still constant with s, but it depended on θ and the surface drag; for slopes less than 0.5°, U_f decreased with s, because the buoyancy force could not overcome the surface drag.

Britter and Linden (1980) also investigated the ratio U_f/U_c. For a Boussinesq plume ($\rho_c/\rho_a - 1 \ll 1$) they found this ratio to be about 0.6. Hence, the following flow feeds contaminant into the head as the plume travels down the incline. When ρ_c is much larger than ρ_a, the ratio U_f/U_c approaches unity.

When an instantaneous cloud of dense contaminant is released on an incline, the front velocity U_f is not constant with s (or the travel time t) as it is for a continuous plume. Beghin *et al.* (1981) showed that for $\theta \geq 5°$ the cloud goes first through an accelerating phase in which $U_f \propto t$ and then passes into a decelerating phase in which $U_f \propto t^{-1/3}$. The proportionality constants for these relations are functions of θ.

The models and water-tank experiments that were just described have two shortcomings in regard to dense-contaminant transport: they do not include horizontal diffusion and ambient turbulence. These shortcomings will result in overestimates of the cloud transport in most situations, since the decrease of ρ_c with downstream distance will be underestimated. Additionally, the water-tank experiments did not have an ambient mean wind, so their applicability to dense-contaminant diffusion is even more restricted. But the one-dimensional models and water-tank experiments are presently the only sources of information about buoyancy-driven transport.

2.2. Diffusion

The diffusion of a dense-contaminant cloud generally involves a sequence of phases (Hunt *et al.*, 1984; Havens and Spicer, 1985). A specific combination of forces characterizes the diffusion during each phase; however, every phase may not be present during a particular release. The initial phase of diffusion is the buoyancy-dominated phase. During this phase the buoyancy force is the main source of energy for diffusion. It not only causes the cloud to slump and spread horizontally over the ground, but also creates turbulent kinetic energy within the cloud. This phase may not appear if the ambient flow has enough energy to disrupt the buoyancy-driven motions. For a surface release, the ratio of the buoyancy force to the force exerted by the ambient flow is given by the Richardson number

$$Ri_* = g\frac{\rho_c - \rho_a}{\rho_a}\frac{H}{u_*^2}\,, \qquad (5)$$

where u_* is the friction velocity and H is the height of the cloud. When $Ri_* \ll 1$, the deformation of the cloud resulting from the ambient flow (see Rottman *et al.*, 1987) masks the effects of buoyancy, so the cloud can be treated as a passive contaminant. When $Ri_* \gg 1$, the buoyancy force dominates, and the gravitational slumping of the cloud must be accounted for. More precise criteria for Ri_* are discussed in Section 4.

During the buoyancy-dominated phase the larger hydrostatic pressure within a dense cloud causes the cloud to spread horizontally over a flat surface. Several researchers have investigated the characteristic structure of the cloud during this phase (Benjamin, 1968; Simpson and Britter, 1979; Rottman and Simpson, 1984). Figure 2 is a schematic representation of this structure. Qualitatively, this flow is similar to the flow on an incline (Fig. 1). At the cloud's boundary a head forms that is about twice as deep as the center of the cloud. Within the head a horizontal vortex forms with upward motion on the outer edge of the head and downward motion on the inner edge. Most of the entrainment of ambient air occurs not horizontally through the cloud's sides, but vertically in a wake region behind the head.

The horizontal spread of a dense cloud causes a corresponding decrease in the height of the cloud. If an instantaneous release of dense contaminant is assumed to have a cylindrical form with radius R, height H, and volume $V = \pi R^2 H$, the rate of change

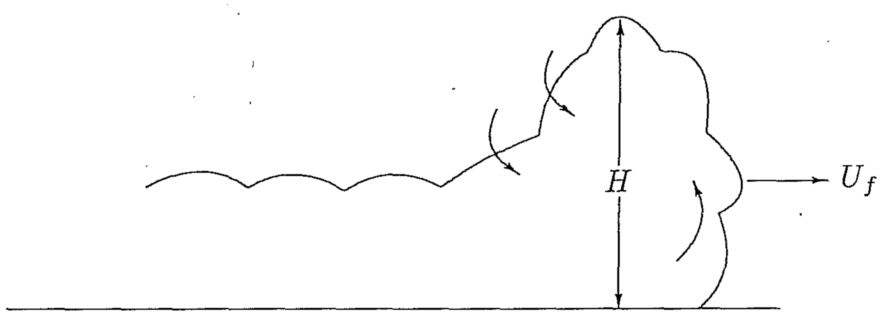

Figure 2. Schematic illustration of the structure within a dense cloud during the buoyancy-dominated phase.

