R. M. Eckman

NOAA Technical Memorandum ERL ARL-171

THE SUITABILITY OF DIFFUSION AND WIND-FIELD TECHNIQUES FOR AN EMERGENCY-RESPONSE DISPERSION MODEL

Richard M. Eckman
Ronald J. Dobosy

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Richard M. Eckman and Ronald J. Dobosy

Atmospheric Turbulence and Diffusion Division
Oak Ridge, Tennessee

April 1989

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LIST OF SYMBOLS

Symbols are listed below and are also defined in the text. A prime on a variable denotes the fluctuating part of a quantity, and an overbar indicates the mean part of a quantity.

b	denotes an unspecified variable
B_3	buoyancy force in momentum equation
$\hat{B}_3$	buoyancy force for a dense-gas cloud
c	proportionality constant ($\simeq 0.56$) resulting from Lagrangian similarity theory
f_i	empirical function used to estimate σ_i at a given travel time
f_i'	empirical function used to estimate σ_i at a given downwind distance
g	gravitational acceleration
h	release height of contaminant cloud
k_a	von Kármán constant
K_{ij}	eddy diffusivity tensor relating concentration flux in direction i to concentration gradient in direction j
m_i	meandering of a puff's center of mass in direction i
n	number of velocity measurement locations in a region of interest
p	exponent used in distance-weighted interpolation
P_i	pseudo-velocity used in ADPIC model in coordinate direction i
q	contaminant release rate for Gaussian plume
Q	mass of contaminant in Gaussian puff
r_{jk}	distance between two points labeled j and k
$R^L(\tau)$	Lagrangian autocorrelation

S	net source/sink term in continuity equation for a contaminant
$S_i^L(\omega)$	normalized Lagrangian velocity spectrum for direction i
t	time
T	travel time for diffusion
u_i	velocity component in direction i
u_i''	random velocity component in direction i drawn from a statistical distribution
u_{ij}	measured velocity component in direction i at location j
u_*	friction velocity
v_{ik}	interpolated velocity component in direction i at location j
$W(r_{jk})$	weighting function for distance-weighted interpolation
x_i	displacement component in direction i relative to fixed coordinate system
X	downwind distance from source
y_i	displacement component in direction i relative to center of Gaussian puff
z_0	aerodynamic roughness length
Z	mean height of a contaminant cloud
$\delta(\tau)$	delta function
Δt	time increment
η_i	standard deviation of velocity fluctuations in direction i
θ_0	reference potential temperature
θ_s	surface potential temperature
λ	sampling time for diffusion

π	$3.14159\ldots$
ρ_0	ambient air density
ρ_c	density within dense-gas cloud
σ_i	standard deviation of Gaussian plume or puff in direction i
τ	time lag
χ	contaminant concentration
ω	angular frequency

THE SUITABILITY OF DIFFUSION AND WIND-FIELD TECHNIQUES FOR AN EMERGENCY-RESPONSE DISPERSION MODEL

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ABSTRACT. Most atmospheric dispersion models have two separate components: a diffusion component that simulates the dilution of a contaminant by turbulence, and a wind-field component that transports the contaminant away from the source. Many modeling techniques have been developed for each of these components. This report examines the suitability of these modeling techniques for a near-field emergency response model that must simulate the dispersion of a hazardous contaminant out to several kilometers from a source. For an emergency response model that must provide real-time dispersion estimates (a Class A model), a puff model is the most appropriate diffusion technique, and simple interpolation is the most appropriate wind-field technique. For more-complex models that are used for emergency planning and post-accident assessments (Class B models), a puff model is still suitable, but the wind-field technique should be able to remove spurious velocity divergence and channel the wind flow in complex terrain.

1. INTRODUCTION

The rapid advance of computer technology has stimulated the development of atmospheric dispersion models. Most of these computer models have separate diffusion and wind-field components. The diffusion component simulates the dilution of contaminant by atmospheric turbulence; the wind-field component transports the contaminant away from the source. Meteorologists have developed many modeling techniques for each of these components. These diffusion and wind-field techniques vary in their applicability to different release conditions, terrain characteristics, and spatial scales.

Dispersion models are an important part of emergency response systems that must deal with hazardous atmospheric contaminants. The most suitable modeling techniques for a particular emergency response model will depend on the model's purpose. Some of these models simulate dispersion on regional or larger scales. Others simulate near-field dispersion out to several kilometers from a source. Near-field models can be further divided into simple Class A models, which provide real-time estimates of transport and diffusion during accidental releases, and slower, more complex Class B models, which simulate releases in more detail. The Class B models are useful for planning and for post-accident assessments.

In this report we divide diffusion and wind-field modeling techniques into several broad categories. After examining the ability of each category to fulfill the requirements of an near-field emergency response model, we make recommendations concerning the most appropriate diffusion and wind-field categories for Class A and Class B dispersion models.

2. DISCUSSION OF AVAILABLE DIFFUSION TECHNIQUES

The diffusion techniques that meteorologists have developed for computer modeling generally fall into three categories: diffusion-equation, stochastic, and assumed-distribution techniques. In the following sections we will describe these categories and discuss their suitability for emergency response.

2.1. Diffusion-Equation Techniques

These techniques calculate the diffusion of a contaminant by solving the contaminant's continuity equation:

$$\frac{\partial \overline{\chi}}{\partial t} + \overline{u}_i \frac{\partial \overline{\chi}}{\partial x_i} = S - \frac{\partial}{\partial x_i} \overline{u_i' \chi'} \,. \tag{1}$$

Here χ denotes the contaminant concentration, t is time, S is a net source and sink term, and u_i is the velocity component in the direction x_i ($i = 1, 2, 3$); an overbar indicates a mean quantity, and a prime indicates a fluctuating quantity. Unless stated otherwise, we assume summation over repeated indices. The mean velocity component $\overline{u_i}$ on the left-hand side of Eq. (1) could come from one of the wind-field techniques that we will describe later. The mean product $\overline{u_i' \chi'}$ on the right-hand side of Eq. (1) is the turbulent flux of contaminant.

The major problem with diffusion-equation techniques is the well-known closure problem: Eq. (1) is not closed, because $\overline{u_i' \chi'}$ is an unknown second moment. One way to resolve this problem is to assume that the flux is proportional to the gradient of the first moment $\overline{\chi}$:

$$\overline{u_i' \chi'} = -K_{ij} \frac{\partial \overline{\chi}}{\partial x_j} \,, \qquad i, j = 1, 2, 3 \,. \tag{2}$$

This first-order closure assumption has its roots in molecular diffusion, where it works well. The proportionality constants K_{ij} are called eddy diffusivities; the off-diagonal elements are usually set to zero. With first-order closure, Eq. (1) becomes

$$\frac{\partial \overline{\chi}}{\partial t} + \overline{u}_i \frac{\partial \overline{\chi}}{\partial x_i} = S + \frac{\partial}{\partial x_i} K_{ij} \frac{\partial \overline{\chi}}{\partial x_j} \,. \tag{3}$$

Much effort has gone into finding analytical and numerical solutions for Eq. (3). Analytical solutions (Sutton, 1953) were popular before the advent of digital computers. First-order closure is also attractive because it is relatively simple to introduce inhomogeneous turbulence and chemical reactions into Eq. (3).

