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Description and Validation of ERAD: An Atmospheric Dispersion Model for High Explosive Detonations

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Description and Validation of ERAD: An Atmospheric Dispersion Model for High Explosive Detonations

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Abstract

The Explosive Release Atmospheric Dispersion (ERAD) model is a three-dimensional numerical simulation of turbulent atmospheric transport and diffusion. An integral plume rise technique is used to provide a description of the physical and thermodynamic properties of the cloud of warm gases formed when the explosive detonates. Particle dispersion is treated as a stochastic process which is simulated using a discrete time Lagrangian Monte Carlo method. The stochastic process approach permits a more fundamental treatment of buoyancy effects, calm winds and spatial variations in meteorological conditions. Computational requirements of the three-dimensional simulation are substantially reduced by using a conceptualization in which each Monte Carlo particle represents a small puff that spreads according to a Gaussian law in the horizontal directions. ERAD was evaluated against dosage and deposition measurements obtained during Operation Roller Coaster. The predicted contour areas average within about 50% of the observations. The validation results confirm the model's representation of the physical processes.

MASTER

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1.0 Introduction

Acts of terrorism involving the intentional dispersal of radioactive material by use of high explosive can result in severe radiological consequences. The storage and transportation of nuclear weapons raises similar concerns in that accidental detonation of a weapon's chemical explosive may disperse radioactive material over large areas. An important part of the response to these incidents is the capability to make timely estimates of the downwind spread of the cloud of radioactive particles. This is particularly true at locations within a few tens of kilometers from the detonation point where the health hazard is most severe. Results of these calculations can be used to make decisions regarding evacuation and sheltering and to estimate the potential size of the cleanup operation.

When a device containing high explosive and nuclear material is detonated, a large portion of the energy released heats the surrounding air to form a warm gaseous cloud, or thermal. The cloud rises, entrains ambient air, and cools as it moves downwind. The explosion breaks the nuclear material within the device into small particles which initially rise and move along with the cloud of heated gases. These particles, with aerodynamic[†] diameters ranging from tenths to hundreds of micrometers, continue to move with the cloud until gravitational or turbulent forces cause them to break away from the cloud and fall toward the ground. Once free from the cloud's influence, the particles do not assume simple ballistic trajectories but, instead, follow random paths determined by the turbulent atmospheric flow.

This report describes the Explosive Release Atmospheric Dispersion (ERAD) model. ERAD is a three-dimensional numerical simulation of particle dispersion in the atmosphere that includes initial cloud dynamics, buoyancy effects and turbulent diffusion. The model was developed to provide real-time predictions of the near-field radiological hazards which result from an explosive release[‡] using a small field-deployable computer. In this context, near-field refers to dispersion on a scale of several tens of kilometers from the source.

A defensible assessment of an atmospheric dispersion model's performance can only be made by comparing predictions with observations; evaluations based on inter-model comparisons prove very little. The best available empirical information on dispersal from high explosive detonations was collected during the Operation Roller Coaster field program. In this report, ERAD is tested by comparison with dose and deposition measurements from two of the Roller Coaster events: Double Tracks and Clean Slate 1. The validation studies confirm the efficacy of the ERAD dispersion algorithms and demonstrate the model's ability to provide reliable predictions in real-time.

[†] The aerodynamic diameter is defined as the diameter of a unit density sphere with the same gravitational settling velocity as the particle of interest (e.g., Hinds, 1982). All particle diameters used in this report refer to aerodynamic diameter.

[‡] The ERAD model has been extended to treat buoyant, continuous (e.g., fire) and nonbuoyant sources. Documentation of the continuous source plume rise model is in preparation. The treatment of a nonbuoyant release, whether instantaneous or continuous, is straightforward — all buoyancy terms are set to zero.

The approach used in ERAD can be conveniently separated into two parts: buoyant cloud rise and particle diffusion. Separating the two components in this way is possible because the dynamics and thermodynamics of the cloud of warm gases that forms on detonation are insensitive to the presence of the particles, i.e., the particles can be treated as a passive tracer moving freely within the buoyant cloud and ambient. With this conceptualization, the gaseous cloud is treated as a localized region within the atmosphere whose properties differ from those of the ambient flow. The combination of these two components together with a wind field model provides a complete description of the dispersing ensemble of particles as a function of time.

2.0 Cloud Rise

The cloud formed following detonation of a high explosive is initially very buoyant; a typical value of the initial plume density is 20% less than that of the surrounding air. To take into account buoyant rise, many predictive models use empirical correlations to determine an effective "final rise" or "stabilized cloud height" which is a function of the energy released (Church, 1969). Using an empirical initial distribution of particle mass within the cloud, the dispersion is then tracked from this stabilized condition. In reality, for some meteorological conditions, "final rise" may not occur within any downwind distance of practical interest. Further evidence of the importance of buoyant rise has been shown in laboratory investigations. Willis and Deardorff (1983) and Willis and Hukari (1984) have demonstrated in a series of convection tank experiments the highly skewed nature of the vertical concentration profile and the substantial reduction in ground-level concentration due to plume buoyancy.

To realistically treat buoyancy effects from time zero onward, the cloud of warm gases which forms when the explosive detonates is modeled using the integral technique. The governing equations are obtained by integrating the three-dimensional partial differential conservation equations for mass, momentum and energy across the cloud cross section. The resulting integral equations are reduced to a set of coupled ordinary differential equations on the cloud centerline variables by making assumptions regarding (a) cloud symmetry, (b) the shape of the property profiles across the cloud, and (c) the methodology for treating entrainment and the effects of the pressure drag force. Only the macroscopic plume characteristics, e.g., cloud radius, height, temperature and velocity, are predicted with this technique; details of the cloud's internal structure are ignored.

The cloud is assumed to be composed of an equilibrium mixture of dry air, water vapor and liquid water. Particulate material and gases formed on detonation are neglected since they constitute a very small fraction of the thermal mass. This approach represents an improvement over simple empirical formulas for stabilized height since it provides a complete description of both the physical and thermodynamic properties of the gaseous cloud as functions of time, accounting for ambient density stratification and cross flow. Details of the cloud rise model can be found in Boughton and DeLaurentis (1987).

3.0 Particle Diffusion

In ERAD, particle dispersion is treated as a stochastic process which can, in turn, be simulated using a discrete time Lagrangian Monte Carlo method. The stochastic process approach provides a more general description of particle dispersion than the conventional continuum methods and allows for a more fundamental treatment of buoyancy effects, droplet evaporation, calm winds and time or space variability in meteorological conditions. Contemporary descriptions of atmospheric turbulence can also be incorporated within the framework of this modeling approach.

The underlying mathematical model is described in terms of the governing stochastic differential equations in section 3.1. This is followed by a section which relates the continuous time stochastic process to a discrete time Lagrangian Markov chain. In section 3.3, we describe the behavior of the process as it interacts with the ground and present a method for simulating boundary conditions in which the deposition flux is proportional to the concentration. Subsequently, in section 3.4, we introduce a kernel density estimation method that improves simulation convergence by tracking "puffs" instead of individual particles. The final section of this chapter discusses the extension from a monodisperse to a polydisperse release and develops a stratified sampling variance reduction technique for the polydisperse case.

3.1 The Stochastic Differential Equations

In the Monte Carlo simulation, ensemble statistics such as dose and deposition are calculated by following the trajectories of a few thousand individual particles. The probability density for the stochastic process governing particle trajectories satisfies a Fokker-Planck equation that is derived from the mass conservation equation for a passive aerosol. Displacements of the individual particles are derived from the set of stochastic differential equations for this process. Using a rectangular coordinate system with x in the direction of the mean wind, y in the horizontal crosswind direction and z directed vertically upward, the particle position $(X(t), Y(t), Z(t))$ is a random vector whose components satisfy the stochastic differential equations

$$dX(t) = \mu_1(X, Y, Z, t) dt + \sigma_1(t) dB_1(t) \quad (3-1a)$$

$$dY(t) = \mu_2(X, Y, Z, t) dt + \sigma_2(t) dB_2(t) \quad (3-1b)$$

$$dZ(t) = \mu_3(X, Y, Z, t) dt + \sigma_3(Z, t) dB_3(t) \quad (3-1c)$$

where

$$\mu_1(x, y, z, t) = u_x(x, y, z) \quad (3-2a)$$

$$\mu_2(x, y, z, t) = u_y(x, y, z) \quad (3-2b)$$

$$\mu_3(x, y, z, t) = \frac{\partial}{\partial z} K(z, t) - w_s(t) + w_p(x, y, z, t) \quad (3-2c)$$

and

$$\sigma_3(z, t) = \sqrt{2K(z, t)}. \quad (3-3)$$

Here, $u_x(x, y, z)$ and $u_y(x, y, z)$ are the components of the mean wind in the x - and y -directions, respectively, $K(z, t)$ is the vertical diffusivity, $w_s(t)$ is the particle gravitational settling velocity and $w_p(x, y, z, t)$ is a contribution to the particle's velocity from the thermal. Equations (3-1) through (3-3) represent a continuous time Markov process model of three-dimensional particle motion in turbulent shear flow.

The drift functions $\mu_j(X, Y, Z, t)$ can be identified with deterministic motions such as advection and gravitational settling. The term $\partial K/\partial z$ in Equation (3-2c) implies that for cases in which the diffusivity is a function of the vertical coordinate, there is an effective drift toward larger values of K , i.e., a countergradient flux. Since the diffusivity increases with height in the lower atmosphere, neglecting this term produces an unrealistic accumulation of particles close to the ground and results in an overestimate of ground-level concentration. For particles within the thermal's boundaries, buoyancy effects are introduced by including the puff velocity w_p in the expression for μ_3 . This approach permits cloud buoyancy to influence particle movements from time zero onward, eliminating the stabilized cloud assumption.

Turbulent effects enter through the second term on the right-hand side of Equation (3-1). The random forcing functions $dB_j(t)$, $j = 1, 2, 3$ are independent increments of the Wiener process; a Gaussian random process that is a mathematical model of free-particle Brownian motion. The random movements are then similar to a Brownian motion except that the size of the random displacement is scaled by the function σ_j .

The formulation of the coefficients in Equation (3-1) in terms of meteorological parameters is described in Chapter 5.

3.2 The Discrete Time Process

To numerically simulate particle trajectories, we approximate the continuous time process by a discrete time Markov chain. Using an integer subscript to index time, Equation (3-1) may be discretized as

$$X(t_{i+1}) - X(t_i) = \mu_1(X, Y, Z, t_i) \Delta t_i + \sigma_1(t_i) \Delta B_1(t_i) \quad (3-4a)$$

$$Y(t_{i+1}) - Y(t_i) = \mu_2(X, Y, Z, t_i) \Delta t_i + \sigma_2(t_i) \Delta B_2(t_i) \quad (3-4b)$$

$$Z(t_{i+1}) - Z(t_i) = \mu_3(X, Y, Z, t_i) \Delta t_i + \sigma_3(Z, t_i) \Delta B_3(t_i), \quad (3-4c)$$

where $\Delta t_i = t_{i+1} - t_i$ and the terms $\Delta B_j(t_i)$, $j = 1, 2, 3$ are independent Gaussian random variables with mean zero and variance Δt_i . For a source located at height z_0 at the moment $t_0 = 0$, the initial conditions are $X(t_0) = 0$, $Y(t_0) = 0$, and $Z(t_0) = z_0$.

The first term on the right-hand side of Equation (3-4) represents the drift of the process during a small interval of time Δt_i ; the second represents the random movement exhibited by the particle during Δt_i . Roughly, the process is locally Brownian, i.e., for a short interval of time the process behaves as a three-dimensional Brownian motion with constant drift and variance given by the $\mu_j's$ and $\sigma_j's$, respectively. The discrete time process is constructed by patching together the various local processes from each time step. In the limit as Δt_i approaches zero, the Markov chain converges in mean square to the continuous time process (Gihman and Skorohod, 1972).

3.3 The Boundary Condition at the Ground

The motion of particles sufficiently far above the ground is governed by the set of stochastic differential equations given in Equation (3-1) or the set of difference equations in Equation (3-4). The process must be modified as the particles interact with the earth's surface. In particular, the model must account for removal of airborne material as particles strike the ground and either rebound or deposit. In this context, the term "ground" is loosely construed to include vegetation and structures which extend above the ground and which affect particle removal. Deposition includes the effects of surface roughness impaction, adsorption, electrostatic forces, thermal diffusion and interactions with the vegetative canopy as well as gravitational settling.

Previous stochastic models typically include the simplifying assumption that the ground is a perfectly reflecting barrier. A partially absorbing surface can be specified using the boundary condition

$$K(0, t) \frac{\partial}{\partial z} c(0, t) + w_s(t) c(0, t) = w_d c(0, t), \quad (3-5)$$

where $c(0, t)$ is the concentration at the surface and w_d is the deposition velocity. In this formulation, the various removal mechanisms other than settling are grouped together into a single term $w_d c(0, t)$ in which the rate of removal is assumed to be proportional to the ground-level concentration.

Numerous investigators have attempted to measure deposition velocities; extensive reviews of these measurements are given by Sehmel (1980) and Hosker and Lindberg (1982). Results of these studies indicate that for larger particles (diameters greater than 30 to 40 μm), the deposition velocity is very nearly equal to the settling velocity implying that deposition by settling is the dominant process. For smaller particles, the deposition velocity is found to appreciably exceed the settling velocity indicating that removal by other mechanisms is significant. For the

smallest particles (diameters less than 0.1 μm), deposition by other processes, e.g., Brownian diffusion, is dominant over deposition by settling due to their negligible mass.

The boundary condition (Equation 3-5) is simulated by estimating the probability that a particle is absorbed during a short interval of time. This probability is used to determine the fraction of particles that are removed from further transport downwind. The method we present was chosen for its computational efficiency. For alternative approaches see, e.g., Stone (1963), Gihman and Skorohod (1972) and Gerardi et al. (1983).