of H with time t is given by

$$\frac{dH}{dt} = \frac{1}{\pi R^2}\frac{dV}{dt} - 2\frac{H}{R}\frac{dR}{dt}\,. \tag{6}$$

The first term on the right side of this equation represents the increase in H that results from entrainment of ambient air; the second term is the decrease in H that results from the radial spread of the cloud. During the buoyancy-dominated phase of diffusion, the magnitude of the second term is larger than that of the first, so H decreases with time (*i.e.*, slumping). In fact, dH/dt can only become positive if ambient turbulence is present as a source of energy for entrainment (van Ulden, 1987).

If ambient turbulence is present, a dense-contaminant cloud eventually reaches a condition in which the entrainment term in Eq. (6) exceeds the slumping term, and dH/dt then becomes positive. This marks the beginning of what Havens and Spicer (1985) call the stably stratified phase. In this phase the diffusion is determined by a combination of buoyancy forces and the external turbulence. For diffusion in the surface layer the first term on the right side of Eq. (6) scales with the friction velocity u_*. Hence, the stably stratified phase begins when

$$u_* \sim 2\frac{H}{R}\frac{dR}{dt}\,. \tag{7}$$

The aspect ratio H/R is generally significantly less than unity by the time the stably stratified phase is reached, and Eq. (7) may therefore be fulfilled well before u_* becomes comparable to the spreading velocity dR/dt (Hunt *et al.*, 1984). This indicates that the stably stratified phase may be further subdivided into two parts. In the first part the horizontal diffusion is still dominated by gravity, but entrainment by ambient turbulence has halted the cloud's slumping. The second part begins when dR/dt falls to a value comparable to u_*, and the ambient turbulence is then important for both horizontal and vertical diffusion, although the cloud's stable stratification still influences the diffusion.

Eventually, a dense-contaminant cloud becomes diluted enough that buoyancy is no longer significant. This is the final passive phase of diffusion, when the ambient turbulence dominates the diffusion process.

3. DESCRIPTION OF MODELING TECHNIQUES FOR DENSE CONTAMINANTS

Meteorologists have developed several modeling techniques to simulate the transport and diffusion of dense contaminants. Most of these techniques treat the dense contaminant's diffusion in detail, but assume that the transport results only from the ambient wind with speed U. Such models are only valid for releases in flat terrain with no significant obstacles. The most complex models are able to handle sloping terrain and obstacles, although they do not treat the transport and diffusion as separate, independent components, as is the case with modeling techniques for passive contaminants (Eckman and Dobosy, 1989). In fact, the transport and diffusion of dense contaminants are difficult to separate, because the transport in sloping terrain depends on the cloud's density ρ_c, and ρ_c depends in turn on the rate of diffusion.

Several authors, including Havens and Spicer (1985) and Koopman *et al.* (1989), have separated dense-contaminant models into broad categories. For the purposes of emergency preparedness, three categories are used in this report: simple similarity models, advanced similarity models, and dynamic models. The following subsections discuss these categories in some detail.

3.1. Simple similarity models

These models are the simplest of the three categories, and they represent the first generation of models developed for simulating dense contaminants. Most treat an instantaneous release of dense contaminant as a cylinder with horizontal radius $R(t)$, height $H(t)$, and uniform density $\rho_c(t)$, where t is time. Simple equations are used to calculate the front velocity dR/dt and the rate of entrainment of ambient air. Van Ulden (1974) developed the prototype for this model category, and other examples are the models by Cox and Carpenter (1980), Eidsvick (1980, 1981), and Fay and Zemba (1985).

All the simple similarity models use the following equation for the radial spreading of the cloud:

$$\frac{dR}{dt} = U_f = c\sqrt{g\frac{\rho_c - \rho_a}{\rho_a}H}\,. \tag{8}$$

Here, ρ_a is the ambient density and c is a constant close to unity (van Ulden, 1974).*

* Some authors use ρ_c as the denominator on the right side of Eq. (8), but ρ_a is the correct density.