First-order closure has not generally been successful in simulating atmospheric diffusion, because Eq. (2) is only valid when the fluid motions responsible for the diffusion are small compared to the size of the contaminant cloud; this is clearly unrealistic for most situations in the atmosphere. The one situation where first-order closure appears to be adequate is for the vertical diffusion resulting from a surface release (Pasquill and Smith, 1983, Chapter 3).

To avoid the problems of first-order closure, meteorologists have developed second-order closure (Donaldson, 1973). Second-order closure introduces additional equations for the turbulent fluxes in Eq. (1). The resulting system of equations is still not closed, because the flux equations contain unknown third moments. To close the equations, meteorologists assume that the third moments are known functions of the first and second moments. Second-order closure produces more-realistic solutions than first-order closure, but it also requires considerable amounts of computer time.

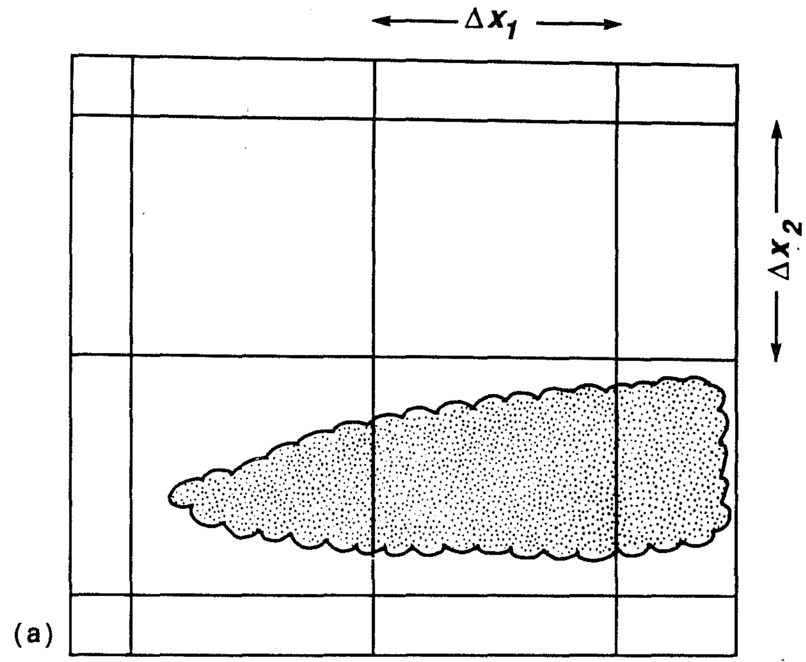
A limitation of all diffusion-equation techniques is that the computer grid size must be small enough to adequately resolve the contaminant cloud (Fig. 1). In first-order closure, for example, the resolution must be sufficient to calculate the local concentration gradient in Eq. (2). Such resolution is not difficult when the contaminant cloud has dimensions of kilometers or tens of kilometers, but for the near-field diffusion that is important in emergency response, adequate resolution may not be practical.

One emergency response system that uses a diffusion-equation technique is the Atmospheric Release Advisory Capability (ARAC; Dickerson *et al.*, 1985). ARAC uses a diffusion-equation technique called ADPIC (Lange, 1978), which, assuming incompressibility, combines the advection and flux terms in Eq. (3) to form a pseudo-velocity P_i at each grid cell:

$$P_i = \overline{u}_i - \frac{K_{ij}}{\overline{\chi}} \frac{\partial \overline{\chi}}{\partial x_j} \,. \tag{4}$$

ADPIC uses this field of pseudo-velocities to transport a cloud of contaminant particles through the model grid. A major advantage of this approach is that it can produce irregular concentration distributions in a complex flow field, provided the wind field has adequate resolution.

Although diffusion-equation techniques may be adequate for the large-scale diffusion covered by ARAC, we do not recommend them for Class A or Class B emergency response models that simulate dispersion in the near field. The ability of



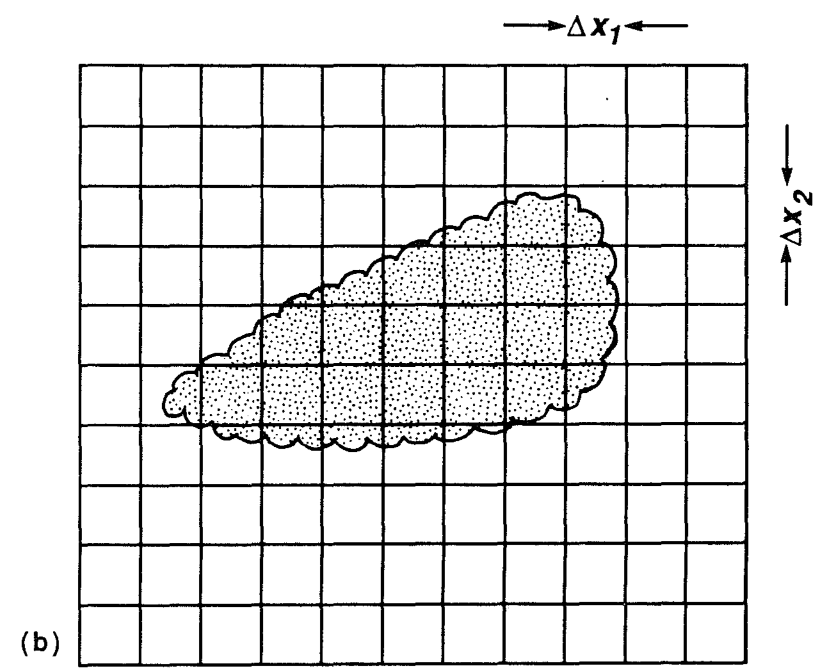


Figure 1. Schematic illustration of the grid-resolution problem encountered in diffusion-equation techniques. In (a), the grid size is not sufficient to resolve the contaminant cloud. In (b), the cloud is resolvable. The situation shown in (b) is not difficult to attain on larger scales, but it would be difficult to attain on the local scales important for emergency response.

models like ADPIC to produce irregular concentration distributions in complex terrain is a distinct advantage, but this is offset in near-field diffusion by the problems with first-order closure, the high grid resolution required, and the large amount of computer time needed to advect a large number of particles.

