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LA-6103

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Reporting Date: September 1975

Issued: January 1976

Monte Carlo Simulation of the Turbulent Transport of Airborne Contaminants

by

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**UNITED STATES
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION
CONTRACT W-7405-ENG. 36**

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Printed in the United States of America. Available from
National Technical Information Service
U S Department of Commerce
5285 Port Royal Road
Springfield, VA 22151
Price: Printed Copy \$4.00 Microfiche \$2.25

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SYMBOLIC LIST

Δt = time-step taken.
 t = time.
 $t_j \equiv \tau_j$ = travel time up to step j , measured from t_0 .
 t_0 = starting time for a particle trajectory.
 L_x = time-mesh size.
 $\tau_j \equiv \Delta t$ = time-resolution limit for the trajectory.
 τ = lag time.
 $x = (x, y, z, u)$ = the phase-space of interest.
 $x_j = (x_j, y_j, z_j, u_j)$ = phase-space location of a particle at step j .
 x_0 = phase-space location of the starting point of a trajectory.
 $(1,0)$ = National Meteorological Center rectangular-coordinate system.
 n = number of time steps per trajectory.
 N = number of trajectories in the cloud simulation.
 ν = frequency.
 $\vec{r}_{jc} = (x_{jc}, y_{jc}, z_{jc})$ = position of source-cloud centroid at step j .
 $\vec{r}_{sc}$ = position of cloud centroid at time t_0 .
 $\vec{r}_j = (x_j, y_j, z_j)$ = position of a particle trajectory at step j .
 $\vec{r}_0$ = trajectory starting position at time t_0 .
 $\Delta \vec{r}_j = (\Delta x_j, \Delta y_j, \Delta z_j)$ = trajectory displacement during step j .
 $\vec{r}_j = (x_j - x_{jc}, y_j - y_{jc}, z_j - z_{jc})$ = radial position of a particle at step j as measured from the cloud centroid.
 $\vec{r}_0$ = radial position of trajectory starting point at time t_0 .
 $\vec{u}_j = (u_j, v_j, w_j)$ = local wind vector at $\vec{r}_j$.
 (u_j, v_j, w_j) = components of $\vec{u}_j$ in the y -, x -, and z -directions, respectively (CFOUR code).
 $\Delta \vec{u}_j = (\Delta u_j, \Delta v_j, \Delta w_j)$ = a random sample from the probability density function describing small-scale (one-step) wind fluctuations at $\vec{r}_j$.

NOTATION (cont)

* = expected value.

$\bar{u}_j = \langle \vec{u}_j \rangle = \langle u_j, v_j, w_j \rangle = (\bar{u}_j, \bar{v}_j, \bar{w}_j)$ = mean wind at z_j .

$f(\vec{r}_0)$ = initial cloud-particle distribution about the cloud centroid.

$f_A(\lambda)$ = probability density function of A .

$p(u)$ = probability density function for the small-scale (one-step) fluctuations of u .

$\phi(u, \sigma_u^2)$ = normal distribution function with mean = 0, variance = σ_u^2 .

$\phi_{ij}(\tau) = \langle (u_j - \bar{u}_j)(u_{j+\tau} - \bar{u}_{j+\tau}) \rangle$ = autocovariance function for u_j at lag time τ .

$\Phi(\nu)$ = turbulent-energy power spectral density at frequency ν .

R = ratio of dissipation to Kolomov time scales of turbulence.

$\hat{r}_{j,i}$ = velocity-recursion-relationship correlation parameter between steps j and i .

$\hat{r}_w$ = "one-term" velocity-recursion-relationship correlation parameter for vertical transport.

$\sigma_{\vec{r}_j}^2$ = variance of $\vec{r}_j$ distribution for N trajectories.

$\sigma_{z_j}^2$ = variance of $(z_j - z_{jc})$ distribution for N trajectories.

$\sigma_{u,j}^2, \sigma_{w,j}^2$ = variances of $p(u)$ and $p(w)$, respectively.

$\sigma_{u_j}^2$ = variance of u_j distribution for N trajectories.

$\sigma_{u_1}^2, \sigma_{u_2}^2$ = variance of velocity distribution for total observation time T_2 with resolution T_1 .