Benjamin (1968) derived this equation by assuming that the difference $g(\rho_c - \rho_a)H$ in hydrostatic pressure between the ambient fluid and the contaminant cloud is balanced by the dynamic pressure $0.5\rho_a U_f^2$ exerted by the ambient fluid near the gravity current's leading edge.

The similarity models simulate the entrainment of ambient fluid into the cloud by defining one entrainment velocity w_e for the cylinder's top and another u_e for the cylinder's side. Different models use significantly different equations to estimate these entrainment velocities, which modify the cloud's volume V through the equation

$$\frac{dV}{dt} = 2\pi RHu_e + \pi R^2 w_e \, . \tag{9}$$

Most of the simple similarity models assume that u_e is either negligible or is directly proportional to U_f. The entrainment velocity w_e is usually calculated with a relation of the form

$$\frac{w_e}{u_\ell} = f(Ri) \, , \tag{10}$$

where u_ℓ is an ambient turbulence velocity scale such as the friction velocity u_*, and $f(Ri)$ is some function of a cloud Richardson number such as Ri_* in Eq. (5).

Picknett (1978) and Cox and Carpenter (1980) use the function

$$f(Ri) = \frac{c_1}{Ri} \, , \tag{11}$$

where c_1 is a constant, to model the vertical entrainment. Turner (1968) and Kato and Phillips (1969) found that this equation provided a good fit to entrainment data from water-tank experiments. At small values of Ri, Eq. (11) produces an unbounded increase in w_e, so $f(Ri)$ is set to a constant when Ri falls below a specified value. To provide for a smooth transition to a constant value at small values of Ri, Eidsvik (1980), Fay and Ranck (1983), and others have used an expression of the form

$$f(Ri) = (c_2 + c_3 Ri^n)^{-\frac{1}{n}} \, . \tag{12}$$

In this equation c_2, c_3, and n are constants. Eidsvik (1980) chose $n = 1$, whereas Fay and Ranck (1983) used $n = 2$. Equation (12) reverts to Eq. (11) for large values of Ri; hence, $c_3^{-1/n}$ should equal c_1. In Eqs. (10)–(12) the entrainment velocity w_e depends on the level of ambient turbulence, so these equations are better suited for the stably stratified phase of diffusion than they are for the buoyancy-dominated phase.

The models discussed above are for instantaneous releases of dense contaminant. Several simple similarity models have also been developed for continuous releases (Cox and Carpenter, 1980; Raj and Morris, 1987). These models assume that the plume of contaminant has a rectangular cross section, and they use spreading and entrainment relations similar to those for dense puffs.

Most of the simple similarity models have a transition to passive-contaminant diffusion when the cloud is sufficiently diluted. Usually, Gaussian plumes and puffs are used in this passive phase. In Cox and Carpenter's (1980) model, the transition to the passive phase occurs when the horizontal growth given by Eq. (8) becomes equal to the rate of growth given by the Pasquill-Gifford curves (see *e.g.*, Hanna *et al.*, 1982) for passive diffusion. Other models make the transition to passive diffusion when U_f falls to a value comparable to u_* (van Ulden, 1974) or when a cloud Richardson number Ri falls below a critical value (Raj and Morris, 1987).

3.2. Advanced similarity models

Like the simple similarity models, the advanced similarity models assume that the contaminant cloud's concentration distribution has a specific mathematical form (*e.g.*, a cylindrical puff, rectangular plume, rectangular plume with Gaussian tails, *etc.*). But they use more complex equations to estimate the radial spreading and entrainment of the cloud. These equations may include momentum and energy budgets and possibly thermodynamic interactions between the cloud and environment. The models discussed by Morgan *et al.* (1983), van Ulden (1984), Havens and Spicer (1985), and van Ulden (1987) fall into this category.

Each of the models in this category uses a somewhat different set of physical equations, so van Ulden's (1987) model for axisymmetric clouds—which only applies to the buoyancy-dominated phase of diffusion—is used here as a representative example. In van Ulden's (1987) model, the axisymmetric cloud is assumed to be a cylinder, and the time rate of change of the cylinder's volume V is given by

$$\frac{dV}{dt} = \pi R^2 w_e \,, \qquad (13)$$

which is the same as Eq. (9) except that the side entrainment term is missing. Van Ulden left out the side entrainment term because observations indicate that little mixing occurs through the sides of a dense-contaminant cloud during the buoyancy-dominated phase; instead, the velocity shear at the head of the slumping cloud creates turbulent kinetic energy, which in turn produces vertical entrainment through the cloud's top.