2.2. Stochastic Techniques

Stochastic techniques treat the turbulent velocity fluctuations of a fluid particle as a Markov process. The equation describing this process is (Smith, 1968)

$$u_i'(t+\tau) = R^L(\tau)u_i'(t) + u_i''(t)\,, \tag{5}$$

where t is time, τ is a time increment, $u_i'(t)$ is the particle's velocity fluctuation, $R^L(\tau)$ is a Lagrangian velocity correlation, and $u_i''(t)$ is a random velocity drawn from a known statistical distribution. Equation (5) implies that the autocorrelation for the particle's acceleration is proportional to the delta function $\delta(\tau)$; such an autocorrelation is only representative of turbulence in the inertial subrange (Sawford, 1984).

The main advantages of stochastic techniques are the simplicity of Eq. (5) and the ability to incorporate spatial variations in turbulence properties. Their major disadvantage is that Eq. (5) must be repeated for a large number of particles. The resulting particle distribution normally represents the time-averaged diffusion of a contaminant.

Simple applications of Eq. (5) for homogeneous turbulence (Smith, 1968) assume that $u_i''(t)$ is a Gaussian random variable with a constant variance. For inhomogeneous turbulence, $u_i''(t)$ can be drawn from more-complex distributions (Thomson, 1984). For the vertical velocity component, Cogan (1985) introduced plume rise into Eq. (5) by adding an extra velocity term to the right-hand side of the equation; this extra term represents the vertical velocity produced by buoyancy effects.

The necessity of repeating Eq. (5) for a large number of particles makes stochastic techniques generally unsuitable for emergency response. Furthermore, the concentration distributions that these techniques produce are often similar to the assumed distributions discussed in the next section. In homogeneous turbulence, for example, stochastic techniques give the same result as an assumed Gaussian distribution. Likewise, the more-complex distributions produced by stochastic techniques often correspond to assumed non-Gaussian distributions (Panofsky and Dutton, 1984, sections 10.3 and 10.6).

2.3. Assumed-Distribution Techniques

These techniques assume that the concentration distribution within a contaminant cloud has a specific mathematical form. The rate of growth of this distribution with travel time or downwind distance must be specified. The well-known Gaussian plume model (Hanna *et al.*, 1982) is one of the simpler assumed-distribution techniques:

$$\overline{\chi} = \frac{q}{2\pi U \sigma_2 \sigma_3} \exp\left[-\frac{1}{2}\left(\frac{x_2}{\sigma_2}\right)^2\right] \left\{\exp\left[-\frac{1}{2}\left(\frac{x_3 - h}{\sigma_3}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{x_3 + h}{\sigma_3}\right)^2\right]\right\} . \quad (6)$$

This model is best suited for elevated sources in flat terrain. In Eq. (6), $\overline{\chi}$ is the mean contaminant concentration, q is the contaminant release rate, $U = \sqrt{\overline{u}_i^2}$ is the (constant) mean wind speed, h is the height of the plume centerline, and σ_i is the plume standard deviation in the direction i. From Eq. (6) onward we will adopt the subscript convention that $i = 1$ is downwind, $i = 2$ is crosswind, and $i = 3$ is the vertical.

An assumed-distribution technique that is more appropriate for complex terrain is the puff model (Ludwig *et al.*, 1977; Mikkelsen *et al.*, 1984). Puff models release a series of contaminant puffs that move and diffuse semi-independently. Normally each puff has a three-dimensional Gaussian distribution:

$$\overline{\chi} = \frac{Q}{(2\pi)^{3/2}\sigma_1\sigma_2\sigma_3} \exp\left\{-\frac{1}{2}\left[\left(\frac{y_1}{\sigma_1}\right)^2 + \left(\frac{y_2}{\sigma_2}\right)^2 + \left(\frac{y_3}{\sigma_3}\right)^2\right]\right\} , \quad (7)$$

where Q is the total mass of contaminant in the puff and y_i ($i = 1, 2, 3$) is the displacement from the puff's center. The advantage of puff models is that only smaller-scale turbulent eddies appear statistically in the diffusion parameters σ_i, while larger-scale eddies appear explicitly in the wind field; in the Gaussian plume model all of the turbulence appears statistically in the diffusion parameters σ_i. This increased resolution in the wind field allows puff models to simulate some flow features in complex terrain. One example of the use of puff models in complex terrain is Rao *et al.*'s (1989) simulation of tracer dispersion in a nocturnal drainage flow.

2.4. Summary of Diffusion Techniques

In Table 1 we summarize the advantages and disadvantages of diffusion-equation techniques, stochastic techniques, the Gaussian plume model, and puff models. Of these techniques, puff models offer the best combination of computation speed and adaptability for emergency response: they do not have the closure and grid resolution problems of diffusion-equation techniques, and they can reproduce many of the results of stochastic techniques without modeling a large number of particles. Puff models are also applicable to a wider range of terrain features and atmospheric conditions than the Gaussian plume model. Because of these advantages, we recommend a puff model for both the Class A and Class B dispersion models.

Table 1. Advantages and disadvantages of various diffusion techniques discussed in text

TECHNIQUE	ADVANTAGES	DISADVANTAGES
Diffusion-equation techniques	Easy to introduce inhomogeneous turbulence and chemical reactions. Analytical solutions possible in simple situations.	Closure problem. Grid resolution problem.
Stochastic techniques	Relatively simple to install on a computer. Can introduce inhomogeneous turbulence.	Must be repeated for many particles. Results often similar to those of simpler techniques.
Gaussian plume model	Simplicity. Limited input requirements.	Not appropriate in complex terrain or nonstationary conditions. Not appropriate for light winds.
Puff models	Relatively simple. Can cope with complex terrain and light winds. Can introduce inhomogeneous turbulence to a limited extent.	Utility decreases if puffs become too large. Computation time rapidly increases with number of puffs.

3. DETERMINATION OF σ_i IN A PUFF MODEL

Normally puff models assume that the puff diffusion is axisymmetric about the vertical axis, so that $\sigma_1 = \sigma_2$. In the following sections we describe some models for σ_2 and σ_3 that may be suitable for an emergency-response puff model. We also discuss the effects of sampling time, wind shear, and negative buoyancy on puff diffusion.

3.1. Relation of puff diffusion to relative diffusion

A source of confusion with the term "puff model" is that many meteorologists use "puff diffusion" as a synonym for "relative diffusion." Actually, the concepts of relative diffusion and absolute diffusion apply equally to both puffs and plumes. When a puff is released into a field of turbulence, it not only diffuses about its center of mass, but the center of mass also meanders about its ensemble-average position, which is determined by the mean wind U. The ensemble-average diffusion about the puff's center of mass represents relative diffusion, whereas the combination of the relative diffusion and the ensemble-averaged meandering represents the absolute diffusion (Fig. 2).