MONTE CARLO SIMULATION OF THE TURBULENT TRANSPORT OF AIRBORNE CONTAMINANTS

by

Clayton W. Watson and Sumner Barr

ABSTRACT

A generalized, three-dimensional Monte Carlo model and computer code (SPOCR) are described for simulating atmospheric transport and dispersal of small pollutant clouds. A cloud is represented by a large number of particles that we "track" by statistically sampling simulated wind and turbulence fields. These fields are based on generalized wind data for large-scale flow and turbulent energy spectra for the micro- and mesoscales. The large-scale field can be input from a climatological data base, or by means of real-time analyses, or from a separate, subjectively defined data base. We introduce the micro- and mesoscale wind fluctuations through a power spectral density, to include effects from a broad spectrum of turbulent-energy scales. The role of turbulence is simulated in both meander and dispersal. Complex flow fields and time-dependent diffusion rates are accounted for naturally, and shear effects are simulated automatically in the ensemble of particle trajectories. An important adjunct has been the development of computer-graphics displays. These include two- and three-dimensional (perspective) snapshots and color motion pictures of particle ensembles, plus running displays of differential and integral cloud characteristics. The model's versatility makes it a valuable atmospheric research tool that we can adapt easily into broader, multicomponent systems-analysis codes. Removal, transformation, dry or wet deposition, and resuspension of contaminant particles can be readily included.

1. INTRODUCTION

An important class of environmental analysis problems deals with the transport and dispersal of localized "puffs" of atmospheric pollutants, such as might result from some type of accidental release, or, of more direct interest to this study, the residual radioactive debris clouds from hypothesized military engagements in which nuclear weapons are used. More specifically, we are interested in modeling the space-time history of an initially small cloud of noxious atmospheric contaminants. We are particularly concerned with the first few hours after release, when the cloud is most concentrated and might affect local populations and before local atmospheric turbulence fields disperse it to an innocuous level.

The Navier-Stokes equations provide a formulation of the general atmospheric diffusion problem. In the general case, however, local wind fields have substantial space and time gradients that make the problem multidimensional and nonstationary. The

numerical ~~integrations~~ required to obtain solutions for other than highly restricted and idealized cases are beyond the capabilities of the most powerful computers. For early transport times (from a few minutes to a few tens of hours) and for small clouds (up to a few tens of kilometers in overall dimension), these difficulties are further aggravated by a need for high time resolution over a range of several orders of magnitude. Statistical fluctuations in the driving turbulence fields are also typically of the same scale as the phase-space dimensions of the cloud and this implies that the problem should be cast in probabilistic terms.

Monte Carlo statistical simulation techniques^{1,2} have been used extensively in the radiation transport field to deal with analogous multidimensional numerical difficulties.³ The Monte Carlo approach is also innately probabilistic and should thus be uniquely appropriate for this class of atmospheric-transport simulation. The remainder of the report discusses a random-walk Monte Carlo model we developed for this purpose.

II. FORMULATION OF THE BASIC DIFFUSION MODEL

A. Problem Definition

To outline the basic concept, we must first define the problem more explicitly. Consider an initial cloud of airborne particles beginning at some specified time t_0 with a known spatial distribution of particles at t_0 ; that is, we have an initial-value problem with initial conditions given in terms of the cloud configuration at time t_0 . Let this initial configuration be $f(\vec{r}_0)$, where

$\vec{r}_0 = (x_0 - x_{oc}, y_0 - y_{oc}, z_0 - z_{oc})$ = radial vector at time t_0 as measured from the point $\vec{r}_{oc}$,

$\vec{r}_{oc} = (x_{oc}, y_{oc}, z_{oc})$ = position of the cloud centroid at time t_0 .

We make two basic assumptions.

- Particle-particle interactions within the cloud are infrequent and can be ignored.

- Particle volumes are small compared with the volume of interstitial air and can be neglected.

These assumptions hold to a high degree of accuracy for the relatively diffuse pollutant clouds of practical interest. They also give necessary and sufficient conditions to ensure that the trajectory of each particle in the cloud can be considered independently from the other particles.

B. Simulating Cloud Diffusion with Random-Walk Particle Trajectories

We represent the initial cloud by a large number of individual particles with starting positions selected from the initial density function $f(\vec{r}_0)$. We then assume the time axis to be divided into small increments Δt and we "track" each particle by generating, in three-dimensional space and time, successive spatial displacements during these Δt 's. The overall cloud is described at any point in time in terms of the ensemble properties of these particle trajectories.

We therefore proceed to consider a single particle's trajectory and begin by making two general points. First, an airborne particle is transported by local wind fields that vary stochastically with time, and the characteristic frequencies of these variations span many orders of magnitude. Thus, the entire transport process is innately probabilistic in nature. A particle trajectory can be viewed as a random variable governed by an unknown, multidimen-

sional probability density function (PDF), and each simulated trajectory constitutes an independent random sample from this PDF. We wish to generate enough of these samples to make statistically significant estimates of certain properties of the PDF, such as the expected-value path of the cloud centroid and the time-space trace of the particles' distribution about this centroid.