Instead of using Eq. (8) for the spreading velocity U_f, van Ulden derives U_f from a momentum equation of the form

$$\frac{dM_r}{dt} = F_s + F_v + F_d + F_a \,, \qquad (14)$$

where M_r is the radial momentum of the slumping cloud, F_s is the static pressure force created by the cloud's buoyancy, F_v is the non-hydrostatic pressure force resulting from vertical accelerations in the cloud, F_d is the dynamic pressure force caused by the cloud's radial motion, and F_a is a reaction force resulting from the acceleration of ambient fluid at the cloud's boundary. Parameterizations can be introduced for the forces on the right side of Eq. (14), and the resulting equation can be solved for dU_f/dt. An important feature of this equation for U_f is that it accounts for the initial radial acceleration of the cloud from rest; this initial acceleration does not appear in Eq. (8).

The other major equation in van Ulden's model is an energy conservation law of the form

$$\frac{d}{dt}\left[P_E + K_E + T_E + I_E\right] = 0\,, \tag{15}$$

where P_E, K_E, T_E, and I_E are respectively the potential energy, the kinetic energy of the mean radial motion, the turbulent kinetic energy, and the internal energy. Since the production of turbulent kinetic energy drives the entrainment of ambient fluid, the solution of this equation for T_E produces an estimate of the entrainment velocity w_e. Hence, the combination of Eqs. (14) and (15) gives an estimate of the radial spreading and entrainment in a dense-contaminant cloud.

In van Ulden's (1987) analysis, the only source of internal energy I_E is the dissipation of turbulent kinetic energy. But in general the internal energy can also be changed by heat transfer between the cloud and its surroundings and by chemical reactions. Havens and Spicer's (1985) model for the buoyancy-dominated phase, which otherwise resembles van Ulden's, accounts for heat transfer between the cloud and its surroundings by introducing an equation for the enthalpy of the dense-contaminant cloud.

Van Ulden's (1987) model applies only to the buoyancy-dominated phase of dense-contaminant diffusion. At the end of his report he has a general discussion of the additions and alterations that would be required to model the stably stratified and passive phases, but this discussion contains no mathematical results. Havens and Spicer's (1985) model does include the stably stratified and passive phases in a manner similar to Colenbrander's (1980) earlier model. In both of these models the vertical diffusion of the cloud in these phases is determined by an eddy diffusivity K_z of the form

$$K_z = \frac{k_a u_* z}{\phi(Ri_*)}\,, \tag{16}$$

where k_a is the von Kármán constant, z is height above ground, and ϕ is an empirical function of Ri_*; the horizontal diffusion is given by Eq. (8) during the stably stratified phase and by an eddy diffusivity K_y based on the Pasquill-Gifford curves during the passive phase. Colenbrander's (1980) model and the stably stratified and passive phases in Havens and Spicer's (1985) model are in some respects more representative of simple similarity models, although they do provide for a continuous transition from an initially uniform cloud distribution in the horizontal crosswind direction to a purely Gaussian distribution in the passive phase (Fig. 3).

The main advantage of the advanced similarity models is that they retain the simple cloud distributions used by the simple similarity models while providing a more detailed