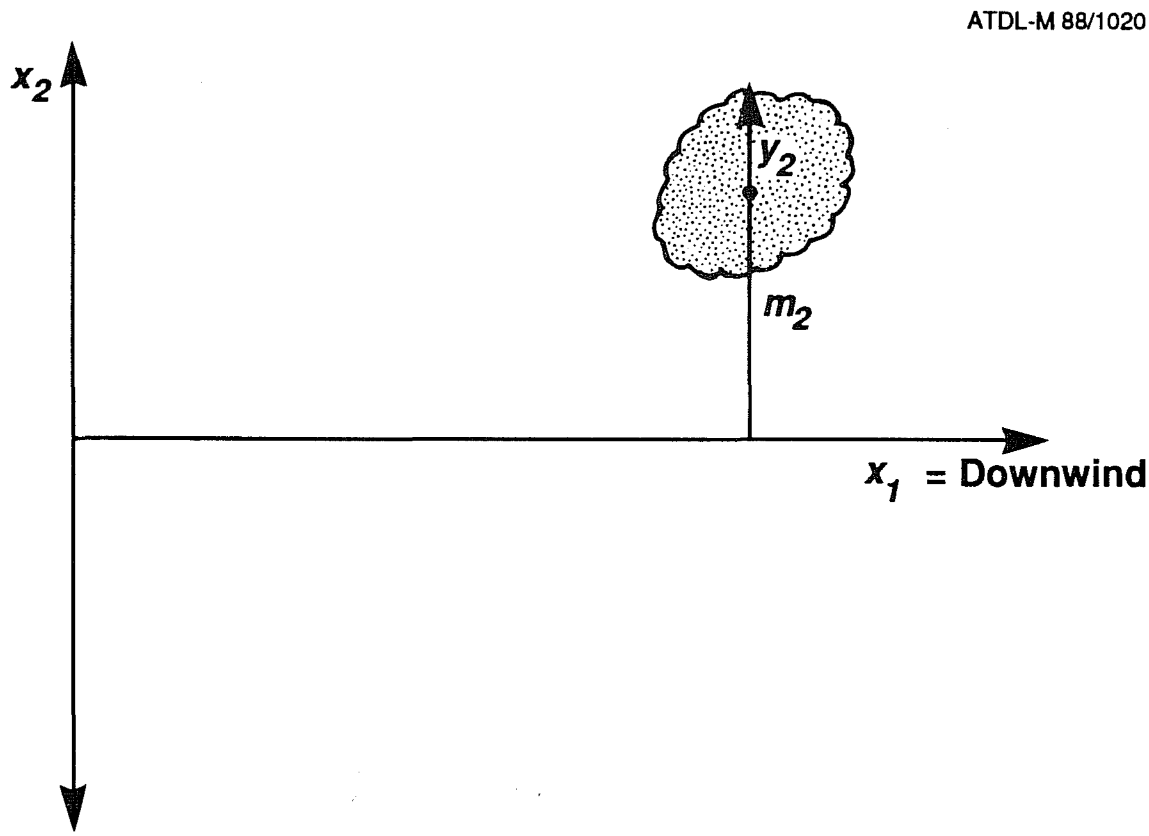


Figure 2. When a puff is released, it will not only undergo relative diffusion about its center of mass $(\overline{y_2^2})$, but the center of mass will also meander about the downwind axis $(\overline{m_2^2})$. The sum of $\overline{y_2^2}$ and $\overline{m_2^2}$ gives the absolute diffusion.

In practice, U and other velocity statistics are not ensemble averages, but time averages over an interval of length λ; therefore, the puff's absolute diffusion in this turbulence field will not contain contributions from turbulent eddies with time scales greater than λ. This high-pass filtering for puff diffusion is equivalent to the filtering that occurs when a continuous plume is sampled over a finite interval λ.

3.2. Models for σ_2 and σ_3

At the present time, the best models for σ_2 and σ_3 use direct measurements of the lateral and vertical velocity standard deviations η_2 and η_3 (Hanna *et al.*, 1977; Irwin, 1983). These models start with a form of Taylor's (1921) equation:

$$\sigma_i^2 = \eta_i^2 T^2 \int_0^\infty S_i^L(\omega) \frac{\sin^2(\omega T/2)}{(\omega T/2)^2}\, d\omega\,, \qquad \text{no summation implied,} \tag{8}$$

where T is travel time and $S_i^L(\omega)$ is the normalized Lagrangian velocity spectrum for angular frequency ω. (No summation over indices is implied in this section). If a function $f_i(T)$ is defined as

$$f_i^2(T) = \int_0^\infty S_i^L(\omega) \frac{\sin^2(\omega T/2)}{(\omega T/2)^2}\, d\omega\,, \tag{9}$$

then (8) reduces to

$$\sigma_i = \eta_i T f_i(T)\,. \tag{10}$$

Most practical applications of diffusion theory use the downwind distance X instead of T, so meteorologists usually replace Eq. (10) with the equation

$$\sigma_i = \eta_i \frac{X}{U} f_i'(X/U)\,. \tag{11}$$

The mean wind U is usually measured at the release height. As long as the ratio X/U is a good estimate of T, $f_i'(X/U)$ in Eq. (11) will be similar to $f_i(T)$ in Eq. (10).

Since no general theoretical relations are available for f_i', Pasquill (1976), Draxler (1976), and others have developed empirical models for this function. Comparisons of these models with data have produced somewhat confusing results. Irwin (1983) compares several models for f_i' ($i = 2, 3$) with data from surface and elevated releases. He finds three models (his Models 1, 3, and 4) that perform reasonably well in both stable and unstable conditions. Irwin's (1983) models for f_i', however, do not fit Hanna's (1986) more-recent data from elevated releases. Doran *et al.* (1978) cloud the issue further by showing that f_i' can vary with the sampling time of the σ_i measurements, the averaging time of the η_i measurements, and several other factors.

Emergency response models will usually be dealing with accidental releases that are at or near the surface. Since there is no consensus on the best forms of f_i' for a surface release, we recommend the following:

$$\frac{1}{f_2'} = 1 + 0.9\sqrt{\frac{X}{300U}}, \tag{12a}$$

$$\frac{1}{f_3'} = \begin{cases} 1 & \text{unstable conditions} \\ 1 + 0.9\sqrt{\frac{X}{50U}} & \text{stable conditions.} \end{cases} \tag{12b}$$

Equation (12a) is Draxler's (1976) empirical fit to surface-release data; Eq. (12b) is from Model 3 in Irwin's (1983) paper. This combination is relatively simple and performs well in Irwin's comparisons with surface-release data. The corresponding curves for σ_2 and σ_3 are plotted in Fig. 3.

As we discussed in Section 2.3, σ_i in a puff model represents the effects of small-scale turbulent eddies that do not appear explicitly in the wind field. If the wind field is an average over an interval of length λ, then σ_i should represent diffusion with a sampling time λ. Although the actual variation of σ_i with sampling time is complicated, a rough estimate using Eq. (11) is to calculate the velocity statistic η_i from a turbulence sample of length λ.