Suppose that at the moment t_i a particle is near the ground, say, at the height $z_i \approx 0$. During the next short time interval the vertical component behaves like a Brownian motion with constant drift and variance given by Equations (3-2c) and (3-3) evaluated at the surface. For this particle, $\partial K/\partial z = 0$ (the diffusivity formulas presented in section 5.6 satisfy this condition) and, by virtue of the no-slip boundary condition for a turbulent flow, $w_p = 0$. Using these results, we can express the diffusion along the vertical approximately as the solution to the stochastic differential equation

$$dZ(t) = -w_s(t_i) dt + \sqrt{2K(0, t_i)} dB_3(t), \quad (3-6)$$

where $Z(t_i) = z_i$ and $t \in [t_i, t_{i+1}]$.

The transition probability density for the stochastic process derived from Equations (3-5) and (3-6) is given by the solution to the initial-boundary-value problem (e.g., Gihman and Skorohod, 1972)

$$\frac{\partial}{\partial \tau} q(z, \tau; z_i) = w_s(t_i) \frac{\partial}{\partial z} q(z, \tau; z_i) + K(0, t_i) \frac{\partial^2}{\partial z^2} q(z, \tau; z_i) \quad (3-7a)$$

$$K(0, t_i) \frac{\partial}{\partial z} q(0, \tau; z_i) + w_s(t_i) q(0, \tau; z_i) = w_d q(0, \tau; z_i), \quad (3-7b)$$

where $z \geq 0$, $p(z, \tau; z_i) \rightarrow \delta(z - z_i)$ as $\tau \rightarrow 0$ and $q(z, \tau; z_i)$ denotes the estimate of the probability density for particles close to the ground. For a particle initially at height z_i , the probability $q(z, \tau; z_i) dz$ represents the probable occurrence of various values of z a short time τ after t_i , where $\tau \in [0, \Delta t_i]$. The solution to Equation (3-7) can be written as (Chandrasekhar, 1954; Monin, 1959)

$$\begin{aligned} q(z, \tau; z_i) = & \frac{1}{2\sqrt{\pi K \tau}} \exp \left[-\frac{(z - z_i + w_s \tau)^2}{4K\tau} \right] [1 - P_I(z, \tau; z_i) P_A(z, \tau; z_i)] \\ & + \frac{1}{2\sqrt{\pi K \tau}} \exp \left[-\frac{(z + z_i - w_s \tau)^2}{4K\tau} \right] \exp \left[-\frac{w_s z}{K} \right] [1 - P_A(z, \tau; z_i)] \end{aligned} \quad (3-8a)$$

$$P_A(z, \tau; z_i) = \beta \sqrt{\frac{\pi \tau}{K}} \exp \left[-\frac{(z + z_i + \beta \tau)^2}{4K\tau} \right] \Phi \left[-\frac{z + z_i + \beta \tau}{\sqrt{2K\tau}} \right] \quad (3-8b)$$

$$P_I(z, \tau; z_i) = \exp \left[-\frac{zz_i}{K\tau} \right], \quad (3-8c)$$

where $z \geq 0$, $\beta = 2w_d - w_s$, $w_s = w_s(t_i)$, $K = K(0, t_i)$ and $\Phi(\zeta)$ is the standard Gaussian distribution function (i.e., $\Phi(-\infty) = 0$, $\Phi(0) = 0.5$, $\Phi(\infty) = 1$).

In the numerical model, Equations (3-8b) and (3-8c) are used in the following algorithm to simulate the boundary condition. The particle is first moved as if no boundary were present. Let us suppose that at the moment $\tau = \Delta t_i$, the new vertical position of the particle is z . The probability of survival P_S when $z \geq 0$ is given by $P_S(z) \equiv 1 - P_I(z, \Delta t_i; z_i) P_A(z, \Delta t_i; z_i)$; for $z < 0$, $P_S(z) \equiv \exp(-w_s|z|/K) [1 - P_A(|z|, \Delta t_i; z_i)]$. If a uniform random number on the interval $[0, 1]$ is less than $P_S(z)$, the particle survives and we set $Z(t_{i+1}) = |z|$. Otherwise, the particle is absorbed by the ground and is removed from further consideration. Every particle is followed until it either deposits or moves beyond the boundaries of the problem. Applying the rules for conditional probabilities, we can show that the preceding algorithm yields the probability density given in Equation (3-8).

Boundary behaviors in which only a fraction of the ground-level particles are absorbed, as well as the extreme cases of perfect reflection and complete absorption, can be simulated using this procedure. To demonstrate that the algorithm exhibits the correct qualitative behavior, we consider two limiting cases. If $w_d = w_s = 0$, the flux at the ground equals zero and the entire collection of particles must remain airborne. This corresponds to a perfectly reflecting barrier and Equation (3-8) gives the probability density for a standard Brownian motion with a reflecting boundary, as desired. If $w_d \rightarrow \infty$, the boundary condition in Equation (3-7b) becomes $q(0, \tau; z_i) = 0$. In this case, all particles reaching the ground must be absorbed. Using an asymptotic expression for $\Phi(\zeta)$, we can show that $P_A(z, t; z_i)$ in Equation (3-8b) tends to one as $w_d \rightarrow \infty$ and $q(z, \tau; z_i)$ takes the form

$$q(z, \tau; z_i) \sim \frac{1}{2\sqrt{\pi K \tau}} \exp \left[-\frac{[z - z_i + w_s \tau]^2}{4K\tau} \right] [1 - P_I(z, \tau; z_i)], \quad w_d \rightarrow \infty, \quad (3-9)$$

where $z \geq 0$. The density in Equation (3-9) represents a completely absorbing process. For this process, the term $P_I(z, \tau; z_i)$ can be viewed as the probability of interaction with the ground during a time interval of duration τ given that the height of the "unrestricted process" equals $z > 0$ at the moment τ (Breiman, 1968).

3.4 Probability Density Estimation

A model used for consequence assessment of radiological problems must be able to provide dispersion estimates in real time. The need to track many thousands of particles to obtain a meaningful estimate of the ensemble concentration has made previous simulations based on the stochastic technique inappropriate for real-time applications, particularly in the three-dimensional case. In a stochastic model, the ensemble mean concentration is calculated from the transition probability density $p(\mathbf{r}, t, \mathbf{r}', t')$ using

$$c(\mathbf{r}, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} p(\mathbf{r}, t, \mathbf{r}', t') S(\mathbf{r}', t') d\mathbf{r}' dt', \quad (3-10)$$

where $\mathbf{r} = (x, y, z)$ is the position vector of the point at which the concentration prediction is desired and S is the source distribution function. For an instantaneous point source of strength Q , $S(\mathbf{r}, t) = Q\delta(\mathbf{r} - \mathbf{r}_0)\delta(t)$ and Equation (3-10) becomes

$$c(\mathbf{r}, t) = Qp(\mathbf{r}, t, \mathbf{r}_0, 0), \quad (3-11)$$

where p is the transition probability density for the occurrence of a displacement $\mathbf{r}$ at time t given that the particle was initially released at $\mathbf{r}_0 = (x_0, y_0, z_0)$. Equations (3-10) and (3-11) show that calculating the concentration becomes a problem of estimating the transition density. For a stochastic model to be effective in a real-time application, efficient computational algorithms must be used without compromising the reliability of the density estimate. Making use of results from atmospheric tracer and wind field studies, we have developed a methodology which minimizes the number of particles required to determine the transition density and which eliminates the need to take random steps in the horizontal directions.

Although there is overwhelming observational evidence of the non-Gaussian nature of the vertical dispersion, systematically non-Gaussian distributions are not observed in the case of lateral diffusion (Deardorff and Willis, 1975; Gryning et al., 1978; Nieuwstadt and van Duuren, 1979; Gryning and Lyck, 1980; Eberhard et al., 1988). The lateral dispersion may be viewed as the combined effect of turbulence and shear in the wind direction (section 5.5). In ERAD, the first of these processes is treated by using Monte Carlo "particles" that grow according to a Gaussian law in the horizontal directions. The growth of each two-dimensional puff is made according to an empirical function of travel time which relates the spread of the distribution to the standard deviation of the lateral wind fluctuations. Tracking two-dimensional puffs rather than points in space improves simulation convergence and reduces by as much as a factor of four the number of "particles" required to obtain reliable ensemble statistics.

Field observations show that for all but the most unusual combinations of meteorology and terrain, the mean wind speed is a stronger function of height than position in the horizontal plane. The drift terms μ_1 and μ_2 can then be approximated as $\mu_1(X, Y, Z, t) \approx \mu_1(Z, t)$ and $\mu_2(X, Y, Z, t) \approx \mu_2(Z, t)$. With this result, we can decompose $(X(t), Y(t))$ into a drift

(mean) term $(\bar{X}(t), \bar{Y}(t))$ that involves only $Z(t)$ and a random term $(\tilde{X}(t), \tilde{Y}(t))$ such that $(X(t), Y(t)) = (\bar{X}(t), \bar{Y}(t)) + (\tilde{X}(t), \tilde{Y}(t))$ where

$$\bar{X}(t) = x_0 + \int_0^t \mu_1(Z, s) ds \quad (3-12a)$$

$$\bar{Y}(t) = y_0 + \int_0^t \mu_2(Z, s) ds. \quad (3-12b)$$

The random components $(\tilde{X}(t), \tilde{Y}(t))$ are independent Gaussian processes with independent increments, variances $\tilde{\sigma}_1^2(t) = \int_0^t \sigma_1^2(s) ds$ and $\tilde{\sigma}_2^2(t) = \int_0^t \sigma_2^2(s) ds$, respectively, and zero expectations.

A further simplification is possible if we assume that the vertical drift can be written as $\int_0^t \mu_3(X, Y, Z, s) ds \approx \int_0^t \mu_3(\bar{X}, \bar{Y}, Z, s) ds$. Using this assumption, we can express the Z component of the stochastic process as

$$Z(t) = z_0 + \int_0^t \mu_3(\bar{X}, \bar{Y}, Z, s) ds + \int_0^t \sigma_3(Z, s) dB_3(s). \quad (3-13)$$

The heuristic reasoning which leads to this approximation is based primarily on the assumption that the process $(\bar{X}(t), \bar{Y}(t), Z(t))$ spends very little time in the transition region between the ambient and the plume. The estimate given by Equation (3-13) represents the first term in a Taylor series expansion of μ_3 about the centerline variables or drift terms $(\bar{X}(t), \bar{Y}(t))$. Since the dependence of the vertical drift on the x - and y -coordinates is due solely to the appearance of the plume velocity in μ_3 , we need only estimate the error for points inside and in the vicinity of the plume. For points in the interior of the plume or in the ambient near the plume, we assume that the derivatives of μ_3 with respect to x and y are small. Further, we assume that the amount of time, in the mean square sense, that the process $(\bar{X}(t), \bar{Y}(t), Z(t))$ spends in the transition region (interface between the ambient and interior of the plume) is small. The result is that the integral over time of the higher order terms is negligible in the mean square sense compared with the first integral in Equation (3-13).

These observations allow us to decompose the particle's position into the sum of two independent random vectors, namely, $(X, Y, Z) = (\bar{X}, \bar{Y}, Z) + (\tilde{X}, \tilde{Y}, 0)$. The probability density for the sum of independent random variables is given by the convolution of their densities, i.e.,

$$p(\mathbf{r}, t, \mathbf{r}_0, 0) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(x - \bar{x}, y - \bar{y}, t) h(\bar{x}, \bar{y}, z, t) d\bar{x} d\bar{y} \quad (3-14a)$$

$$g(\tilde{x}, \tilde{y}, t) = \frac{1}{2\pi\tilde{\sigma}_1(t)\tilde{\sigma}_2(t)} \exp\left[-\frac{\tilde{x}^2}{2\tilde{\sigma}_1^2(t)} - \frac{\tilde{y}^2}{2\tilde{\sigma}_2^2(t)}\right], \quad (3-14b)$$

where $g(\tilde{x}, \tilde{y}, t)$ is the joint probability density of $(\tilde{X}, \tilde{Y})$ and $h(\bar{x}, \bar{y}, z, t)$ is the joint conditional probability density of $(\bar{X}(t), \bar{Y}(t), Z(t))$. This expression indicates that the transition density p can be estimated by convolving the Gaussian function $g(\tilde{x}, \tilde{y}, t)$ with an estimate of $h(\bar{x}, \bar{y}, z, t)$.

To determine the joint probability density of $(\bar{X}(t), \bar{Y}(t), Z(t))$, we employ a kernel density estimation method (Silverman, 1986; Thompson and Tapia, 1990). The kernel method is a meshless, nonparametric approach that, when properly applied, can produce results which are statistically superior to estimates obtained by simply counting particles in cells of a computational grid (e.g., Gingold and Monaghan, 1982). At each time step, the Monte Carlo simulation yields a set of particle heights Z^k and drift locations $(\bar{X}^k, \bar{Y}^k)$, where $k = 1, 2, 3, \dots, N$ indexes particle number. The drift variables are completely determined by the vertical process, i.e., random steps are taken explicitly in only the vertical. The joint probability density of $(\bar{X}(t), \bar{Y}(t), Z(t))$ is estimated from the particle positions using

$$\hat{h}(\bar{x}, \bar{y}, z, t) = \frac{1}{N} \sum_{k=1}^n p_N(z - Z^k, t) \frac{1}{\Delta^2} f\left(\frac{\bar{x} - \bar{X}^k}{\Delta}, \frac{\bar{y} - \bar{Y}^k}{\Delta}\right), \quad (3-15)$$

where $n \leq N$ is the number of particles in the air,

$$p_N(z - Z^k, t) = \frac{1}{\sqrt{2\pi}\sigma_N\Phi(z/\sigma_N)} \exp\left[-\frac{(z - Z^k)^2}{2\sigma_N^2}\right] \quad (3-16)$$

is the kernel for the vertical direction and $\Phi(\zeta)$ is the standard Gaussian distribution. The function f is a smoothing kernel for the x - and y -directions whose integral over the domain is unity and the time-dependent resolution bandwidths in the horizontal and vertical directions are Δ and σ_N , respectively.