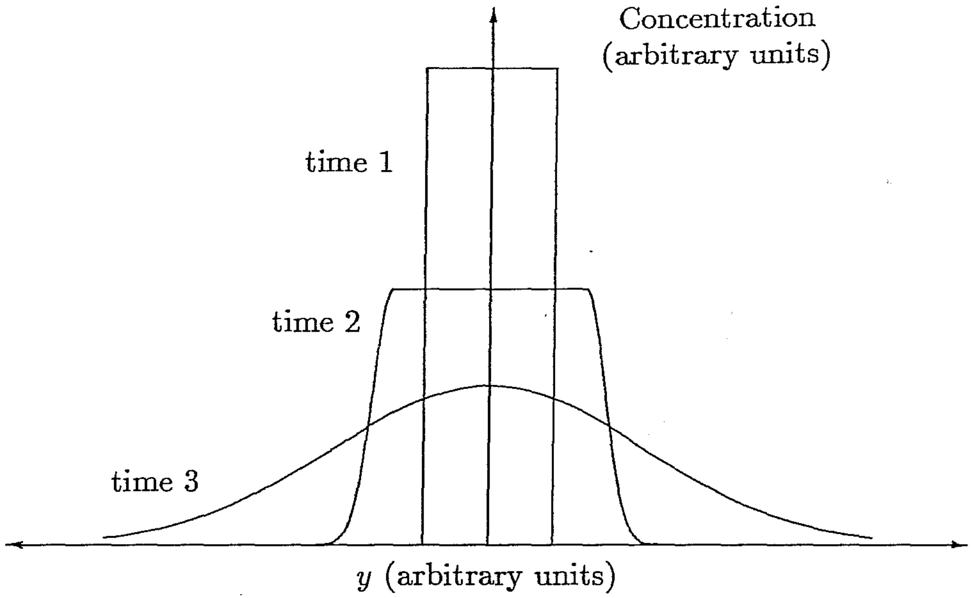

Figure 3. In the models described by Colenbrander (1980) and Havens and Spicer (1985), the horizontal cloud distribution varies continuously from an initially uniform distribution to a purely Gaussian distribution.

description of the physics involved in dense-contaminant dispersion. Yet these models are significantly easier to use than the dynamic models that are discussed in the next subsection.

3.3. Dynamic models

Dynamic models use a full system of prognostic primitive equations to simulate the development of a dense-contaminant cloud in three dimensions. In principle they can simulate a wide range of phenomena in dense-contaminant diffusion, including the velocity distribution within a slumping cloud and the effects of sloping terrain and obstacles. But they suffer from the same problems as the dynamic techniques discussed by Eckman and Dobosy (1989): they require large amounts of computer resources, a closure assumption for the flux terms in the primitive equations, and a spatial and temporal grid spacing that is sufficiently small to resolve the developing cloud. Examples of dynamic models specifically designed for dense contaminants include FEM3 (Chan, 1983; Chan *et al.*, 1987) and HEAVYGAS (Deaves, 1984).

Normally, the system of equations in dynamic models includes three momentum equations, the first law of thermodynamics, a continuity equation for both the contaminant-air mixture and the contaminant species alone, and the equation of state. In FEM3 and most other dynamic models, these equations are closed using first-order closure (*i.e.*, K theory). This is a major weakness of these dynamic models, because the assumptions required to justify first-order closure are not generally fulfilled in atmospheric diffusion (see *e.g.*, Pasquill and Smith, 1983, Sections 3.1 and 3.2; Eckman and Dobosy, 1989, p. 3). HEAVYGAS and some other models attempt to mitigate the problems with first-order closure by using what Deaves (1984) calls k–ϵ closure models. These closure models use estimates of the turbulent kinetic energy (k) and the rate of dissipation of turbulent kinetic energy (ϵ) to estimate the eddy diffusivities. But k–ϵ closure models still essentially involve first-order closure, because the diffusion is proportional to the local gradient of the mean concentration.

4. SUITABILITY OF DENSE-CONTAMINANT MODELS FOR EMERGENCY RESPONSE

Clearly, the suitability of the model categories described above varies from one application to another. Dynamic models, for example, are useful in basic-research applications, because physical completeness is a primary consideration in such applications. But in emergency-preparedness applications, the physical completeness of a model must be weighted against other important considerations. For dense-contaminant dispersion these other considerations are basically the same as the criteria given by Eckman and Dobosy (1989) for wind-field techniques:

(*a*) The diffusion model should be appropriate for the range of terrain features, atmospheric conditions, and source characteristics that can exist during an accidental release.

(*b*) The model should not require types or quantities of input data that would be difficult or impossible to obtain during an accidental release.

(*c*) The execution time of the model on a computer should be within the limits set for Class A and Class B models. Class A models must provide real-time estimates at the time of a release; Class B models need not run in real time, but they should be able to complete a simulation within a reasonable period of time (30 minutes, say).

(*d*) More complex models do not automatically perform better than simpler models. For their intended applications, more complex models should be able to demonstrate an improved performance over their simpler counterparts.

Although dynamic models are physically complete—and therefore fulfill criterion (*a*)—they have difficulty fulfilling criteria (*b*), (*c*), and perhaps (*d*). For dense-contaminant releases, dynamic models require rather detailed input regarding the spatial distribution of the wind, the thermodynamic variables, and the characteristics of the contaminant source. Additionally, they require considerable execution times even on large mainframe computers. Because of these limitations, dynamic techniques are better suited for research applications than they are for operational use in an emergency preparedness system (Koopman *et al.*, 1989).