The second point is that we can model a wind-driven trajectory in general terms. In fact, we can model specific problems to almost any degree of detail we want in terms of random-walk time-series processes of the sort outlined in Sec. II-B,⁴ provided Δt is chosen small enough. Naturally, no such model offers a panacea for atmospheric transport problems, and the resulting formulation will necessarily have parameters that must be fixed by fundamental meteorological data if quantitative results are to be realistic. Indeed, the burden of physical accuracy is intentionally shifted by this approach to the adequacy of the input data upon which it is based. Specifics of the final model will be determined by what types of atmospheric data we choose for these inputs. We will later illustrate this more explicitly.

C. Modeling the Atmospheric Turbulence Field for a Single Trajectory

We turn to the detailed simulation of a single particle trajectory. The problem becomes that of sequentially specifying a local displacement vector for each small time step along the particle's path. We generate this series of small displacements by applying local wind velocity vectors obtained by statistically sampling the governing time- and space-dependent PDFs as determined by the local wind fields at each step.

It will be instructive at this point to anticipate later discussions and consider the structure of the continuum of time scales of action (or frequencies) implicit in atmospheric turbulence fields. We can view the frequency spectrum as being made up of the following three distinctive regimes. (1) A small-scale regime in which turbulent wind fluctuations occur with characteristic periods smaller than the inherent time-resolution limit Δt of the model, (2) an intermediate-scale regime with wind variations on time scales comparable to the cloud transport times of interest (between Δt and a few tens of

hours), and (3) a large-scale regime with wind periods that are large (days to years) compared with the maximum transport times of interest. We delineate these three regimes because it will be convenient (and advantageous from the standpoint of computing time) to model the different regimes in different ways.

In the small-scale regime, the time- Δt size Δt establishes the lower limit of resolution available in the simulation.* Detailed particle trajectories on time scales smaller than Δt are presumably of no interest; otherwise, a smaller Δt should have been chosen. It is therefore sufficient to know only the relatively small expected net particle displacement during Δt . We can describe this displacement in terms of a PDF for the one-step displacement vectors, or, what is equivalent, a PDF giving the one-step distribution of net resultant wind vectors, as determined by the small-scale wind field, averaged over a travel time Δt .**

The large-scale winds determine bulk, or coherent, flow of the particle ensemble as measured, for example, by the path of the cloud centroid. Intermediate- and small-scale winds, on the other hand, determine dispersal, or incoherent particle flow, as measured, for example, by the particle distribution about the centroid. We can take advantage of the fact that we are interested primarily in simulating cloud dispersal characteristics for specific, representative, large-scale wind fields, and only secondarily in estimating the expected mean path of the centroid (over weeks or years) or in the corresponding dispersion of such cloud paths about their mean. It will therefore be sufficient and possibly more instructive to introduce the large-scale winds into the calculation deterministically from a previously prepared input data base. Considerable computer time will be saved by eliminating the statistical-

sampling requirement for these large-scale fields. Variations and sensitivities in the cloud transport as a function of changes in the large-scale winds can still be studied by simply running different simulations with different large-scale wind fields.

The time- and space-dependent cloud properties of principal interest (dispersal) will be determined predominantly by the intermediate continuum of turbulent wind fluctuations. The intermediate regime also constitutes a transition region between the small and the large scales of motion, and any detailed transport model must include the correct mix of influences from these two regions as modified by the superimposed intermediate field at every point in the cloud's history. A key variable is the travel time τ (time from t_0). Both the cumulative fraction of the intermediate spectrum that affects the particle's trajectory and the relative mix of influences from the two extreme regimes are functions of τ . If $(\tau - t_0)$ is small, particle trajectories will be determined mainly by the small-scale step-to-step velocity fluctuations, and a pronounced random character will be evident. As τ increases, the effect of these small-scale fluctuations will decrease, the cloud transport will become increasingly dominated by intermediate-scale winds, and the ensemble properties will be increasingly affected by gradients in the large-scale field ("shear" effects).

These discussions identify some key characteristics of the random-walk particle-trajectory model we describe later. Specifically, small-scale wind variations will be modeled by an explicit PDF, to be determined by input data, giving the step-to-step stochastic components $\Delta \vec{p}$ for the trajectory wind vectors. A deterministic large-scale wind field also will be imposed, and intermediate-scale wind contributions will be inferred from an input turbulent-energy field having a continuous frequency spectrum. The overall model will include these components in proportions to be determined, as a function of travel time, by the input turbulence spectrum.

We emphasize that, although delineation of separate turbulence regimes is useful, the model still considers bulk transport and dispersal simultaneously as different manifestations of the same

* We typically have used a Δt of 0.1 h in our calculations.