Now, allowing Δ to become small and substituting Equation (3-15) into Equation (3-14) we arrive at the desired result

$$p(\mathbf{r}, t, \mathbf{r}_0, 0) \approx \hat{p}(\mathbf{r}, t, \mathbf{r}_0, 0) = \frac{1}{N} \sum_{i=1}^n g(x - \bar{X}^k, y - \bar{Y}^k, t) p_N(z - Z^k, t), \quad (3-17)$$

where $\hat{p}$ is the estimator for the probability density p . Associated with each Monte Carlo particle is a weighting function that grows according to a Gaussian law in the horizontal directions. Since every airborne particle contributes to the estimate of the concentration, the number of particles required to produce reliable ensemble statistics is reduced. The principal advantage of this approach is that the three-dimensional density calculation is reduced to essentially a one-dimensional estimate.

Only particles with $|z - Z^k| \leq \sigma_N$ contribute significantly to the estimate. The bandwidth σ_N must be chosen so as to strike a balance between the bias and variance of the approximation. For estimating ground level concentrations ($z = 0$ in Equation 3-17), the asymptotically optimal bandwidth in the sense of minimizing the mean square error is proportional to $N^{1/3}$ (Silverman, 1986). For estimates of concentration at locations well above the ground ($z \gg 0$ in Equation 3-16), the asymptotically optimal bandwidth in the sense of minimizing the *integrated* mean square error grows proportional to $N^{1/5}$ (Rosenblatt, 1971; Silverman, 1986). The analysis of the *integrated* mean square error uses the symmetry of the kernel (for $z \gg 0$) and so does not directly apply to our ground level estimate. In the ground-level case, the root mean square error is of order $N^{-1/3}$ while in the latter case the root mean *integrated* square error has order $N^{-2/5}$.

The Gaussian law for the horizontal diffusion arises naturally from the lateral wind fluctuations, however, the kernel p_N should not be construed as having a physical interpretation in the context of atmospheric dispersion physics. The fact that we have used a Gaussian kernel in the vertical does not imply our methods are applicable only to atmospheric conditions for which the underlying density is essentially Gaussian. Kernel density estimation is a mathematical device for approximating probability densities and converges regardless of the underlying distribution (assuming, e.g., that the unknown density has derivatives of all orders).

The essential step in this analysis is the formulation of the drift variables in terms of the vertical process as given by Equations (3-12) and (3-13). This allows us to express the three-dimensional process as the sum of two independent random variables, namely, $(X, Y, Z) = (\bar{X}, \bar{Y}, Z) + (\tilde{X}, \tilde{Y}, 0)$. Given $Z(t)$, the processes in the horizontal directions are now deterministic, simulating advection by the wind, including directional shear. Smaller-scale turbulent effects are simulated in the growth of the individual puffs with time. With this simplification, random movements are made explicitly in only the vertical direction. This approach results in a less computationally intensive model, while still accounting for the variation of the turbulence parameters with height which allows the vertical distribution of particles to be non-Gaussian.

3.5 Polydisperse Release

A model of particle transport for explosive releases must be able to simulate dispersion over a wide range of particle sizes. The calculation required for a large number of distinct particle siz-

es, using conventional continuum methods, is prohibitively expensive. One of the strengths of the stochastic approach is the ability to model polydisperse releases in an efficient manner. Extension to a polydisperse source is achieved by allowing the coefficients of the stochastic differential equations to depend not only on position and time, but also on particle diameter. The ensemble mean concentration $c(\mathbf{r}, t)$ is calculated from the transition probability density $p(\mathbf{r}, t, \mathbf{r}_0, 0; \alpha)$, for a particle of size α , using

$$c(\mathbf{r}, t) = \int Q p(\mathbf{r}, t, \mathbf{r}_0, 0; \alpha) F(d\alpha), \quad (3-18)$$

where $\mathbf{r} = (x, y, z)$ is the position vector of the point at which the concentration prediction is desired, $F(\alpha)$ is the particle size distribution, Q is the source strength of an instantaneous point source located at $\mathbf{r}_0 = (x_0, y_0, z_0)$ and $p(\mathbf{r}, t, \mathbf{r}_0, 0; \alpha)$ is the transition probability density for the occurrence of various points $\mathbf{r}$ at time t given that the particle of size α was initially released at $\mathbf{r}_0$. Estimates of the monodisperse densities $p(\mathbf{r}, t, \mathbf{r}_0, 0; \alpha)$ are provided by the numerical model as discussed in the preceding sections.

A stratified sampling technique is used to reduce the variance in the estimate of the polydisperse concentration (Hammersley and Handscomb, 1964). In stratified sampling, the range of integration is divided into subintervals such that the variation within any subinterval is approximately the same and then crude Monte Carlo is applied to each subinterval separately. This allows the simulation to expend more effort computing the densities for particles with larger statistical variation and less effort on particles that are more deterministic in nature. The result is that the variance of the simulation is reduced; equivalently, fewer particles are needed to achieve the same accuracy.

To this end, we divide the domain of integration into several small subintervals, namely, $\alpha_l < \alpha \leq \alpha_{l+1}$, where $\alpha_1 < \alpha_2 < \dots < \alpha_m$. The estimator for Equation (3-18) has the form

$$\hat{c}(\mathbf{r}, t) = Q \sum_{l=1}^m \frac{\Delta F_l}{n_l} \sum_{k=1}^{n_l} \hat{p}(\mathbf{r}, t, \mathbf{r}_0, 0; \alpha_l + \Delta \alpha_l \xi_{kl}), \quad (3-19)$$

where $\Delta F_l = F(\alpha_{l+1}) - F(\alpha_l)$, $\Delta \alpha_l = \alpha_{l+1} - \alpha_l$, the ξ_{lk} 's are independent, uniformly distributed random variables on $(0, 1]$, and $\hat{p}(\mathbf{r}, t, \mathbf{r}_0, 0; \alpha_l + \Delta \alpha_l \xi_{kl})$ is a point estimate of the probability density for a particle of size $\alpha_l + \Delta \alpha_l \xi_{kl}$. Here, we have decided to sample n_l points from the l^{th} subinterval, $n_l \geq 1$. In words, for every subinterval, we select n_l particles of size $\alpha_l + \Delta \alpha_l \xi_{kl}$, $1 \leq k \leq n_l$, and assign to each the mass fraction $Q \Delta F_l / n_l$. The mean and variance of the estimator are given by

$$E [\hat{c} (r, t)] = Q \sum_{l=1}^m \int_{\alpha_l}^{\alpha_{l+1}} E [\hat{p} (r, t, r, 0; \alpha)] \frac{\Delta F_l}{\Delta \alpha_l} d\alpha, \quad (3-20a)$$

$$\text{var} [\hat{c} (r, t)] = Q^2 \sum_{l=1}^m \frac{\Delta F_l^2}{n_l \Delta \alpha_l} \int_{\alpha_l}^{\alpha_{l+1}} \text{var} [\hat{p} (r, t, r_0, 0; \alpha)] d\alpha, \quad (3-20b)$$

where $E [\hat{p} (r, t, r, 0; \alpha)]$ and $\text{var} [\hat{p} (r, t, r_0, 0; \alpha)]$ are the mean and variance, respectively, of the point estimate for the density of a particle of size α . The mean of the estimator $\hat{c} (r, t)$ converges to $c (r, t)$ whenever the lengths of the subintervals decrease to zero and the bias of $\hat{p}$ ($\text{bias} [\hat{p}] = E [\hat{p}] - p$) goes to zero. The square of the statistical error, $\text{var} [\hat{c} (r, t)]$, goes to zero as the ΔF_l 's decrease to zero or if the n_l 's tend to infinity (assuming the variance of $\hat{p}$ is bounded).

The variance in stratified sampling with a fixed number of particles is typically less than the variance in crude Monte Carlo where the sample points are selected according to the underlying distribution $F (\alpha)$. When the number of particles are fixed ($\sum_{l=1}^m n_l = n$) and the stratification points are prescribed, the optimal strategy is to distribute the samples so that n_l^2 is

proportional to $\frac{\Delta F_l^2}{\Delta \alpha_l} \int_{\alpha_l}^{\alpha_{l+1}} \text{var} [\hat{p} (r, t, r_0, 0; \alpha)] d\alpha$. One method for selecting the stratification

is to choose the α_l 's such that the ΔF_l 's are equal to some small prescribed value. The variance, $\text{var} [\hat{p}]$, can be determined from numerical experiments. As might be expected, the random displacements for the smaller particles exhibit the largest statistical fluctuations. The use of uniform deviates can be eliminated by breaking each subinterval into smaller pieces, say, n_l sections of the same length, and selecting one point (deterministically) from each piece.

With this approach, the computing effort can be concentrated on simulating particles that demonstrate the largest statistical fluctuations. Since random variates from the distribution F are not required, stratified sampling also provides a technique for simulating cases in which the particle size distribution is only known empirically or is difficult to sample directly. The principal advantage for this application is the reduction in the number of particles required to produce reliable ensemble statistics.

4.0 The Wind Field Model

The wind field model is used to calculate the spatial variation of the mean atmospheric flow. The techniques available to determine the wind field fall into three broad categories: (a) interpolation, (b) diagnostic, mass-consistent models and (c) prognostic methods. Moving from interpolation through to a prognostic approach involves a substantial increase in model complexity in terms of both the required number of input parameters and computational effort.

Interpolation techniques use a distance-weighted average of multiple soundings or tower wind speed measurements to calculate the wind field. An inverse distance weighting is common, with a $1/r^2$ interpolation the most widely used. Here, r is the horizontal distance from the measurement station to the point at which the wind speed is desired. This approach is readily integrated into a wide range of dispersion models and has an almost negligible impact on turn-around time compared to a simulation using a single sounding. Interpolation can resolve terrain-induced flow features, e.g., thermally-driven winds, waves and wake phenomena, which are inherent in the input wind measurements, but without a sufficient number of measurement stations to delineate the flow field, will not provide the resolution required to handle steep terrain gradients or sharp changes in roughness elements.

Generally, the wind field derived from an interpolation technique does not satisfy conservation of mass, i.e., the resulting flow field is divergent $\nabla \cdot \mathbf{u} \neq 0$. A flow field with significant divergence can produce artificial sources and sinks of mass. Diagnostic, mass-consistent models start with an interpolated wind field and use the incompressible continuity equation as a constraint to calculate a final wind field that is divergence free. Unfortunately, the continuity equation alone does not specify a unique solution. Additional constraints, usually in the form of a stability parameter which governs the relative amount of adjustment to the horizontal and vertical components of the wind, must be imposed to select a single solution from the many that satisfy the continuity condition. Theoretically, the stability parameter should be a function of the Froude number based on the height scale of the local topography and may need to be a function of position to accommodate varying terrain features. In practice, the stability parameter is most often taken as a constant for the entire computational domain with a value assigned subjectively that is only crudely dependent on atmospheric stability (Sherman, 1978; Traci et al., 1978; Davis et al., 1984; Guo and Palutikof, 1990). Ross et al. (1988), using conservation of energy arguments, developed a framework relating the stability parameter to the Froude number for neutral and stably stratified flows. This more objective approach had only limited success in predicting wind tunnel and tow tank measurements of flow past an ideal hill. In a subsequent paper, Ross and Fox (1991) evaluate a revised formulation for the stability parameter by comparing model predictions with measurements of plume behavior in the vicinity of a roughly axisymmetric, isolated hill. As in the first study, the best predictive performance was achieved for neutral atmospheric conditions in which case the potential flow solution provides an adequate approximation to the flow field. The sensitivity of the winds predicted by a diagnostic model to the stability parameter and the initial, interpolated wind field has been demonstrated by Traci et al. (1979), Lewellen et al. (1982), Kitada et al. (1983), Barnard et al. (1987) and Mathur and Peters (1990).

Because the mass-consistent models do not explicitly include energy and momentum conservation, they can only generate flow features that are reflected in the input wind observations and offer no advantage over interpolation in this respect. In the absence of representative observational data, a diagnostic wind model cannot by itself produce physical features of the flow field which may play an important role in the transport problem, e.g., wave phenomena on the leeward side of a hill in stable flow (Ross et al., 1988; Ross and Fox, 1991), sea breezes and eddy circulations (Hanna et al., 1991).

The prognostic methods (Pielke, 1974; Mahrer and Pielke, 1977; Yamada and Bunker, 1988, 1989; Kessler and Douglas, 1991) solve a complete set of conservation equations, sometimes referred to as primitive equations, and are the most complex of the wind field modeling techniques. Whereas interpolation and the mass-consistent models yield steady-state solutions, the prognostic methods predict the time-dependent flow field. The strength of this modeling approach lies in its ability to generate on its own such features as upslope/downslope winds, sea breezes and eddies. Initialization of a prognostic model involves specification of an extensive set of parameters. A typical simulation requires gridded terrain information; domainwide profiles of wind, temperature and specific humidity; an estimate of the ground surface albedo; and characterization of the soil including the heat diffusivity, specific heat and moisture content. It may also be necessary to assign values to constants which influence the numerical integration scheme. Clearly, many of these parameters cannot be deduced from routine meteorological measurements.

In ERAD, the wind components (u_x and u_y in Equation 3-2) are computed from multiple upper-air soundings using a $1/r^2$ interpolation formula. A mass-consistent model was judged inappropriate because of the strong dependence of the calculated winds on the choice of certain input parameters, the need to maintain a terrain (and vegetation) database and the additional computational costs relative to interpolation. Moreover, the available evidence does not indicate that use of a diagnostic method would result in a model with a statistically significant improvement in predictive performance. Lange (1985) compared concentration predictions with measurements while varying the wind field component of the dispersion model. The percentage of predicted concentrations within a factor of five of the observed values was used as a performance statistic. For a case with three surface wind measurements and one vertical profile, this statistic increased by only 2% when going from interpolation to a diagnostic model. Similar results were obtained as the number of input wind observations was increased. Prognostic models are computationally intensive and impractical for applications requiring real-time predictions. Furthermore, the prognostic approach is not adequately supported by the available input data.