Criterion (a) is a major problem for both the simple and advanced similarity models. Many of the models in these categories are only valid for dense-contaminant releases into calm environments, and none of them can deal with sloping terrain. The transport of a dense-contaminant cloud on a terrain slope differs significantly from that of a passive contaminant, so an emergency-preparedness model should be able to accommodate buoyancy-driven transport. Another problem with the similarity models is that they simulate only the relative diffusion of a cloud; in practice it may also be necessary to account statistically for the meandering of a cloud's center of mass. Large scale atmospheric motions with length scales that are significantly larger than a cloud's dimensions are the source of this meandering. For a plume, the meandering represents the lateral fluctuations of the cloud's centerline about its average position during a sampling interval, whereas the meandering of a puff is an ensemble-average statistic that quantifies the uncertainty associated with the position of the puff's center. (Eckman and Dobosy, 1989, Section 3.1).

The main conclusion of the discussion above is that none of the current models for dense contaminants is entirely suitable for emergency preparedness. Dynamic models are too complex to be used in an operational mode, whereas both categories of similarity models are presently too restricted in their applicability. However, dense-contaminant modeling is a relatively new and active field, so better models may appear in the near future.

5. RECOMMENDATIONS AND CONCLUSIONS

Although none of the present dense-contaminant models is entirely suitable for emergency-preparedness applications, the simple and advanced similarity models seem to have more potential than the dynamic models. The dynamic models may be useful for making detailed simulations of hypothetical releases, but they do not seem to have much capability for operational applications, even considering the recent increases in computer speed. Similarity models can be used operationally and have the advantage that they are relatively simple to combine with the puff-model technique that Eckman and Dobosy (1989) recommended for passive contaminants. But at present they are too limited in their applicability to different atmospheric conditions and terrain features.

For an emergency-preparedness system it is recommended that a puff-model technique be used for both dense and passive contaminants. But when the contaminant is dense, the normal algorithm for Gaussian puff diffusion should be replaced by a similarity model for dense cylindrical clouds. Also, the transport of the puffs should be modified to account for buoyancy forces, possibly using a bulk model like Ellsion and

Turner's (1959). A number of more specific recommendations concerning the use of a puff model to simulate dense-contaminant diffusion are given below:

(*a*) Criteria must be established to determine whether the puffs in a puff model will initially act like a dense contaminant (buoyancy-dominated or stably stratified phases) or a passive contaminant. Havens (1988) presents criteria based on Ri_* in Eq. (5). He suggests that a cloud will start in the buoyancy-dominated phase when $Ri_* \geq 30$, in the stably stratified phase when $1 \leq Ri_* \leq 30$, and in the passive phase when $Ri_* \leq 1$. These criteria are reasonable for emergency preparedness, since Ri_* represents a direct estimate of the relative importance of the buoyancy force and the ambient flow, but is still relatively simple to estimate.

(*b*) Careful consideration must be given to the procedures a puff model should use to account for puff interactions. Passive puffs that overlap do not create many problems, because they move and diffuse independently. But this is not true of dense puffs; overlapping puffs will increase the effective cloud density ρ_c, which will affect both the transport and diffusion of dense puffs. A simple way to account for overlapping is to make the effective density of each puff equal to the sum of its own density and the density contributions of nearby puffs.

(*c*) The buoyancy-dominated phase generally has a short duration, so it should be reasonable to assume that this phase is a source effect that alters only the initial size and position of each puff. Havens and Spicer (1985) used a similar assumption in their model. Van Ulden's (1987) model for a dense-contaminant cylinder is a good choice for simulating this phase of dense-puff diffusion, because it has a good combination of physical completeness and mathematical simplicity. The only problem with this model is that it requires flat terrain. Equations (14) and (15) would have to be modified to account for sloping terrain. Additionally, a momentum equation for the bulk downslope velocity U_c would be required. This modified model would be run until the buoyancy-dominated phase is completed, and the final dimensions of the puff would then be used as the starting point for the later phases of diffusion in the puff model.

d) By the time the stably stratified phase is reached, Eqs. (8) and (10) should respectively give a good estimate of the cloud's horizontal spread and vertical entrainment. A simple similarity model will thus be useful for simulating this phase. Since Eq. (16) is conceptually similar to Eq. (10), Havens and Spicer's (1985) model is also a good choice for this phase. The latter model has the additional attribute that the cloud distribution changes continuously from uniform to Gaussian.

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