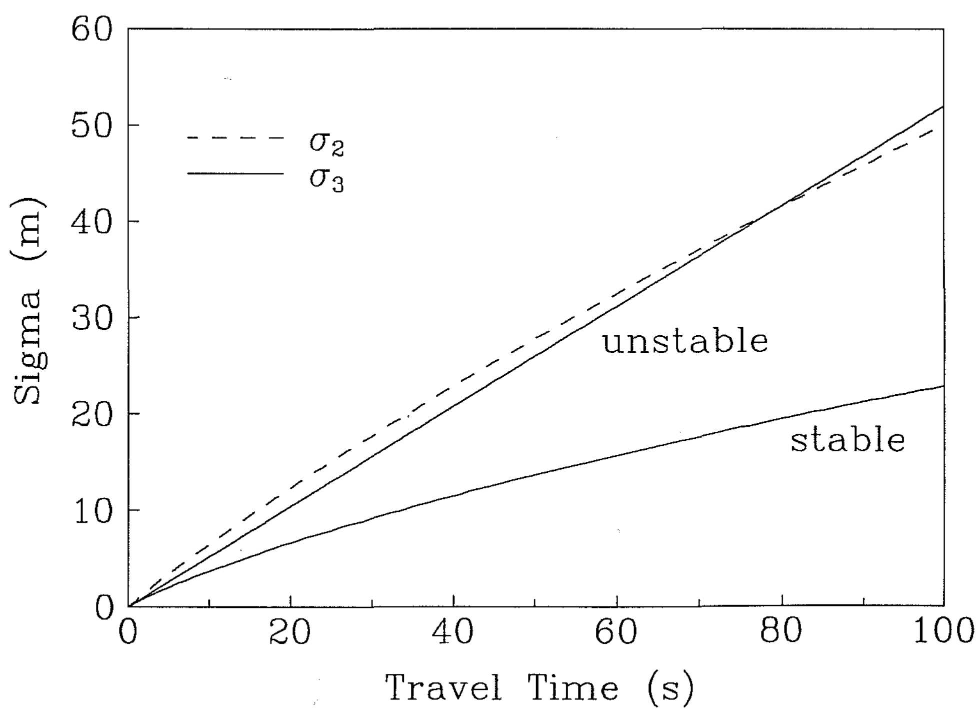


Figure 3. Empirical curves for σ_2 and σ_3. The velocity standard deviations η_2 and η_3 were estimated as $1.9u_*$ and $1.3u_*$, respectively (u_* = friction velocity = $0.4\,\text{m/s}$).

When measurements of η_i are not available at a site, more empirical estimates of the diffusion are necessary. The most common of these empirical methods is the Pasquill-Gifford curves (Hanna *et al.*, 1982, Chapter 4). Each curve for σ_2 and σ_3 in this set corresponds to one of the six Pasquill stability classes, which range from A (very unstable) to F (moderately stable). An observer estimates the stability class at a particular location by looking at wind speed, insolation, and cloud cover. An emergency response model should only use the Pasquill-Gifford curves and similar schemes as a last resort when no turbulence data are available.

The Pasquill-Gifford curves were derived from surface-release data with sampling times of a few minutes. The curves will hence be most appropriate in puff models that use winds averaged over a few minutes. However, the curves are often used for hour-average diffusion, mainly because no alternatives are available.

3.3. Effects of wind shear and negative buoyancy

For elevated releases, the ratio X/U will usually be a good estimate of the travel time T. For surface releases, however, the vertical wind shear complicates matters. This wind shear will alter the relation between T and X, which will in turn alter the relation between f_i in Eq. (10) and f_i' in Eq. (11). In the following paragraphs we will show that the empirical model for f_i' in Eq. (12a) may be at least partly due to the effects of wind shear.

For a surface release in neutral conditions, Lagrangian similarity theory predicts that the mean downwind distance X and mean height Z of a contaminant cloud will be related through the logarithmic wind profile (Batchelor, 1964):

$$\frac{dX}{dT} = \frac{u_*}{k_a} \ln\left(\frac{cZ}{z_0}\right) , \tag{13}$$

where u_* is the friction velocity, k_a is the von Kármán constant ($\simeq$ 0.4), z_0 is the aerodynamic roughness length, and c is a constant with an approximate value of 0.56 (Chatwin, 1968). Lagrangian similarity theory also predicts that dZ/dT should be proportional to u_* in neutral conditions (Batchelor, 1964):

$$\frac{dZ}{dT} = k_a u_* . \tag{14}$$

The combination of Eqs. (13) and (14) gives X for a surface release as a (nonlinear) function of T. We can use this relation to obtain a simple model for f_2'. The first step is to combine Eqs. (10) and (11) into an equation for f_2':

$$f_2'(X/U) = \frac{UT}{X} f_2(T) . \tag{15}$$

The functions f_2 and f_2' will not be equal for surface releases, because of the nonlinear relation between T and X. If we now assume that $f_2 = 1$ and that Eqs. (13) and

(14) determine the relation between T and X, then the solid curve in Fig. 4 shows the resulting variation of f_2' with X. To obtain this curve we assumed that the release height h is 2 m (typical for field experiments), $u_* = 0.4\,\mathrm{m/s}$, and $z_0 = 5\,\mathrm{cm}$. The wind speed U was determined by using $Z = h = 2\,\mathrm{m}$ in Eq. (13). Because we set f_2 equal to unity, the only source of variation in this model for f_2' is the transformation from T to X.

The dashed curve in Fig. 4 is Eq. (12a). This curve uses U at the (near-surface) release height, which is the normal procedure in applications of Eq. (12a). The resemblance of the two curves in Fig. 4 suggests that the variation of f_2' in Eq. (12a) is at least partly due to the nonlinear relation between X and T that results from vertical wind shear. The empirical model for f_3' (Eq. (12b)) may also reflect the effects of wind shear, although the situation is more complicated for vertical diffusion, because η_3 is a function of height in the surface layer (Panofsky and Dutton, 1984). One reason that Irwin (1983) also obtained a result resembling Eq. (12a) for elevated sources may be that most of his elevated-release data comes from experiments with receptors at or near the surface.