5.0 Parameterization of the Planetary Boundary Layer

The performance of an atmospheric dispersion model depends strongly on its meteorological component, more specifically, the scaling used to describe the structure of the planetary boundary layer (PBL). Reviews by Smith (1984), Bowne et al. (1985) and Hayes and Moore (1986) have shown that most applied models use parameterizations that are substantially out of date with contemporary understanding of turbulence and diffusion in the PBL. The meteorological component in ERAD is based on state-of-the-art scaling derived from observational, laboratory and numerical studies. Examples are the use of Monin-Obukhov similarity theory in the surface layer, convective scaling in the unstable boundary layer and local scaling in the stable boundary layer. A more thorough discussion of the various scaling regimes can be found in Nichols and Readings (1979), Olesen et al. (1984) and Holtslag and Nieuwstadt (1986). We begin by describing the PBL in general terms, followed by more detailed presentations of how particular parameters are calculated.

The PBL can be defined as the lowest layer of the atmosphere where surface friction and the diurnal heating and cooling cycle strongly influence the turbulent flow field. One common measure of the stability of the atmospheric flow is the potential temperature gradient (Monin and Yaglom, 1971)

$$\frac{\partial \theta}{\partial z} = \frac{\partial T}{\partial z} - \Gamma, \quad (5-1)$$

where the adiabatic lapse rate $\Gamma = -0.0098^\circ\text{C/m}$ is the rate at which the temperature of a parcel of dry air decreases with height when lifted adiabatically through the atmosphere. If the potential temperature gradient is less than zero, an upwardly displaced parcel of air would be warmer than its surroundings and will continue to rise vertically. The boundary layer under these conditions is called convective or unstable. If the potential temperature gradient is positive, an upwardly displaced parcel would be cooler than its surroundings and will return to its original position. These conditions are termed stable. For potential temperature gradients close to zero, there is no tendency for a displaced parcel to move from its new position and the atmosphere is said to be neutrally stable.

A convective boundary layer (CBL) forms during the daytime when there is solar heating of the earth's surface. Under these conditions, the temperature decreases with height more rapidly than the adiabatic lapse rate, i.e., the potential temperature gradient is negative, and there is an upward heat flux at the ground. The CBL extends from the ground to the base of an elevated layer of stable air and typically reaches a height of 1 to 2 km over land at midafternoon. Updrafts of warm air from the surface and downdrafts of cooler air from the inversion produce complete vertical mixing. In simplest terms, the vertical structure of the CBL can be broken into three layers: surface, mixed and entrainment. (A more detailed analysis would include a fourth scaling regime: the free convection layer, which is a matching region between surface layer and mixed layer scaling.) The approximate extent of each layer can be given in terms of the boundary layer depth h , which defines the thickness of the fully turbulent region next to the

ground. This is also called the mixing height, since pollutants are well-mixed within it. In the CBL, we have $h \cong z_i$, where z_i is the height of the temperature inversion.

Both wind shear and thermal effects influence turbulence in the surface layer ($z < 0.1h$). Because the fluxes of momentum and sensible heat are treated as constants in this layer, the characterization of turbulence is relatively simple and well established (Businger, 1973). Monin and Obukhov (1954) first introduced the basic scaling parameters for the surface layer. The appropriate velocity and length scales are the friction velocity u_* and Monin-Obukhov length L . The friction velocity, given by

$$u_* = \sqrt{\tau_0}, \quad (5-2)$$

where τ_0 is the surface kinematic shear stress, determines the production of turbulence by shear at the surface. The surface fluxes of heat and momentum define the length scale as

$$L = \frac{-u_*^3}{\kappa (g/\theta_0) Q_0}, \quad (5-3)$$

where $\kappa = 0.4$ is von Karman's constant (Högström, 1985), g is the gravitational acceleration and θ_0 is the potential temperature at the surface. The turbulent kinematic heat flux Q_0 is related to the vertical flux of sensible heat at the ground q_0 by

$$q_0 = \rho c_p Q_0, \quad (5-4)$$

where ρ is the air density and c_p is the specific heat at constant pressure. The Monin-Obukhov length reflects the relative importance of turbulence produced by shear and buoyancy. When the heat flux is positive (unstable conditions), $L < 0$ and $|L|$ provides an estimate of the depth over which shear dominates the flow. At night, when radiative cooling of the surface results in a negative heat flux (stable conditions), $L > 0$. On cloudy days with strong winds and during the dawn and dusk transition periods, the heat flux is essentially zero (neutral stratification) and $|L| \rightarrow \infty$. The structure of the surface layer is described by Monin-Obukhov similarity theory which postulates that the dimensionless variables characterizing the turbulence and mean flow are universal functions of z/L .

In the mixed layer ($0.1h < z < 0.8h$), mechanical turbulence generated by surface stress becomes unimportant compared to convective turbulence. Numerical simulations by Deardorff (1970, 1972) showed that the most important length and velocity scales in the mixed layer are the CBL depth or mixing height h and the convective velocity

$$w_* = \left(\frac{g Q_0 h}{\theta_0} \right)^{1/3} = u_* \left(\frac{-h}{\kappa L} \right)^{1/3}. \quad (5-5)$$

The mean wind speed, wind direction, potential temperature and turbulence components are nearly constant with height in this layer. The validity of convective scaling has been confirmed

by field data obtained during the Minnesota (Kaimal et al., 1976) and Ashchurch (Caughey and Palmer, 1979) experiments.

The characteristics of the capping inversion and air from above the CBL influence the turbulent structure through the entrainment layer ($0.8h < z < 1.2h$). At present, the structure of this region is poorly understood and no universal scaling parameters can be given (Deardorff et al., 1980; Driedonks and Tennekes, 1984). Fortunately, the entrainment layer is located at levels too high to play a significant role in most applications.

A stable boundary layer (SBL) forms on clear nights when the ground cools faster than the upper air due to long wavelength radiation heat transfer. Turbulence in the SBL is driven by shear stress. The downward heat flux acts to suppress turbulence and, consequently, the mixing height h is typically smaller than the depth of the ground-based inversion. Understanding of the SBL is much less advanced than the CBL due to the very low turbulence levels and the accompanying measurement problems. In addition, the turbulence structure is often masked by other coexisting processes including gravity waves, drainage flows and intermittency. Three major scaling regimes can be identified in a SBL with continuous turbulence: the surface layer, the local scaling layer and the z -less scaling layer. For strongly stable cases, an intermittency regime exists in which turbulence is weak and sporadic. Currently, no scaling theory exists for the intermittent SBL.

The stable surface layer ($z < 0.1h$) can be described using Monin-Obukhov similarity theory as in the CBL. Above the surface layer, Nieuwstadt (1984a, 1984b) and Sorbjan (1986a, 1986b) have shown that the turbulence scales with local values of the momentum and heat fluxes. Local scaling is an extension of Monin-Obukhov theory to heights much greater than the surface layer. For a stationary boundary layer, this approach is equivalent to the gradient transfer hypothesis, i.e., K -theory (Nieuwstadt, 1984b). A local Monin-Obukhov length is defined as

$$\Lambda = \frac{-\tau^{3/2}}{\kappa(g/\theta)Q}, \quad (5-6)$$

where τ and Q are local values of the kinematic momentum and heat flux. The nondimensional turbulent variables are then expressed as functions of z/Λ . Holtslag and Nieuwstadt (1986) show that over a large part of the SBL, $\Lambda \approx L$ which implies that local scaling is nearly equivalent to surface layer similarity. In fact, Holtslag (1984), Holtslag and De Bruin (1988) and Beljaars and Holtslag (1991) have shown that Monin-Obukhov similarity wind and temperature profiles are in good agreement with observations well above the surface layer, to $z/L \approx 7$. At large values of z/Λ , the turbulent eddies are not influenced by the presence of the ground and z is no longer an important length scale. In this region, z -less scaling applies (Wyngaard, 1973) and the dimensionless turbulence variables are constant with height (Nieuwstadt, 1984a; Sorbjan, 1986a).

Advanced models of atmospheric transport and diffusion rely on detailed descriptions of the PBL. Most models require estimates of the mixing depth, the surface fluxes of sensible heat

and momentum and vertical profiles of temperature, wind and turbulence. Because direct measurements of all the required meteorological variables are seldom available, they must be parameterized in terms of routinely available data. The boundary layer parameterization used in ERAD is based on scaling theory. Formulas similar to those presented here have been suggested by Wilczak and Phillips (1986), Gryning et al. (1987), Irwin and Paumier (1990) and Hanna and Chang (1992). Parameterizations of this type have accuracies of 20 to 30% over a broad range of meteorological conditions. For complex cases, e.g., strong stability and transition periods, performance is less satisfactory and errors can be as large as the estimates themselves.

5.1 The Surface Fluxes and Monin-Obukhov Length

The surface fluxes of heat and momentum are needed to calculate the Monin-Obukhov length (Equation 5-3) and the convective velocity scale (Equation 5-4). They determine the mean profiles within the surface layer and influence to a large extent the structure of the entire PBL. Direct flux measurements require fast response instrumentation that is not often available. Indirect estimates may be derived from Monin-Obukhov surface layer similarity theory and measurements of wind speed and temperature close to the ground using the profile method (Irwin and Binkowski, 1981; DeHeer-Amissah et al., 1981; Berkowicz and Prahm, 1982; Holtslag and van Ulden, 1983; Byun, 1990). As input, this technique requires a single wind speed, an effective surface roughness (section 5.2), air temperature and a potential temperature difference near the surface. Nieuwstadt (1978), Holtslag and van Ulden (1983), Holtslag and De Bruin (1988) and Beljaars and Holtslag (1991) have demonstrated that flux estimates obtained with the profile method using an effective roughness length are in agreement with direct turbulence measurements and with predictions of techniques which parameterize the sensible heat flux.

A fundamental hypothesis of the Monin-Obukhov theory is that the dimensionless flux-gradient relationships can be written as

$$\frac{\kappa z}{u_*} \frac{\partial u}{\partial z} = \phi_m(z/L) \quad (5-7a)$$

$$\frac{\kappa z}{\theta_*} \frac{\partial \theta}{\partial z} = \phi_h(z/L), \quad (5-7b)$$

where ϕ_m and ϕ_h are universal functions of z/L only and the temperature scale θ_* is related to the surface heat flux by

$$q_0 = -\rho c_p u_* \theta_*. \quad (5-8)$$

Integrating Equation (5-7) between the surface and a height z , we obtain the surface layer wind and temperature profiles

$$u(z) = \frac{u_*}{\kappa} \left[\ln \left(\frac{z}{z_0} \right) - \psi_m(z/L) \right] \quad (5-9a)$$

$$\theta(z) - \theta_0 = \frac{\theta_*}{\kappa} \left[\ln\left(\frac{z}{z_0}\right) - \psi_h(z/L) \right], \quad (5-9b)$$

where z_0 is the effective roughness length and the stability functions ψ_m and ψ_h are given by

$$\psi_{m,h}(z/L) = \int_0^{z/L} \frac{1 - \phi_{m,h}(\zeta)}{\zeta} d\zeta. \quad (5-10)$$

In a neutrally stratified boundary layer ($1/L = 0$), $\phi_{m,h} = 1$ and Equations (5-9a) and (5-9b) reduce to the well-known logarithmic profiles.

Similarity theory does not specify the functional dependence of ϕ_m and ϕ_h on z/L , so the gradient functions must be determined from experimental observations. Several different empirical relations have been proposed, with no single formulation finding universal acceptance. In a reassessment of many of the earlier proposals, Högström (1988) concludes that the widely-used results of Dyer and Hicks (1970) and Businger et al. (1971) provide a good representation of the observational data for convective conditions. These expressions may be written

$$\phi_m = \left(1 - 19 \frac{z}{L}\right)^{-1/4} \quad (5-11a)$$

$$\phi_h = \left(1 - 14 \frac{z}{L}\right)^{-1/2} \quad (5-11b)$$

incorporating the refined values of the constants developed by Högström (1988) for ϕ_m and Dyer and Bradley (1982) for ϕ_h .

For stable conditions, it is common to assume equality of the gradient functions for wind and temperature, i.e., $\phi_m = \phi_h$ (e.g., Delage, 1988). The linear relation

$$\phi_m = \phi_h = 1 + 5 \frac{z}{L} \quad (5-12)$$

given by Webb (1970), Businger et al. (1971) and Dyer (1974) fits the data well for $0 < z/L \leq 0.5$. This expression appears to be suitable for slightly stable conditions, but fails in stronger stabilities (Högström, 1988). Carson and Richards (1978) and Holtslag (1984) conclude that a formulation by Hicks (1976) best represents the entire range of stable data. Analyzing surface layer wind profiles from the Wangara Experiment, Hicks found that Equation (5-12) remains valid only up to $z/L \approx 0.5$ followed by a transition region in which ϕ_m tends to a purely logarithmic law. Beyond $z/L \approx 10$, a linear profile was found. Recently, Holtslag and De Bruin (1988) developed a single expression which describes these results

$$\phi_m = \phi_h = 1 + \frac{z}{L} \{0.7 + 0.75 \exp(-0.35 \frac{z}{L}) [1 + 0.35 (14.3 - \frac{z}{L})]\}. \quad (5-13)$$

The assumption $\phi_m = \phi_h$ is supported by SBL observations in the regime of continuous turbulence. However, Hicks (1976) and Kondo et al. (1978) show that as stability increases the heat transfer mechanism becomes far less efficient than mass transfer, i.e., $\phi_h > \phi_m$. In extremely stable conditions (the intermittent regime), Hicks (1976) obtained $\phi_h \approx 2\phi_m$. To account for this Beljaars and Holtslag (1991) propose

$$\phi_m = 1 + \frac{z}{L} \left\{ 1 + 0.667 \exp \left(-0.35 \frac{z}{L} \right) \left[1 + 0.35 \left(14.3 - \frac{z}{L} \right) \right] \right\} \quad (5-14a)$$

$$\phi_h = 1 + \frac{z}{L} \left\{ \left(1 + 0.667 \frac{z}{L} \right)^{1/2} + 0.667 \exp \left(-0.35 \frac{z}{L} \right) \left[1 + 0.35 \left(14.3 - \frac{z}{L} \right) \right] \right\} \quad (5-14b)$$

These expressions satisfy $\phi_h > \phi_m$ for large z/L and are also consistent with the concept of a critical Richardson number. Consideration of a critical Richardson number, above which turbulence disappears, arises from the physical constraint that buoyancy destruction of turbulent kinetic energy must always be less than shear production.