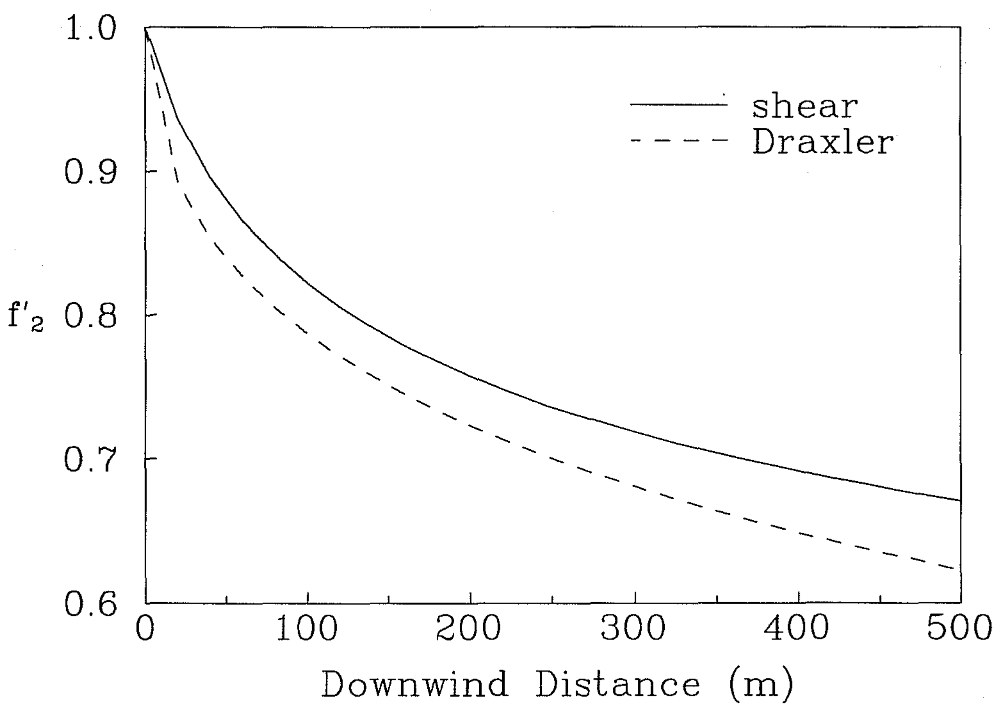


Figure 4. Comparison of Draxler's (1976) model for f_2' and the wind-shear model discussed in text. The similarity of the curves suggests that Draxler's empirical model is at least partly a result of wind shear in the surface layer. The wind-shear model assumes that the release height is 2 m, $u_* = 0.4\,\mathrm{m/s}$, and $z_0 = 5\,\mathrm{cm}$.

Another phenomenon that is potentially important for an emergency response diffusion model is the effects produced by contaminants that are denser than air (*e.g.*, Zeman, 1982). The initial diffusion of dense gases differs from that of passive contaminants in two major ways: gravitational spreading influences the diffusion of dense-gas clouds, and the ambient turbulence is not the dominant source of mixing within dense-gas clouds. We will not discuss dense gas modeling in detail here, but will only mention that several models are available to account for dense-gas effects (*e.g.*, Ermak *et al.*, 1988). These dense-gas effects will be important until the cloud is diluted enough that it behaves like a passive contaminant.

4. DISCUSSION OF AVAILABLE WIND-FIELD TECHNIQUES

So far we have only discussed the diffusion component of an emergency response model. The other important component is the wind field that transports the contaminant. Over the last two decades, the meteorological community has developed many techniques to generate wind fields from scattered measurements. Most of the techniques fall into four categories: interpolation, mass-conservative, diagnostic, and dynamic techniques. These categories are based in part on those defined by Yocke and Liu (1979) and Moussiopoulos and Flassak (1986). We describe these categories in more detail below.

4.1. Interpolation Techniques

These techniques generate a wind field by forcing an arbitrary, smooth transition from one wind measurement to another. They do not contain any physical constraints such as conservation of mass or Newton's second law. Meteorologists have developed several different interpolation techniques for wind fields. We will describe some of the more common techniques in the following paragraphs.

When wind measurements at only one location are available, the most obvious extrapolation is to assume that the wind field is spatially uniform. Gaussian plume models (Hanna *et al.*, 1982) require a spatially uniform wind field that is also constant in time. Mikkelsen *et al.* (1984) also use a spatially uniform wind field in their puff-model simulation of dispersion out to downwind distances of several hundred meters; by retaining the temporal variations in the wind, they can simulate smaller-scale meandering that Gaussian plume models only represent statistically. Clearly, a spatially uniform wind field will only be realistic within a limited area around the measurement location. In flat terrain the single measurement may be representative for at least 1 km downwind of a source (Mikkelsen *et al.*, 1984).

The simple interpolation discussed above is only useful in somewhat special situations. Goodin *et al.* (1979) describe three more-general techniques. The most common of the three is to compute a distance-weighted average of the surrounding measurements. Suppose velocity measurements are available at n locations in the region of interest. Let u_{ij} represent the i'th velocity component ($i = 1,2,3$) measured at location j ($= 1,2,\ldots,n$). Then the interpolated velocity v_{ik} at some arbitrary location k is defined as

$$v_{ik} = \frac{\sum_{j=1}^{n} u_{ij} W(r_{jk})}{\sum_{j=1}^{n} W(r_{jk})} , \tag{16}$$

where $W(r_{jk})$ is a weighting function depending on the separation r_{jk} between locations j and k. A common form for $W(r_{jk})$ is an inverse power:

$$W(r_{jk}) = r_{jk}^{-p} . \tag{17}$$

Most weighted-interpolation models use Eq. (17) with $p = 2$ (Wendell, 1972; Nyren *et al.*, 1984); this is the well-known "$1/r^2$" interpolation technique. The mass-conservative techniques that we will discuss in the next section often use $1/r^2$ interpolation to generate an initial wind field (Sherman, 1978; Davis *et al.*, 1984; Barnard *et al.*, 1987). Goodin *et al.* (1980) and Mulholland and Jury (1987) use Eq. (17) with the less-common power $p = 1$.

Two possible refinements of weighted interpolation are to use only measurements within a certain radius (the "radius of influence") of a given location (Kitada *et al.*, 1983; Ross and Smith, 1986) or to use only the three closest measurements (Sherman, 1978). These restrictions limit the effects at a particular location of distant measurements.

The second, more-complicated technique that Goodin *et al.* (1979) discuss is a least-squares fit of a polynomial either to all the data or to a subset of the data. Panofsky (1949) and Gilchrist and Cressman (1954) use polynomial interpolation for weather-map analysis, but no one, as far as we know, has used it in practice for local wind fields—fitting even a second-degree polynomial requires solving six simultaneous equations. Nonetheless, Goodin *et al.* (1979) conclude that the second-degree polynomial interpolation they use performs better than other techniques they consider.

The third technique Goodin *et al.* (1979) mention is optimum interpolation. This technique uses spatial covariances derived from archived data to interpolate present data. Several meteorologists, including Dartt (1972), have used optimum interpolation for synoptic-scale flow. Porch and Rodriguez (1987) seem to be the only ones so far to use archived covariances in a model for local wind fields.

Interpolation techniques are common in emergency response models. They are easy to install and run on a computer and require only a limited amount of input data. In fact, with only a single meteorological tower at a site, the spatially uniform winds used by Gaussian plume models and some puff models may be the only practical alternatives for emergency response. When a network of towers is available, distance-weighted interpolation becomes an attractive alternative (Mulholland and Jury, 1987).

4.2. Mass-Conservative Techniques

A good approximation for the wind fields in diffusion models is that the atmosphere is incompressible. For an incompressible mean flow the continuity equation is

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0\,. \tag{18}$$

A major problem with interpolation techniques is that the wind fields they create do not generally obey Eq. (18). As discussed by Kitada (1987), significant deviations from Eq. (18) in a diffusion-model wind field will produce fictitious sources and sinks of contaminant. To correct this problem with interpolation, meteorologists have developed techniques that adjust interpolated wind fields so that they do obey the continuity equation. We will call these techniques mass-conservative, because they contain the continuity equation, but no other physical constraints.

Dickerson (1978) and Sherman (1978) discuss one common mass-conservative technique. This technique uses the variational analysis theory developed by Sasaki (1958, 1970) to impose mass conservation on an initial, interpolated wind field. The variational analysis theory finds a mass-conservative wind field that resembles the initial wind field as closely as possible.

Another mass-conservative technique applies a finite-difference form of Eq. (18) directly to each cell in a wind-field grid. Liu and Goodin (1976) use this finite-difference technique to construct a two-dimensional (horizontal) wind field; Goodin *et al.* (1980) and Erasmus (1986) use it to construct three-dimensional wind fields. Since wind adjustments at one grid point will alter the divergence at surrounding points, this finite-difference technique requires several iterations of the divergence reduction procedure.

Equation (18) alone does not produce a unique solution for the wind field, because it contains three unknowns. Mass-conservative techniques must therefore provide a way to choose one solution from the many that satisfy Eq. (18). Usually these techniques use stability parameters (Sherman, 1978) to determine how wind adjustments will be distributed among the three velocity components. In stable conditions the models remove velocity divergence mainly by adjusting the horizontal components; in unstable conditions they mainly adjust the vertical component.

Mass-conservative techniques provide a simple means of including terrain in an emergency response model, although the main justification for these techniques has been their ability to remove spurious velocity divergences. The greater complexity of these techniques relative to interpolation has hindered their use in emergency response. One major system that does use a mass-conservative technique is the ARAC system discussed earlier. ARAC requires about 45 minutes to use the full capability of its mass-conservative model (Dickerson *et al.*, 1985).

4.3. Diagnostic Techniques

Like mass-conservative techniques, diagnostic techniques adjust an initial wind field so that the final, steady-state wind field obeys certain physical constraints. But these techniques use other physical constraints in addition to mass conservation. The additional constraints are often simplified forms of the momentum equation.

Fosberg *et al.* (1976) present an example of a diagnostic technique. This technique simulates the effects of thermal forcing and momentum transfer to the ground by using simplified forms of the divergence equation and the vorticity equation. Fosberg *et al.* eliminate the time dependence in the divergence and vorticity equations by integrating the equations over a square-wave impulse of duration Δt. At each grid point the model initially requires the terrain height, temperature, pressure, and roughness length; the model's initial wind field is spatially uniform.

Lanicci and Ward (1987) describe another diagnostic technique. Their model retains two terms in the momentum equation: the momentum advection term $\overline{u}_j \partial \overline{u}_i / \partial x_j$ and the component of the buoyancy force

$$B_3 = -g \frac{\theta_0 - \theta_s}{\theta_0} \tag{19}$$

that is parallel to the local terrain slope, where θ_s is the surface potential temperature, θ_0 is a reference potential temperature above the surface, and g is the the gravitational acceleration. As in the model by Fosberg *et al.* (1976), this model has no time derivatives, and therefore represents steady-state conditions.

Mass-conservative techniques rely on the initial, interpolated wind field to provide information about major flow features such as buoyancy-driven flows. The two diagnostic techniques discussed above shift the burden of finding the major flow features to the model equations; the initial wind fields in these models are uniform (and represent the large-scale flow). This implies that the model equations can simulate at least some of the important flow features in complex terrain.

Diagnostic techniques have not been used for emergency response, because they are generally more complex than both interpolation and mass-conservative techniques. Lanicci and Ward's (1987) diagnostic model does resemble an emergency response model in some ways; it simulates surface-layer winds during military operations.

4.4. Dynamic Techniques

Dynamic techniques use a full system of primitive equations that govern atmospheric motion. Normally this system will contain forms of Newton's second law, the first law of thermodynamics, the mass continuity equation, and the equation of state. Often dynamic models define these equations in a terrain-following coordinate system. Including water or other atmospheric chemicals in a dynamic model requires additional equations in the system.

Unlike the three other technique categories, dynamic techniques are prognostic in nature: given a set of initial and boundary conditions on a grid, they simulate the temporal evolution of the velocity and thermodynamic variables. Examples of such models are those of Pielke (1974), Anthes and Warner (1978), and Yamada (1981, 1983). Specific applications to pollutant transport include the investigations by McNider (1981) and Garret and Smith (1984) into buoyancy-driven flow over complex terrain, and the paper by Segal *et al.* (1982) concerning the coupling of sea breezes and synoptic forcing in a coastal region. Pielke (1984) gives a good description of dynamic models and their uses in mesoscale meteorology.

Because a dynamic model must solve the primitive equations on a grid with finite space and time increments, some atmospheric phenomena will be too small or too short-lived for the model to resolve explicitly. Each variable b is therefore the sum of an averaged, resolvable component $\overline{b}$, and a subgrid-scale component b':

$$b = \overline{b} + b' \ . \tag{20}$$

This separation produces the same closure problem that was discussed in Section 2.1: the primitive equations for first-moment variables such as $\overline{b}$ will contain second moments such as $\overline{u_i' b'}$. The dynamic models described by Pielke (1974), Garret and Smith (1984), and Moore *et al.* (1987) resolve the closure problem by using first-order closure. Yamada (1981, 1983) uses second-order closure. The drawback to the higher-order closure models is that the number of equations increases rapidly with the order.

No operational emergency response systems presently use dynamic techniques for real-time simulations.

4.5. Effects of Averaging Time, Wind Shear, and Negative Buoyancy

The performance of the wind field in an emergency response model will be affected by the averaging time of the wind measurements, by wind shear, and by negative buoyancy. If the diffusion model is a puff model, the wind-field averaging time is directly proportional to the sampling time for the diffusion parameters σ_i. As the averaging time of the wind field in a puff model decreases, more of the larger-scale turbulent eddies appear explicitly in the wind field instead of implicitly in σ_i. For emergency response, a smaller averaging time will usually be better, because the hazard from accidental releases often results from high short-term concentrations that do not show up in models that predict time-averaged (say, one-hour average) concentrations. However, the benefits of a smaller averaging time must be weighted against the potential increases in equipment investments and computer time.

As we discussed in Section 3.3, the empirical equations for f_i' ($i = 2, 3$) seem to account for near-surface wind shear to a limited extent. For most situations, we feel the the effects of local wind shear on pollutant transport will be of secondary importance compared to the problem of identifying the major flow features in complex terrain. Therefore, we recommend that an emergency-response puff model use the wind at or near the puffs' centers to transport the puffs. For surface releases, the wind at several meters above the local surface would be a reasonable estimate of the transport wind.