The ERAD model uses the Businger-Dyer formulas (Equation 5-11) for convective conditions ($z/L < 0$) and the Beljaars-Holtslag relations (Equation 5-14) for stable atmospheres ($z/L > 0$). These functions are shown with the Lövsta experiment data (Högström, 1988) in Figures 1 and 2. The formulas are a good approximation to the observations. There is, however, considerable scatter in the data particularly for stable air, typical of direct turbulent flux measurements (Businger et al., 1971; Dyer and Bradley, 1982).

Performing the integral in Equation (5-10) with these choices for the nondimensional wind and temperature gradients we obtain

$$\psi_m = \begin{cases} 2 \ln \left(\frac{1 + \phi_m^{-1}}{2} \right) + \ln \left(\frac{1 + \phi_m^{-2}}{2} \right) - 2 \operatorname{atan} (\phi_m^{-1}) + \frac{\pi}{2} & z/L \leq 0 \\ 0.667 \left(14.3 - \frac{z}{L} \right) \exp \left(-0.35 \frac{z}{L} \right) - \frac{z}{L} - 9.52 & z/L > 0 \end{cases} \quad (5-15)$$

$$\psi_h = \begin{cases} 2 \ln \left(\frac{1 + \phi_h^{-1}}{2} \right) & z/L \leq 0 \\ 0.667 \left(14.3 - \frac{z}{L} \right) \exp \left(-0.35 \frac{z}{L} \right) - \left(1 + 0.667 \frac{z}{L} \right)^{3/2} - 8.52 & z/L > 0 \end{cases} \quad (5-16)$$

where ϕ_m and ϕ_h refer to the convective boundary layer expressions given in Equation (5-11).

In the profile method, estimates of the fluxes of sensible heat and momentum are obtained from the surface layer wind and temperature profiles. Starting with a prescribed value of the effective surface roughness, a single wind speed measurement at height z_1 and a potential temperature difference between two levels z_2 and z_3 , we can solve for u_* and θ_* by iteration. First, we

Figure 1. Lövsta experiment data (Högström, 1988) and surface layer similarity dimensionless wind and temperature gradient functions for convective conditions.

Figure 2. Lövsta experiment data (Högström, 1988) and surface layer similarity dimensionless wind and temperature gradient functions for stable conditions. Open circles with error bars represent stability group averages.

assume a value for the Monin-Obukhov length, say, $L = \infty$ (this implies $\psi_m = \psi_h = 0$). Next, estimates of u_* and θ_* are computed by inverting Equation (5-9)

$$u_* = \kappa u(z_1) \left[\ln \left(\frac{z_1}{z_0} \right) - \psi_m(z_1/L) \right]^{-1} \quad (5-17a)$$

$$\theta_* = \kappa [\theta(z_3) - \theta(z_2)] \left[\ln \left(\frac{z_3}{z_2} \right) - \psi_h(z_3/L) + \psi_h(z_2/L) \right]^{-1}. \quad (5-17b)$$

Using these values, L is computed by substituting Equations (5-4) and (5-8) into (5-3), i.e.,

$$L = \frac{u_*^2}{\kappa (g/\theta_0) \theta_*}. \quad (5-18)$$

Finally, this new value of L is substituted in Equation (5-17) to obtain improved estimates of u_* and θ_* . This procedure is repeated until successive estimates of L converge.

The Monin-Obukhov length defined in Equation (5-18) ignores the contribution of water vapor to buoyancy. To account for moisture effects, the kinematic heat flux in Equation (5-3) is replaced by the virtual heat flux. Correcting for water vapor buoyancy multiplies the denominator of Equation (5-18) by

$$1 + 0.07/B_r, \quad (5-19)$$

where the Bowen ratio B_r is the ratio of sensible to latent heat flux at the surface. Values of B_r range from 0.1 over water to 10 for desert. The moisture correction has less than a 10% effect on the calculated value of L over a land surface.

The method we have described to calculate the surface fluxes is strictly valid only when the required wind and temperature measurements are all made within the surface layer. However, field studies show good agreement between observations and the surface layer wind and temperature profiles well above the surface layer (up to $|z/L| \approx 7$) for both convective (Garratt et al., 1982; Holtslag, 1984; Wilczak and Phillips, 1986) and stable stratification (van Ulden and Holtslag, 1985; Holtslag and De Bruin, 1988; Beljaars and Holtslag, 1991).

5.2 The Surface Roughness Length

The accuracy of the profile method relies on the assumed value of the effective surface roughness. Formally, the concept of a surface roughness length applies only to terrain with a uniform distribution of roughness elements. Fiedler and Panofsky (1972) introduced the "effective" roughness length as a means to characterize terrain with heterogeneous roughness elements. The intent is to derive a roughness value such that flux estimates obtained from boundary layer similarity theory are representative of spatial-averages over scales of a few kilometers and in this way account for varying landscape features. This length is typically a factor of two to ten times larger than the roughness length characterizing the local terrain owing to the effects of

surface inhomogeneities in the upwind direction, e.g., relatively smooth fields with occasional obstacles such as ditches, trees, fences and houses. Beljaars et al. (1983) found that the effective roughness length for the Cabauw site in The Netherlands to be ~ 15 cm whereas the local roughness length is about 1 cm (typical for short grass).

The turbulent velocity fluctuations in the horizontal direction are largely determined by eddies with dimensions comparable to the PBL height. These large eddies adjust very slowly to changing surface features and carry with them characteristics of the upstream terrain (Panofsky et al., 1982; Beljaars, 1987). This is demonstrated in the results of Beljaars et al. (1983) which show that the horizontal velocity fluctuations are influenced by obstacles a few kilometers in the upwind direction and that the variances scale not on the local friction velocity but on a friction velocity representative of a much larger area. As a result of this memory effect, a roughness length derived from horizontal turbulence quantities takes into account terrain characteristics on scales of 3 to 10 kilometers.

A number of different approaches exist to estimate the effective roughness length z_0 . The choice of a particular methodology depends on the available set of observed meteorological parameters. If measurements of wind speed and the standard deviation of wind speed σ_u or wind direction σ_ϕ are available, z_0 can be estimated from the wind profile in neutral conditions (see Equation 5-9a)

$$u(z) = \frac{u_*}{\kappa} \ln \frac{z}{z_0}. \quad (5-20)$$

For near-neutral atmospheres ($|h/L| \ll 1$), σ_u and $\sigma_\phi = u\sigma_v$, where σ_v is the standard deviation of the horizontal wind component in the crosswind direction, are simple functions of the friction velocity as shown in Equation (5-24). Substituting these relations into Equation (5-20) gives a direct relation between z_0 and either u/σ_u or u/σ_ϕ . An obvious disadvantage of this method is that it requires fast response equipment to measure σ_u or σ_ϕ .

An alternative approach, suitable for use with a standard single-level meteorological station, is described by Wieringa (1976, 1980, 1983). Assuming strong winds (neutral stratification) and a logarithmic wind profile, Wieringa obtains an expression for the effective surface roughness in terms of the gust factor which is defined as the ratio of the maximum to the average wind speed over a 10 minute averaging period. Beljaars (1982) and Holtslag (1984) show that predictions of the profile method using a roughness length derived from gust factor analysis are in agreement with direct flux and wind profile observations.

If no observational data are available, z_0 can be estimated from a visual inspection of the site using the terrain classification scheme presented in Table 1 (van Dop, 1983; Wieringa, 1986). A useful rule of thumb when employing this more subjective procedure is that an area of varying landscape structure tends to attain the roughness corresponding to the roughest features in the area.

Table 1. Effective Surface Roughness Length z_0 in Terms of Terrain Classification[†]

Terrain Category	z_0 (m)
Open water (minimum fetch 5 km)	0.0002
Small lake, snow, mud flats	0.006
Open field, marshland	0.03
Pasture	0.07
Agricultural	0.17
Fields with scattered trees and hedges	0.25
Orchards	0.35
Forest	0.75 - 1.0
Residential area, structure heights < 10 m	1.12
City center, multistory buildings	1.6 - 2.0

[†] Adapted from van Dop (1983) and Wieringa (1986)

The effective roughness values depend both on the local ground cover and mesoscale terrain features in an integrated fashion. This dependency on terrain characteristics a few kilometers away implies that a separate roughness length should be determined for as many wind direction sectors as needed to resolve major variations in upwind roughness elements and topography.

5.3 The Mixing Height

Ideally, the mixing height (PBL depth) should be determined from direct observation. For convective and neutral conditions, the mixing depth can be estimated by inspection of a slow-ascent radiosonde temperature profile using $h = z_i$, where z_i is the height of the kink in potential temperature associated with the capping inversion. In a stable boundary layer, buoyancy forces suppress turbulence which reduces the mixing depth to a height less than that of the ground-based inversion. In this case, direct measurement of h is difficult and requires equipment that is often not available in practical applications, e.g., a doppler acoustic sounder. If measurements are unavailable or the observations are unreliable, the analytical techniques described in this section can be used to estimate the mixing depth.

In a neutrally stratified boundary layer, the turbulence is purely mechanical and dimensional arguments show that the depth of the mixed layer is given by

$$h = c_n \frac{u_*}{f}, \quad (5-21)$$

where $c_n \approx 0.3$ is an empirical constant and f is the Coriolis parameter ($\sim 10^{-4} \text{ sec}^{-1}$ at midlatitudes). This relation together with the logarithmic neutral wind profile (Equation 5-20) indi-

cate that the mixing height under neutral conditions is proportional to wind speed and increases with surface roughness. In practice, the neutral PBL depth may be limited by an elevated inversion at z_i . The mixing height in this case should be taken as the minimum of z_i and the value given by Equation (5-21).

Theoretically, the height of the stable nocturnal boundary layer is best determined by a rate equation model. The time dependence of h is usually expressed as a simple relaxation process in which the actual mixing height approaches an equilibrium value (Nieuwstadt and Tennekes, 1981). The difficulty in applying a prognostic model lies in estimating the initial SBL height at the end of the transition period after sunset. Nieuwstadt and Tennekes (1981) and André (1983) show that this initial height provides a good estimate of h throughout the night because the time scale of the relaxation process is very large, on the order of several hours. The turbulent time scale is very short by comparison (Wyngaard, 1983) suggesting that the SBL may be treated as quasi-stationary. Consequently, reasonable estimates of the mixing depth can be obtained using a steady-state expression first derived by Zilitinkevich (1972) from similarity considerations

$$h = c_s \sqrt{\frac{u_* L}{f}}, \quad (5-22)$$

where c_s is a constant of proportionality. Empirical evaluations of c_s show considerable scatter (Garratt, 1982a) with $c_s \approx 0.4$ consistent with most observations (Caughey et al., 1979; Garratt, 1982b; Lenschow et al., 1988). Arya (1981), Mahrt et al. (1982) and Nieuwstadt (1984b) have demonstrated that this equation gives an acceptable fit to data, although in principle a rate equation should be more appropriate.

Zilitinkevich (1989) combines Equations (5-21) and (5-22) to obtain a simple interpolation formula valid for neutral and stable stratification

$$h = \frac{u_*}{f} \left(\frac{1}{c_n} + \frac{1}{c_s} \sqrt{\frac{u_*}{fL}} \right)^{-1}. \quad (5-23)$$

An alternative expression that satisfies the same neutral and stable limits has been given by Nieuwstadt (1981).

As previously mentioned, a reliable estimate of the mixing height under convective conditions can be determined from radiosonde data using $h = z_i$. Without a current temperature profile, a prognostic (inversion rise) model, initialized with an early morning temperature sound, may be used to calculate the growth of the daytime mixed layer. The simplest models for the growth of the CBL idealize the mixed layer as a slab of air in which the potential temperature is uniform with height, capped by an infinitesimally thin inversion. The inversion is represented as a step change in potential temperature. A set of equations for the evolution of h is obtained from a heat energy balance on this slab (Tennekes, 1973; Carson, 1973). Mixing height estimates are then calculated by a timewise integration of the surface heat flux and friction velocity (Driedonks and Tennekes, 1984; Weil and Brower, 1984; Batchvarova and Gryning, 1990;

Culf, 1992). Garrett (1981) derived a convective mixing depth model from a coupled set of ordinary differential equations which govern the time-dependent virtual temperature profile and inversion strength. The numerical solution is discussed by Driedonks (1982a, 1982b) and Wilczak and Phillips (1986). The method endorsed by the EPA for regulatory studies calculates hourly estimates of the mixing depth using an interpolation between a minimum height at sunrise and a maximum value at midafternoon. The maximum mixing depth is determined from the intersection of a dry adiabat constructed through the maximum afternoon surface temperature with a morning temperature sound. Benkley and Schulman (1979) describe an operational model similar to the EPA scheme. The mixing depth for a given time of day is defined as the height of intersection of a dry adiabat with a morning temperature sounding. In this case, the adiabat is constructed through the existing surface temperature. The effects of large-scale temperature advection are included by adjusting the surface temperature to reflect trends at the 700 mb level. None of the theoretical models address the collapse of the inversion in the late afternoon.

Irwin and Paumier (1990) compared predictions of Carson's (1979) slab model as modified by Weil and Brower (1984), the Garrett (1981) model and the EPA interpolation scheme with observations from three field experiments. All methods performed poorly during the growth stage of the mixed layer between sunrise and midday. The best results were obtained in estimating the late afternoon values when the mixed-layer height varies slowly with time. Estimates of the Garrett model displayed the most scatter; the slab model gave the best overall performance.

ERAD requires an estimate of the height of the lowest temperature inversion z_i to determine the mixing height. For convective atmospheres, we set $h = z_i$. An inversion rise model can be used to obtain h if a representative temperature profile is unavailable. Recently, a useful analytical solution to the Tennekes (1973) slab model equations has been presented by Thomson (1992). In neutral and stable conditions, the mixing height is taken as the minimum of z_i and the value given by the Zilitinkevich formula (Equation 5-23).