Negative buoyancy will be an important consideration for pollutant transport in an emergency response model. On a terrain slope, the transport of dense gas can be decoupled from the ambient wind. Even in flat terrain large dense-gas clouds tend to move slower than the ambient wind (Ermak *et al.*, 1988). A simple way to account for the buoyancy-induced transport of dense gas on a slope is to use the along-slope component of a buoyancy force similar to that in Eq. (19):

$$\hat{B}_3 = -g\frac{\rho_c - \rho_0}{\rho_0} \,. \tag{21}$$

This equation uses the same variables as Eq. (19) except for the gas-cloud density ρ_c (which is a function of time) and the ambient density ρ_0. The transport produced by the buoyancy force $\hat{B}_3$ should be added to the transport produced by the ambient wind. A more refined model for dense-gas transport might also include the effects of frictional retardation on the cloud's movement.

5. SUITABILITY OF THE FOUR WIND-FIELD TECHNIQUE CATEGORIES

Any of the wind-field categories we have discussed could be used with the puff-model technique we recommended in Section 2. But a wind-field technique suitable for an emergency response system should fulfill the following criteria:

(*a*) The technique should be appropriate for the range of terrain features and atmospheric conditions present at the expected release locations.

(*b*) The technique should not require an unrealistically large investment in meteorological and computer equipment.

(*c*) The technique's computation time on a desktop computer or microcomputer should be within the limits set by Class A and Class B diffusion models. A Class A model must provide real-time dispersion estimates at the time of a release; a Class B model does not have to run in real time, but it should be able to run within a reasonable period of time (within 30 minutes, say).

(*d*) In comparisons with observed winds, a more-complex technique should perform better than simpler techniques. If a more-complex technique is unable to do so, then the simpler technique should be used.

Simple interpolation techniques, such as a spatially uniform wind field derived from a single tower measurement, will clearly have difficulty fulfilling criterion (*a*) in complex terrain. Multi-tower interpolation, mass-conservative, diagnostic, and dynamic techniques should all satisfy criterion (*a*) in complex terrain, although interpolation and mass-conservative techniques will do poorly unless the spatial density of wind measurements is sufficient to resolve the important flow features. One situation where the spatial density of measurements may not be sufficient is light winds, when local flow features predominate (Ross and Smith, 1986).

Criterion (*b*) is mainly of concern for dynamic techniques. These techniques require detailed initial and boundary conditions to perform properly (Yocke and Liu, 1979; Moussiopoulos and Flassak, 1986). Small errors in these initial and boundary conditions can propagate and have significant effects on the final wind field. The input data necessary to use a dynamic technique in an emergency response system would require an unrealistic investment in equipment.

Computation-time constraints, criterion (*c*), will be a problem for mass-conservative, diagnostic, and dynamic techniques. A recent test at ATDD of a mass-conservative model showed that the model requires about an order of magnitude more computation time on a microcomputer than $1/r^2$ interpolation (approximately 30 minutes versus 3 minutes for a $67 \times 43 \times 30$ grid-cell array). Optimization procedures (Ross and Smith, 1986) can make mass-conservative techniques fast enough for Class B models, but these optimized versions are probably still not fast enough for Class A models. Diagnostic techniques seem to have computation times comparable to mass-conservative techniques; they may be fast enough for a Class B model. Dynamic techniques will probably be too slow for both Class A and Class B models; they require solving a system of several finite-difference equations on a grid.

Criterion (*d*) is not easy to apply, because an objective, consistent method for evaluating model performance is difficult to develop. The best approach will probably be a set of statistics similar to that described by Fox (1981) for concentration predictions. The literature does not contain many comparisons of different wind-field techniques. The few comparisons that are available often use only a single statistic. Lanicci and Weber (1986), for example, use the root-mean-square difference between observed and predicted wind components to compare an interpolated wind field with the wind field from their diagnostic model. This statistic indicates that their model is not doing any better than interpolation, although they do get better results when some of the meteorological towers are excluded from the input.

An indirect way of assessing the skill of wind-field techniques is to evaluate the concentration predictions of dispersion models that contain different wind-field components. The disadvantage of this kind of comparison is that the wind fields will not be the only source of variations in model skill. A good basis for an indirect wind-field evaluation is the work by Lange (1985). He investigates the variations in dispersion-model skill that occur when both model complexity and the number of wind observations are varied systematically. The statistic he uses is the percentage of predicted concentrations that come within a factor of five of the observed concentrations. Even with 47 surface-wind observations and 8 vertical profiles, Lange's statistic only increases from 38% to 44% when going from a dispersion model with interpolated winds to one with mass-conservative winds (rows 3 and 4 in Lange's Table 5.2); with only three surface stations and one estimated profile, the increase is from 30% to 32%.

Weber and Kurzeja (1984) also present dispersion-model comparisons that are relevant to the evaluation of wind-field techniques. They use a set of statistics to compare observed concentrations with the predictions of several dispersion models. Their results are consistent with Lange's (1985), in that the model with a mass-conservative wind field did slightly better than models with simpler wind fields.

Table 2 is a summary of the discussion in this section.

6. CONCLUSIONS AND RECOMMENDATIONS

We recommend a puff-model technique for both the Class A and Class B dispersion models. Puff models combine simplicity with a limited ability to cope with complex terrain and light-wind conditions. Although the use of wind-sheared puffs is intuitively appealing for surface releases, we do not know whether this addition will improve the performance of a puff model. We do feel that dense-gas effects are important, because the subdued mixing within dense-gas clouds can significantly affect concentrations at ground level.

Our recommendations for wind-field techniques differ for the Class A and Class B models. Because mass-conservative and diagnostic techniques run rather slowly on current desktop computers and microcomputers, distance-weighted interpolation should be the best choice for Class A diffusion models. For Class B models, either a mass-conservative or diagnostic technique will probably be best; both these technique categories account for terrain features and remove spurious divergences in the wind field. Further evaluations are needed to determine whether the more-complex diagnostic techniques actually perform better than the mass-conservative techniques.

Because many hazardous atmospheric contaminants are denser than air, we recommend that both Class A and Class B models provide for the buoyancy-driven transport of dense-gas clouds. This buoyancy-driven transport will dominate during the initial stages of the cloud's dispersion. Once the cloud becomes sufficiently diluted, it will move with the ambient wind.

Table 2. Advantages and disadvantages of various wind-field techniques discussed in text

TECHNIQUE	ADVANTAGES	DISADVANTAGES
Interpolation	Simplicity. Short computation time. Limited input requirements.	Uniform winds inappropriate in complex terrain. Major flow features must be inherent in the input.
Mass-conservative	Removes spurious divergence. Channels flow over complex terrain. Slightly more skill than interpolation.	Long computation time. Major flow features must be inherent in the input.
Diagnostic	Can simulate flow features not inherent in input. Appropriate for complex terrain. Removes spurious divergence.	Long computation time. Large amount of input required.
Dynamic	Can simulate a wide range of atmospheric phenomena.	Very long computation time. Difficult to initialize. Closure problem. Grid resolution problem.

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