5.4 The Turbulence Profiles

Once the friction velocity (surface stress), Monin-Obukhov length (surface stress and heat flux) and mixing height are known, the turbulent velocity profiles can be estimated using similarity scaling laws. In particular, the variances of the horizontal wind components σ_u^2 and σ_v^2 are needed to estimate dispersion in the alongwind and crosswind directions. As discussed in section 5.2, these velocity fluctuations, even at locations close to the surface, are produced primarily by large eddies with diameters of many hundred meters. Because eddies of this size adjust very slowly to changing terrain, scaling which assumes local equilibrium, e.g., Monin-Obukhov surface layer similarity theory, cannot be applied.

In purely mechanical turbulence (near-neutral stratification), the standard deviations of the horizontal wind components, normalized by the friction velocity, are constant within the surface layer. Measurements of σ_u/u_* and σ_v/u_* show some variability from site to site which may be related to mesoscale terrain features, larger values being associated with rough terrain. Most observations are well represented by (Hicks, 1981; Panofsky and Dutton, 1984)

$$\sigma_u/u_* = 2.4 \quad (5-24a)$$

$$\sigma_v/u_* = 2.0. \quad (5-24b)$$

There are no adequate descriptions of turbulence above the surface layer because of the lack of detailed field studies in neutral conditions. Numerical models (Deardorff, 1972) show that, in general, σ_u and σ_v decrease with height. Velocity variances measured over the sea (Grant, 1986) show a weak dependence on height, decreasing through the lower half of the boundary layer.

In the CBL, data from the Minnesota (Kaimal et al., 1976) and AMTEX (Lenschow et al., 1980) field studies as well as laboratory measurements (Adrian et al., 1986) indicate that the horizontal velocity variances are equal and essentially constant with height. Panofsky et al. (1977) demonstrate that σ_u and σ_v do not follow Monin-Obukhov theory in the surface layer, but instead obey mixed-layer similarity and scale with the convective velocity. Fitting an empirical curve to surface layer observations from several field experiments, they find

$$\sigma_{u,v}/u_* = [4 + 0.6(-h/L)^{2/3}]^{1/2} \quad (5-25a)$$

which with the aid of Equation (5-5) may be rewritten

$$\sigma_{u,v} = (4u_*^2 + 0.6\kappa^{2/3}w_*^2)^{1/2} \quad (5-25b)$$

fits the data well except in conditions very close to neutral where equality of σ_u and σ_v is no longer valid. In near-neutral stability, this relation predicts $\sigma_{u,v} = 2u_*$ consistent with Equation (5-24). For very unstable conditions, the standard deviation becomes proportional to w_* and independent of u_* . Taking the limit as $-h/L \rightarrow \infty$, yields $\sigma_{u,v} = 0.57w_*$, in agreement with the observed value of $\sigma_{u,v}$ in the mixed layer (Caughey and Palmer, 1979; Lenschow et al., 1980, Caughey, 1982).

Hicks (1981, 1985) extends the analysis of Panofsky et al. (1977) showing that relationships similar to Equation (5-25), in which the velocity variance is composed of additive contributions from shear-produced turbulence and buoyancy-produced turbulence, apply over the entire CBL. Expressions of this form exhibit the proper behaviors at both the free convection ($-1/L \rightarrow \infty$) and neutral ($1/L \rightarrow 0$) limits. Following Panofsky and Hicks, we obtain the following formulas for convective and neutral boundary layers

$$\sigma_u = (5.8u_*^2 + 0.35w_*^2)^{1/2} \quad (5-26a)$$

$$\sigma_v = (4.0u_*^2 + 0.35w_*^2)^{1/2}. \quad (5-26b)$$

The constants in these relations have been chosen to conform with the neutral values in Equation (5-24) and the generally accepted convective asymptote. Hicks (1985) suggests a somewhat different neutral constant based on the 1968 Kansas experiment (Kaimal et al.,

1972). Predictions of Equation (5-26b) were shown by Hanna and Chang (1992) to be within ~25% of observational data from St. Louis and Indianapolis. In Figure 3, the free convection limit of Equation (5-26), i.e., $\sigma_{u,v}^2 = 0.35w_*^2$, is compared with data from atmospheric and water tank experiments. Similar formulations have been proposed by Gryning et al. (1987) and Britter and Hunt (1988).

Figure 3. Comparison of horizontal variance data from atmospheric and laboratory experiments with free convection limit of Equation (5-26).

Tests with ERAD using these analytical formulas showed that a substantial savings in computational time could be achieved if we used Equation (5-26b) and assumed $\sigma_u = \sigma_v$. The neutral value of σ_u is about 17% low with this simplification; the convective limit remains exact. Model predictions were insensitive to this assumption. Therefore, for convective and neutral conditions we use

$$\sigma_{u,v} = (4.0u_*^2 + 0.35w_*^2)^{1/2}. \quad (5-27)$$

In the stable surface layer, it is often assumed that the variances of the horizontal fluctuating velocities retain their neutral values as given by Equation (5-24). Above this layer, which can be as shallow as a few meters in strongly stable air, the variances decrease as a function of height to a minimum near the top of the boundary layer (Caughey et al., 1979; Lenschow, et al., 1988). The structure of the SBL is sensitive to physical processes unrelated to turbulence, e.g., gravity waves, the effects of sloping terrain and nocturnal low-level jets. Because of these complications, a universal model does not exist which adequately describes the SBL, particu-

larly for very stable conditions in which the variances become large and extremely variable. Sorbjan (1988) examined the turbulent structure of the SBL obtained from aircraft measurements during the Severe Environmental Storms and Mesoscale Experiment (SESAME). The data were collected over rolling terrain in central Oklahoma. Applying local similarity theory he obtained

$$\sigma_u = 2.0u_* (1 - z/h)^{3/4} \quad (5-28a)$$

$$\sigma_v = 2.1u_* (1 - z/h)^{3/4} \quad (5-28b)$$

Lenschow et al. (1988) analyzed the same data set and found

$$\sigma_u = \sigma_v = 2.1u_* (1 - z/h)^{7/8} \quad (5-29)$$

but noted that the scatter in the observations is such that an exponent of 3/4 would be equally justified. Expressions similar to these have been derived from tower data at Cabauw (Nieuwstadt, 1984a) and the Boulder Atmospheric Observatory (Sorbjan, 1987).

Numerical simulations of the SBL by Tjemkes and Duynkerke (1989) corroborate local similarity scaling. However, the results do not show the turbulence vanishing at $z = h$. Britter and Hunt (1988) suggest that the z/h terms in the profile equations be multiplied by 0.9 for undisturbed conditions and by 0.5 for cases with enhanced turbulence due to shear near the top of the surface inversion layer. These recommendations are not inconsistent with the SESAME data considering the large uncertainties in the measurements at the top of the boundary layer. In the ERAD model, we use

$$\sigma_{u,v} = 2.0u_* (1 - 0.8 \frac{z}{h})^{3/4} \quad (5-30)$$

as a compromise between these two results. Equation (5-30) and the SESAME observations are plotted in Figure 4.

5.5 Horizontal Dispersion

As described in section 3.4, ERAD uses a Gaussian formulation to model turbulent dispersion in the horizontal directions. The functions $\tilde{\sigma}_1$ and $\tilde{\sigma}_2$ appearing in Equation (3-14) can be identified as the Gaussian plume parameters σ_x and σ_y , where we have retained the usual notation in which the x and y subscripts refer to the horizontal alongwind and crosswind directions, respectively. Consistent with $\sigma_u = \sigma_v$ (Equations 5-27 and 5-30), we have $\sigma_x = \sigma_y$. The total dispersion σ^2 may be expressed as (Smith, 1965; Pasquill, 1976; Hanna, 1983)

$$\sigma^2 = \sigma_y^2 + \sigma_m^2, \quad (5-31)$$

where σ_y accounts for turbulence with short time scales and σ_m accounts for turbulence with longer time scales. Typically, the sampling time for σ_y is taken as 30 to 60 minutes although the original Pasquill-Gifford curves were based on a 3 minute sampling time (Pasquill, 1961;

Figure 4. Comparison of horizontal variance data from SESAME with Equation (5-30).

1976). The large-scale component σ_m includes contributions from variations in wind direction, mesoscale and synoptic-scale eddies and other phenomena which constitute the low frequency portion of the turbulent energy spectrum, e.g., gravity waves. Here we concentrate on σ_y ; the effects of directional shear with height are handled explicitly in the wind field model.

Often overlooked is the increase in the lateral standard deviation with sampling time, a consequence of including more of the large-scale turbulent energy in the averaging process. Defining a limiting sampling interval beyond which σ_y no longer increases is effectively precluded since the scales of the horizontal turbulent motions can reach hundreds of kilometers and many hours. However, there is usually a gap in the turbulent energy spectrum at a frequency corresponding to a time duration of about 1 hour (e.g., Kaimal et al., 1976) separating the microscale and mesoscale effects. Averages of 30 to 60 minutes are relatively stable; as the sampling period is extended the mean values again exhibit fluctuations. This spectral gap is the basis for the generally accepted practice of choosing sampling times on the order of 1 hour.

It is important to distinguish between dispersion from an instantaneous source, or puff, and a continuous source, or plume. Dispersion from an explosive release clearly falls into the former category. Puff (relative or two-particle diffusion) analyses apply when the sampling time is short; plume (single-particle diffusion) formulas are time-averages and apply when the sampling time is long. To illustrate these differences, suppose a photograph of a continuous plume is taken every 30 sec. The instantaneous width of the plume obtained from a single photograph

yields information on puff diffusion since the sampling time is essentially zero. The width of a mosaic constructed from a sequence of photographs taken over, say, 10 min, provides information on plume dispersion.

The primary difference between a puff and plume is that some measurements indicate that there is a region in which puff diffusion occurs at a rate greater than plume diffusion. Gifford (1977) compiled a set of puff observations including data from radioactive clouds, tetraon pairs, artillery bursts and even soap bubbles. No attempt was made to classify the data according to source or meteorological parameters. The atmospheric measurements extended to travel times of 12 days (downwind distances of 100 km or more). These data support a $\sigma_y \propto t^{3/2}$ growth for travel times up to somewhere between 1000 and 3000 sec, whereas the spreading of continuous plumes is at most $\sigma_y \propto t$. The data do, however, show considerable scatter, σ_y varying by nearly an order of magnitude at 1000 sec. Theoretically, this period of accelerated growth occurs when the puff is growing through dimensions which correspond to the inertial subrange of turbulence energies (Batchelor, 1952).

Model developers are faced with a dilemma when attempting to specify puff dispersion parameters since very little field data exists for instantaneous releases. There have been no major field or laboratory studies of puff diffusion. Without detailed and thorough experimental information, it is impossible to develop and test a general, systematic theory which describes the behavior of the diffusion parameter. These difficulties are underscored in the different and sometimes contradictory evaluations of the available field measurements. As an example, although Gifford's (1977) data exhibit a $\sigma_y \propto t^{3/2}$ regime, Hanna et al. (1982) point out that a $\sigma_y \propto t$ law, consistent with the early growth of a continuous plume, gives the best agreement over the largest part of the observations. More recently, Carras and Williams (1986) found a similar $t^{0.85}$ dependence when analyzing relative diffusion data from four different sites during convective conditions.

Measurements that are comprehensive and of sufficient quality to validate theoretical formulas for σ_y are only available from continuous sources. It would be most useful then if the dispersion parameters obtained from plume studies could be applied to puffs. Hunt and Weber (1979) show that the ensemble statistics of an instantaneous release, obtained by averaging over many puffs, are the same as the statistical properties of a plume if the two-particle Lagrangian velocity correlation is small. They go on to demonstrate that for most situations the effect of this correlation is negligible. Since we are interested in the ensemble mean properties of the distribution, this result implies that at least to a first approximation we can use σ_y relations developed for continuous plumes.

For a continuous source, there is general agreement that the turbulent dispersion parameter is given by the formula (Hanna et al., 1977)

$$\sigma_y = \sigma_v t f_y(t/\tau_{Ly}), \quad (5-32a)$$

where f_y is a dimensionless function and τ_{Ly} is the Lagrangian time scale. The form of f_y is usually chosen so as to satisfy Taylor's (1921) statistical theory of diffusion for stationary, ho-

mogeneous turbulence, i.e., a linear $\sigma_y \propto t$ growth near the source and a $\sigma_y \propto t^{1/2}$ dependence for large times. Field observations (e.g., Hanna, 1986) show that the square-root-of-time asymptote is not often realized owing to the effects of lateral meandering and mesoscale and synoptic-scale eddies. Briggs (1985) argues that for long travel times a $t^{2/3}$ growth is more typical of real-world σ_y values measured near the surface.

Irwin (1983) compared several empirical forms of f_y with field data collected at eleven sites. A form first proposed by Draxler (1976)

$$f_y = \frac{1}{1 + 0.9 (t/T_i)^{1/2}} \quad (5-32b)$$

performed best. The same form was adopted in a later study by Gryning and Lyck (1984). The time scale T_i controls how rapidly the $\sigma_y \propto t^{1/2}$ asymptote is achieved. Hanna (1986) analyzed ground-level σ_y observations from buoyant, stack plumes and showed that Equation (5-32) with $T_i = 15000$ sec is valid out to downwind distances of 50 km. A $\sigma_y \propto t^{1/2}$ relationship was not observed in these data. Li and Meroney (1985) found that a value of 4000 sec for T_i provided an adequate fit to their elevated, non-buoyant source data although, as noted by Gifford (1987), the scatter in the measurements is such that a reasonable argument could be made for $T_i = 15000$ sec as recommended by Hanna (1986). The difference in these two T_i values may reflect the enhancement in σ_y due to the strong buoyancy of the power plant plumes studied by Hanna (1986). Observations of lateral dispersion from sources at heights closer to the ground generally show somewhat smaller values of the time scale. In ERAD, Equation (5-32) with a time scale of $T_i = 10000$ sec is used to compute σ_y in stable atmospheres.

For convective and neutral boundary layers, a more theoretical description can be derived using mixed layer similarity and assuming independent contributions to σ_y from mechanically-driven and buoyancy-driven turbulence (Berkowicz et al., 1985). Following Nieuwstadt and van Duuren (1979) we write

$$\sigma_y = \frac{\sigma_v t}{(1 + t/T_i)^{1/2}} \quad (5-33a)$$

$$T_i = \frac{h}{[(0.24u_*)^2 + (0.91w_*)^2]^{1/2}}, \quad (5-33b)$$

where σ_v is given by Equation (5-27). The constant multiplying the u_* term in the expression for T_i is obtained by equating the neutral form of Equation (5-33) with Equation (5-32). The constant multiplying w_* is chosen so that in the free convection limit ($-h/L \rightarrow \infty$) Equation (5-33) matches the σ_y result developed by Deardorff and Willis (1975) from their convection tank experiments. Nieuwstadt and van Duuren (1979) derive a result similar to Equation (5-33) but use a cubic weighting in their expressions for σ_v and the time scale T_i . Their formula matches Equation (5-32) in neutral conditions but with $T_i = 1000$ sec.

5.6 Vertical Dispersion — The Eddy Diffusivity

A number of investigations have demonstrated that vertical dispersion in the surface layer can be described using an eddy diffusivity derived from Monin-Obukhov similarity theory (Nieuwstadt and van Ulden 1978; van Ulden, 1978; Gryning et al., 1983; Ogawa et al., 1985; Gryning et al., 1987). Empirical evidence suggests that the diffusivity of matter K can be assumed equal to the diffusivity of heat. This implies

$$K(z) = \frac{ku_* z}{\phi_h(z/L)}, \quad (5-34)$$

where ϕ_h is the dimensionless temperature gradient.

Observational data on the vertical distribution of K above the surface layer are incomplete. However, the few limited experiments provide a qualitative picture of the variation of the diffusivity with height. Crane et al. (1977) used concentration measurements from the Los Angeles Reactive Pollution Project to calculate the diffusivity in the CBL. Their analysis shows K increasing through the surface layer, nearly constant at mid-mixing depth and decreasing to a minimum at the top of the boundary layer. The measurements indicate the maximum diffusivity occurs in the region $0.2 < z/h < 0.55$. For convective to neutral conditions, most observations indicate the diffusivity reaches a maximum near $z/h = 0.4$, consistent with the observed peak in the vertical fluctuating velocity variance σ_w^2 (Lenschow et al., 1980). The diffusivity profile calculated from the stable boundary layer data obtained during SESAME (Lenschow et al., 1988) has a maximum near the top of the surface layer ($z/h \sim 0.1$). Above this level, K decreases with height and remains non-zero to about $z/h = 1.4$. The early efforts to develop analytical diffusivity formulas (O'Brien, 1970; Agee et al., 1973; Shir, 1973; Businger and Arya, 1974), based largely on empiricism, exhibit these qualitative features.

In the CBL, strong vertical mixing results from updrafts and downdrafts that extend over the entire depth of the boundary layer. Observations show that the updrafts are more energetic and occupy a smaller fraction of the horizontal area than the downdrafts. The fast rising thermals cause a positive skewness in the probability density of the vertical turbulent velocity (Lenschow et al., 1980) and produce regions of countergradient transport. Obviously, an eddy diffusivity formulation based on local gradients (local K theory) cannot be applied to cases in which the flux is counter to the concentration gradient. This problem is evident in the diffusivity profiles developed from similarity arguments by Sorbjan (1986c, 1989, 1990) which show a singularity near the middle of the mixed layer and become negative above this height.

A useful framework for analysis of vertical diffusion in the CBL is obtained by decomposing the process into top-down and bottom-up components (Wyngaard and Brost, 1984). The top-down component is driven by the entrainment flux at the top of the mixed layer with zero surface flux. The bottom-up diffusion is driven by the surface flux with no flux at the top. Wyngaard (1987) and Schumann (1989) use this decomposition and find that although the top-down diffusion is well behaved, the bottom-up diffusivity exhibits a singularity due to countergradient flux. Holtslag and Moeng (1991) derive a countergradient correction using the results

of a large eddy simulation by Moeng and Wyngaard (1989) which eliminates the singularity. Their formulation combines local gradient transport and a nonlocal countergradient term related to the skewness in the vertical turbulent velocity field. The kinematic model of Wyngaard and Weil (1991) also demonstrates the link between velocity skewness and the breakdown of local K theory. Holtslag and Moeng (1991) find the eddy diffusivity for a conservative scalar, i.e., heat, humidity or contaminant, may be written as

$$K(z) = \frac{[1 - z/h + R(z/h)] K_t K_b}{(1 - z/h) K_t + R(z/h) K_b}, \quad (5-35)$$

where the top-down and bottom-up diffusivities are given by

$$K_t = 7w_* h \left(\frac{z}{h}\right)^2 \left(1 - \frac{z}{h}\right)^3 \quad (5-36a)$$

$$K_b = w_* h \left(\frac{z}{h}\right)^{4/3} \left(1 - \frac{z}{h}\right)^2 \quad (5-36b)$$

and R is the ratio of the entrainment flux at the top of the CBL to the surface flux for the scalar. Typical values of R are -0.4 to -0.1 for heat and 0.5 to 1.5 for moisture. For small z/h , Equation (5-35) matches the results of surface layer similarity theory.

For the stably stratified boundary layer, the available eddy diffusivity observations are well represented by

$$K(z) = \frac{\kappa u_* z (1 - z/h)^n}{\phi_h(z/L)}, \quad (5-37)$$

a form first derived by Brost and Wyngaard (1978) using a second-order closure model. They show the calculated diffusivity profile with $n = 1.5$ agrees with measurements made over Antarctica. Nieuwstadt (1984a) and Sorbjan (1986a, 1986c) obtain the same expression from local similarity theory. Nieuwstadt found $n = 2$ for Cabauw observations collected two to three hours after sunset in near-stationary conditions. The Minnesota data analyzed by Sorbjan were taken close to sunset in an evolving boundary layer and show $n = 1$. The SESAME observations indicate an exponent between 1 and 2 (Lenschow et al., 1988; Sorbjan, 1988). Degrazia and Moraes (1992) derive a very similar diffusivity relation applying local scaling to the energy spectra of the turbulent velocities. More recent numerical studies of the SBL by Lacser and Arya (1986), using a one-dimensional turbulent kinetic energy model, and Garrat (1987), using a two-dimensional primitive equation mesoscale model, confirm the applicability of Equation (5-37). The average value of n was 1.6 for the range of stable conditions ($3 < h/L < 7.5$) considered by Lacser and Arya.

The ERAD model uses Equation (5-35) to compute the eddy diffusivity for convective atmospheres and Equation (5-36) with $n = 1.5$ for stable conditions. To provide closer agreement with both numerical and experimental results which show a non-zero K at the top of the boundary layer, the $(1 - z/h)$ terms are replaced by $(1 - 0.95z/h)$.

6.0 The Roller Coaster Data

The first U.S. attempts to characterize plutonium dispersion resulting from accidental detonation of the high explosive in a nuclear weapon were made at the Nevada Test Site in November 1955 and January 1956 in Project 56. Subsequently, a more extensive experiment, TG57, was carried out as part of Operation Plumbob in April 1957. Recognizing the shortcomings of TG57, a joint U.S.-U.K. effort, Operation Roller Coaster, was conducted in May through June of 1963 near the Tonopah Test Range in southwest Nevada. Specifically, these experiments were to obtain more detailed measurements of the source term and an improved description of the dispersion process that could assist in developing storage criteria for overseas sites where proximity to densely populated areas was a concern. With ratification of the Limited Test Ban Treaty in the fall of 1963, additional field programs like Roller Coaster in which plutonium aerosol would be dispersed in the atmosphere were prohibited.

Each of the four Operation Roller Coaster events: Double Tracks, Clean Slate 1, Clean Slate 2 and Clean Slate 3, addressed a different weapon storage configuration. In each test, one or more devices containing about 48 kg of high explosive was detonated at a single point simulating accident conditions. One unit in each experiment contained plutonium and depleted uranium, all others were entirely depleted uranium. Double Tracks involved a single device held on a stand one foot above an eight foot square steel plate anchored to a concrete pad. The surrounding soil was oil-soaked to minimize entrainment. In Clean Slate 1, nine devices on stands were detonated on a twenty foot square concrete pad representing an accident occurring under open storage conditions. The detonation sequence simulated propagation from the center plutonium-bearing device to the eight surrounding depleted uranium units. Clean Slate 2 and 3 evaluated the effects of earth-covered storage igloos. To avoid complications associated with igloo disassembly and particle interactions with the earth overburden, only the two open-air shots, Double Tracks and Clean Slate 1, were used to validate the ERAD model. A summary of these experiments is given in Table 2.

Table 2. Operation Roller Coaster Event Descriptions

Event Designation	Date	Shot Time (PDT)	Number of Units	HE Mass (kg)
Double Tracks	15 May 1963	0255	1	47.6
Clean Slate 1	25 May 1963	0416	9	428.4

6.1 Meteorological Measurements

Titus (1965) documents the meteorological measurements made in support of Operation Roller Coaster. The on-site observational data for each test included radiosonde temperature measurements to about 5000 ft above the surface. Wind speed and direction profiles were determined using a radar system which tracked an aluminum target carried aloft by a 100 g balloon. For Double Tracks and Clean Slate 1, three weather balloon release stations were sited along the sampling array centerline. Augmenting the upper air observations were a number of tower and

balloon-based instruments deployed around the detonation point. Wind data were collected from towers at 30, 60 and 120 ft levels. The U.K. provided temperature measurements to a height of 900 ft using a series of thermistors attached to a captive balloon cable at 100 ft intervals. Temperature differences measured with the thermistors were purportedly accurate to $\pm 0.3^\circ\text{C}$. This balloon was tethered about 1600 ft from the radiosonde launch site. Surface winds were also obtained from 30-ft towers at three or four additional locations within the aerosol sampling grid.

The radiosonde potential temperature profiles and U.K. thermistor data are shown in Figure 5. Immediately obvious is the discrepancy between the two measurement systems. At all heights the thermistor values are larger than the radiosonde data. The best agreement is at the surface with differences as large as 4°C at higher elevations. Similar trends are evident in the Clean Slate 2 and Clean Slate 3 data. No explanation of these results is offered in any of the Roller Coaster documents. Church (1991) confirms that there were no known problems with the radiosonde equipment. Since we were unable to resolve these discrepancies, our validation studies were based on the temperature sound data alone. Unfortunately, the radiosonde observations provide little resolution, with only one or two measurements in the surface layer.

Figure 5. Double Tracks and Clean Slate 1 temperature profile observations.

The vertical profiles of wind speed obtained from the ground zero balloon release stations are presented in Figure 6. The Double Tracks wind and temperature profiles are typical of the near-neutral atmospheric boundary layer. Clean Slate 1 conditions are more stable with considerable

shear in both wind speed and direction near the surface; in the lowest 50 m the directional shear was about 100 degrees.

Figure 6. Double Tracks and Clean Slate 1 wind speed profile observations.

6.2 Aerosol Measurements

This section includes an exhaustive re-examination of the Roller Coaster aerosol data with particular emphasis placed upon estimates of uncertainties in model performance metrics which result from variabilities in individual observations. This has been a very tedious process complicated by discrepancies between the different data sources, the complexity of the measurements and the age of the information. This effort has, however, been necessitated because the only method of evaluating the physical descriptions embodied in the ERAD model is by comparing predictions with field measurements and the Roller Coaster data remain the best available.

As shown in Figure 7, the primary sampling array for each event consisted of a 90 degree sector divided into a number of arcs, labeled A through R. Surveyed along each arc at angular intervals of 3/4 degree were 121 sampling stations. On arcs B through R, a two foot square concrete pad was located at each station for alpha survey measurements. The Double Tracks array extended to 48000 ft downwind (arc R); the Clean Slate 1 grid to 35000 ft (arc P). A climatological study conducted during the months prior to the Roller Coaster field phase established that the dominant terrain features induced a north-south flow and, therefore, the sampling grids were oriented toward the south.

Figure 7. Operation Roller Coaster primary sampling array.

6.2.1 Dosage

Dosage (time-integrated concentration) was measured by air samplers attached to 4.5 ft steel posts on alternate arcs beginning with arc B. The angular spacing between adjacent samplers varied from 1.5 to about 9 degrees. In addition to the ground array, a curtain of air samplers was suspended from a large balloon positioned on arc B. The sampler pumps were activated some minutes before shot time and operated up to 3 hrs afterwards to insure complete time integration of concentration.

Aerosol samples were collected using Casella Mark II and Anderson cascade impactors and three different types of total material samplers (Maloney, et al., 1965). All of these instruments were ineffective at sampling particles with diameters larger than about 50 μm . Reported "total" dosage values are, therefore, not representative of the entire particle size distribution but only include contributions from particles with diameters less than this approximate cutoff. Comparing observations from stations in which two or more samplers were located shows that differ-

ences of a factor of five between supposedly identical measurements are common. Luna et al. (1971) use a statistical technique to analyze the replicate samples and find that respirable dose[†] data obtained from the cascade impactors demonstrate the least variability. Only the respirable measurements will be used to validate the ERAD model.

Based on the principle of inertial impaction, a cascade impactor separates a source aerosol into a number of size classes according to aerodynamic diameter. In particular, the fraction of the source which is respirable, i.e., capable of reaching the lower (pulmonary) portion of the lung, can be defined. The Casella Mark 2 has four impaction stages followed by an afterfilter. The Anderson impactor was a modified version of the unit commercially available at the time. This modification permitted use of glass plate rather than Petri dish aerosol collection surfaces. In modified form, the Anderson impactor consists of five stages (the commercial unit had six) and a final filter. Both impactors require a nominal flow rate of 18 lpm.

Thomas (1965) summarizes the performance characteristics of the impactors. Sampling efficiency curves for each stage and the resulting cut-points are given. A quantitative assessment of internal particle losses and the inlet sampling efficiency as a function of particle diameter was not made. Qualitatively, the largest losses were found on the upper surface of stage one of the Anderson impactor. For the respirable aerosol, the calibration data suggest the Casella and Anderson units perform comparably.

Roughly 220 Casella and 90 Anderson impactors were fielded on each Roller Coaster event. Not all these samples were selected for radiochemical analysis. With the exception of Clean Slate 1, selections were guided by the preliminary alpha survey plots and field laboratory counting of respirable and total plutonium in air samples. Since the activity levels in the Clean Slate 1 dosage samples were extremely low, sample selection was based solely on the alpha survey. As a result, only a narrow segment of the Clean Slate 1 sampling array was analyzed. Myers (1964) gives a complete listing of the samples chosen for chemical assay and special studies. The results of the air sampler radiochemical analysis are tabulated in Church et al. (1970). All experimental results shown here are have been obtained directly from this data but a correction has been made for an error in sampler locations that appeared in the original documentation.

The operational performance of the cascade impactors was evaluated by examination of samples from individual stages (Sherwood, 1966). Evidence of anisokinetic sampling and varying degrees of particle collection on internal surfaces other than the impaction plates (internal losses) were observed. A number of Casella impactors showed signs of overloading with large particles found on stages 3, 4 and the afterfilter. As might be expected, this was most apparent at locations close to ground zero, e.g., on the arc B balloon curtain, where the aerosol concentration was high. Overloading distorts the particle size distribution causing the respirable fraction to be overestimated.

[†] The respirable dose includes only those particles with aerodynamic diameters less than 10 μm .

Although the respirable dose data are considered more reliable than the total aerosol measurements, there is still significant scatter in the observations. Data from the twenty five Double Tracks and Clean Slate 1 sampling stations where two or more cascade impactors were used to make simultaneous measurements are shown in Figure 8. Excluding those stations in which one of the samplers read zero, "identical" measurements differ by as much as two orders of magnitude.

Figure 8. Double Tracks and Clean Slate 1 respirable dosage measurements for stations in which two or more cascade impactors were collocated.

To better characterize the scatter in the data, the distribution of a simple performance statistic derived from the replicate samples was determined. Specifically, for each station with m non-zero samples we calculate m ratios

$$R_i = \frac{C_i}{(C_1 C_2 \dots C_m)^{1/m}} \quad i = 1, 2, \dots, m \quad (6-1)$$

where the C_i are dosage measurements and, in our case, m is either two or three. The ratios for all replicate sampler stations taken together form a set of dimensionless variables with a geometric mean of one. The geometric standard deviation σ_g of the R_i 's provides a measure of the variability in the data. Treating the Casella and Anderson impactor observations in Figure 8 as a single population, we obtain $\sigma_g = 2.3$. Luna et al. (1971) use a similar approach but there are several inconsistencies in their results which make interpretation difficult.

In Figure 9, a lognormal distribution with geometric mean one and geometric standard deviation 2.3 is superimposed on the cumulative distribution function of R_i . Visual inspection of the two functions indicates that a lognormal hypothesis is plausible. A Kolmogorov-Smirnov (KS) test was used to examine the assumption that the observations came from a lognormal distribution. The KS-test is based on the difference between the empirical and theoretical curves. More precisely, we form the two statistics KS^+ and KS^- , where KS^+ measures the maximum deviation above the lognormal curve and KS^- measures the maximum deviation below the lognormal function. The maximum separations are then multiplied by the square root of the number of samples (this magnifies the statistics so that their standard deviations are independent of sample size). The KS-test applied to this data gives 0.60 and 0.88 for KS^+ and KS^- , respectively. If either value was greater than the 95% level of the KS distribution function, namely 1.22, we would consider the lognormal assumption suspect. For the replicate sampler data shown in Figures 8 and 9, the KS-test indicates that the R_i can be adequately represented by a lognormal distribution.

Figure 9. Cumulative distribution function of ratios defined by Equation (6-1) for Double Tracks and Clean Slate 1 respirable dosage measurements.

The random samples $\log R_i$ are, therefore, approximately normally distributed with mean zero and standard deviation given by the logarithm of the geometric standard deviation $\log 2.3$. The probability is then 68% that a random sample lies in the interval $-\log 2.3 < \log R_i < \log 2.3$. Taking exponentials this interval becomes $1/2.3 < R_i < 2.3$, which shows that the R_i exhibit random fluctuations that are roughly a factor of 1/2.3 smaller or 2.3 larger than one.

Contours of the observed respirable dosage are presented in Figure 10. The distinct broadening of the Double Tracks contours beyond 10 km downwind occurs as the atmospheric flow moves around Stonewall Mountain which lies immediately to the south of the sampling array. The large amount of energy released in the Clean Slate 1 detonation produced a very buoyant cloud which carried most of the small particles above the mixing depth and caused the markedly lower levels of respirable dose compared to Double Tracks. Unfortunately, not all features of the dosage plots can be ascribed to physical phenomena; some are artifacts of the number and location of samples selected for analysis. This is particularly the case for Clean Slate 1 where, based on ground deposition levels, only a narrow sector of the 90 degree sampling array was assayed. In Figure 11, the measurement locations are overlaid on the dosage contours. Only two samples define the east side of the Double Tracks array. The observations suggest that the width of the Clean Slate 1 dosage pattern has been artificially constrained by the measurement domain and may not be representative of the actual dispersal, e.g., values on the east boundary of the array, close to ground zero, exceed $1 \mu\text{g-sec}/\text{m}^3$. On the more distant arcs, dosage increases from east to west. The extension of the $0.1 \mu\text{g-sec}/\text{m}^3$ contour west of the sampling grid is based on a numerical extrapolation of the dosage surface. Although there is little reason to believe that this extrapolation is accurate, the trends in the data provide strong physical evidence that the available measurements do not encompass the entire dosage pattern. These uncertainties diminish the value of a model comparison with the Clean Slate 1 results.

With the conclusion that the R_i are lognormally distributed, it is possible to develop a first order estimate of the uncertainty bounds on the areas enclosed within the respirable dosage contours. As an upper bound, areas were determined from a set of dosage values which were all a factor of σ_g larger than the actual measurements. Similarly, a lower bound was derived from the observed values divided by σ_g . Because the area calculation is nonlinear, it is not possible to develop a mathematical relationship between these bounds, obtained from setting each sampler to its one-standard-deviation level, and bounds determined directly from the (unknown) probability distribution for area. The contours for the two bounding cases are shown in Figure 12 for Double Tracks and Figure 13 for Clean Slate 1. Tables 3 and 4 summarize the contour area information. A better approach, which is the subject of a future study, is to perform numerical experiments in which lognormal variates are sampled at each station. The resulting contour area distribution function can then be used to estimate confidence intervals.

Table 3. Double Tracks Respirable Dosage Contour Areas

Dosage Level ($\mu\text{g-sec}/\text{m}^3$)	Observed (km^2)	Lower Bound (km^2)	Upper Bound (km^2)
10	19	2.6	56
30	2.0	0.95	13
100	0.56	0.10	1.5

Figure 10. Observed respirable dosage contours.

Figure 11. Measurement locations superimposed on observed respirable dosage contours.

Figure 12. Double Tracks respirable dosage contours for lower and upper bound cases.

Figure 13. Clean Slate 1 respirable dosage contours for lower and upper bound cases.

Table 4. Clean Slate 1 Respirable Dosage Contour Areas

Dosage Level ($\mu\text{g}\cdot\text{sec}/\text{m}^3$)	Observed (km^2)	Lower Bound (km^2)	Upper Bound (km^2)
1	1.7	0.72	9.8
3	0.50	0.032	1.5

6.2.2 Deposition

Sticky paper deposition samplers were placed at alternate stations on alternate arcs starting with arc B (Krey et al., 1965). For Double Tracks, all deposition samples from arc B and samples from stations 030 to 070 on the more distant arcs were recovered. Clean Slate 1 samples from stations 000 to 060 on all arcs were recovered and available for subsequent radiochemical analysis. Less reliable deposition estimates over a larger portion of the sampling array were obtained from the alpha surveys conducted shortly after each event.

The deposition contours and contour areas shown in Figure 14 and Table 5 are taken from the interim summary report by Shreve and Thomas (1965). These results are consistent with those in the final report which remains classified. The measurements from which the deposition contours were constructed are unavailable. This precluded a determination of uncertainty estimates as was done for the respirable dosage data. Deposition results obtained from chemical analysis were most reliable; for the alpha surveys, factor of two to three variations across a 2 ft square sampling pad were common.

Table 5. Deposition Contour Areas

Deposition Level ($\mu\text{g}/\text{m}^2$)	Double Tracks Observed (km^2)	Clean Slate 1 Observed (km^2)
10	10	7.2
15	5.3	5.6
30	2.0	2.7
50	0.52	0.97
100	0.05	0.31

The dosage contours presented in Figures 10 through 13 were produced using a numerical surface fitting procedure which smooths the large variations in the measurements. The deposition results given in Shreve and Thomas (1965), reproduced here in Figure 14, were hand-drawn through the observations and fully reflect the small-scale spatial variations in the data. This leads to jagged, discontinuous curves which do not represent average values. Note also that the eastern portion of the Double Tracks 1 $\mu\text{g}/\text{m}^2$ contour was based entirely on alpha survey measurements.

Figure 14. Observed deposition contours. Double Tracks contours outside of dash-dot lines were determined by alpha survey data alone.

6.2.3 Particle Size Distribution

The aerosol formed in each Roller Coaster experiment was comprised of particles with diameters from tenths to several hundred micrometers. Because no single instrument is capable of efficiently sampling over such a wide range of sizes, an estimate of the complete particle size distribution was obtained by piecing together measurements from several different types of samplers. Obviously, the uncertainties associated with this subjective procedure are extremely large. This is compounded by variability in the observations and errors introduced by sampler overloading and anisokinetic sampling.

Composite particle size distributions representative of the aerosol at arc B, 2500 ft from ground zero, were derived for each event (Friend and Thomas, 1965). Balloon curtain cascade impactor observations defined the size distribution in the respirable range. For larger diameters, Cassella stage 1 data and results from three special particulate studies (Dunn and Bersin, 1965; Fuller et al., 1965; Sherwood, 1966) were used. These studies involved more detailed examination of deposition samples, sticky wire samples from the balloon curtain, total material air samples and individual particles using, e.g., optical and electron microscopy, electron diffraction, x-ray diffraction, electron microprobe analysis and nuclear track autoradiography.

The Double Tracks and Clean Slate 1 particle size distributions were identical within the accuracy of the data and estimation methodology. For the purposes of the model evaluation, the size distribution data from these two experiments were fit with a single truncated lognormal distribution. The parameters of the lognormal fit are: minimum diameter 0.1 μm , maximum diameter 200 μm , median diameter 43 μm and geometric standard deviation 3.5.

7.0 Validation Results and Closing Remarks

Previous to this study, the plume rise simulation was tested by comparing predictions of cloud top height with field measurements made during a series of fifteen high explosive experiments, including Double Tracks and Clean Slate 1. The mean relative error was less than 10% and, with few exceptions, the predictions were within 25% of the observations (Boughton and De-Laurentis, 1987). The Monte Carlo transport and diffusion algorithms were first verified against known analytical solutions of the atmospheric dispersion problem for nonbuoyant releases. Agreement between these solutions and the Monte Carlo results was excellent (Boughton et al., 1987). In this chapter, the complete ERAD model (described in Chapters 2 through 5) is evaluated using the respirable dosage and deposition observations from Double Tracks and Clean Slate 1. Visual inspection of the contour plots provides a qualitative assessment of predictive capability. A quantitative measure of model performance is obtained by comparing predicted and observed contour areas.

Figure 15 shows ERAD predictions for Double Tracks. In general, the qualitative features of the observations (Figures 10 and 14) are reflected in the simulation results. The predicted dose and deposition patterns are ensemble means and do not show the small-scale spatial variations evident in the data. A comparison of ERAD contour area predictions with the measured values is given in Figure 16. The top and bottom of the respirable dosage error bars correspond to the upper and lower bounds discussed in section 6.2.1. For the deposition contour areas, we have assigned factor-of-two error bars.

Clean Slate 1 results are presented in Figures 17 and 18. The ERAD computational domain was chosen to approximate the narrow region of the sampling array from which samples were selected for analysis. The deposition contours and contour areas are in close agreement with the observations. The dosage results are less definitive. The strongly buoyant cloud rapidly escapes the shallow ground-based inversion layer, carrying with it nearly all the respirable-sized particulate material. Many of the larger particles that contribute to the deposition remain within the stable surface layer. The dispersion of the small particles is then dominated by processes above the mixed layer where a reliable parameterization of transport and diffusion does not yet exist. In contrast to the smooth deposition contours, the dosage prediction is marked by a series of "hot" spots. This random pattern is caused by small numbers of particles reentering the inversion layer from above and slowly mixing toward the ground.

A common and accepted statistical measure for assessing the performance of an atmospheric dispersion model is the average fractional bias F_b (Cox and Tikvart, 1985; Hanna, 1989) which may be written

$$F_b = \frac{1}{N} \sum_{i=1}^N \frac{2(P_i - O_i)}{(P_i + O_i)}, \quad (7-1)$$

where P_i and O_i are the predicted and observed contour areas, respectively, and N is the number of data points. The Double Tracks and Clean Slate 1 dosage and deposition model-data comparisons taken together yield a set of fifteen contour area pairs (P_i, O_i) from which we

Figure 16. Respirable dosage and deposition contour area comparison for Double Tracks.

Figure 17. Predicted respirable dosage and deposition contours for Clean Slate 1.

Figure 18. Respirable dosage and deposition contour area comparison for Clean Slate 1.

find $F_b = 0.53$. This implies that on average the ERAD contour area predictions differ from the observed values by about 50%. Clearly, this result falls within the uncertainties of the measurements.

In summary, the ERAD model is a numerical simulation of atmospheric dispersion based on first-order physical principles. It employs a state-of-the-art boundary layer description and runs on a small, notebook computer with typical execution times of about two minutes. Most importantly, ERAD duplicates the results of the Operation Roller Coaster experiments within the uncertainties of the data. To further enhance its utility, a graphical user interface is being developed which will permit practitioners with a minimum of training to apply the model.

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