** We can imagine, for example, a real, microscopic, particle trajectory starting at any time t with velocity $\vec{p}$. At time $t + \Delta t$, the particle will have a velocity $\vec{p} + \Delta \vec{p}$, where $\Delta \vec{p}$ is a stochastic net change in the particle's velocity during Δt . The one-step wind-vector distributions are most conveniently given in terms of a PDF for the distribution of $\Delta \vec{p}$ values about the mean. For relatively small values of Δt , these PDFs have means of approximately zero to a good approximation.

basic atmospheric mass- and energy-transfer processes. Even though we treat part of the spectrum deterministically, thereby reducing complexity and computing costs at the expense of certain types of information of secondary interest, the role of turbulence will still be modeled (in both meander and dispersal of the cloud, for example) over the complete spectrum. Complex, large-scale, flow fields and time-dependent diffusion rates will be accounted for naturally, and shear effects are included implicitly and automatically in the ensemble of particle trajectories.

D. A Specific Random-Walk Model

To formulate the specific model we refer to the table of nomenclature* and note that

$$\begin{aligned}\vec{\Delta R}_j &= (\Delta x_j, \Delta y_j, \Delta z_j) = (v_j \Delta t, u_j \Delta t, w_j \Delta t) \\ &= \text{particle displacement during step } j,\end{aligned}$$

and

$$\Delta \omega_j = (\Delta x_j, \Delta y_j, \Delta z_j, \Delta t) = (v_j \Delta t, u_j \Delta t, w_j \Delta t, \Delta t).$$

Implicit in the idea of a deterministic large-scale wind field is the idea of a mean wind field to which the simulation must adhere, in the sense of an expected value. If our simulation is to be inherently realistic and internally consistent, each trajectory must conform (in the statistical limit as the number of trajectories goes to infinity) to the deterministically imposed large-scale wind field. This requirement gives us a condition on the PDFs from which the local wind vectors are sampled.** The expected value of $\vec{\rho}_j$ (at any ω_j) must equal the input large-scale (mean) wind vector at ω_j . If we adopt the convention that the input mean wind data will be denoted by overbars and the expected values of trajectory random variables by brackets $\langle \rangle$, the

formal condition is

$$\langle \vec{\rho}_j \rangle = \vec{\rho}_j, \quad (1)$$

that is, for every ω_j ,

$$\langle (u_j, v_j, w_j) \rangle = (\bar{u}_j, \bar{v}_j, \bar{w}_j),$$

where $(\bar{u}_j, \bar{v}_j, \bar{w}_j)$ is the input large-scale mean wind vector at ω_j .

We can simplify the model and the subsequent statistical analyses with a third assumption: that statistical fluctuations in the wind components u_j , v_j , and w_j about their respective means $\bar{u}_j$, $\bar{v}_j$, and $\bar{w}_j$ are mutually independent. Experimental evidence seems to justify this assumption for the middle troposphere, at the scales where our principal interests lie. We would also expect the net cloud-ensemble properties to be relatively insensitive to existing correlations in this regime. (Discussed in Sec. III.) The available meteorological data in this regime are probably inadequate to support the inclusion of such correlations in our model anyway, although this could be done in a straightforward manner.

This assumption allows us to consider each of the three wind components independently. Therefore, for the remainder of the discussion, we can limit our attention to, say, the y-component, v , and note that the other two components are to be treated analogously. The implication of this assumption is that, at every ω_j , the overall PDF for $\vec{\rho}_j$ is the product of three independent, one-dimensional, conditional PDFs* (for the three components). The condition in Eq. (1) suggests that it will be convenient to consider these PDFs as functions of the random variables $(u_j - \bar{u}_j)$, $(v_j - \bar{v}_j)$, and $(w_j - \bar{w}_j)$; that is, if

$$f_{\rho}(\vec{\rho}_j) = \text{PDF for } \vec{\rho}_j,$$

then

$$f_{\rho}(\vec{\rho}_j)$$

$$= f_{u-\bar{u}}(u_j - \bar{u}_j) f_{v-\bar{v}}(v_j - \bar{v}_j) f_{w-\bar{w}}(w_j - \bar{w}_j), \quad (2)$$

*An analogous statement also holds for the one-step PDF for the small-scale fluctuations $\Delta \vec{\rho}_j$ at ω_j .

* Also see Appendix A for relationships between the (x,y) and (I,J) coordinate systems.

** We are not referring here to the PDF giving small-scale wind fluctuations $\Delta \vec{\rho}$, but to the overall PDFs from which the $\vec{\rho}_j$ values are sampled. The former is a simple, invariant PDF to be given by basic input data, whereas the latter is an unknown, multidimensional PDF that varies with all the phase-space dimensions along a trajectory, including travel time.

where $f_{u-\bar{u}}$, $f_{v-\bar{v}}$, and $f_{w-\bar{w}}$ are one-dimensional PDFs for $(u_j - \bar{u}_j)$, $(v_j - \bar{v}_j)$, and $(w_j - \bar{w}_j)$, respectively.

These PDFs need not be specified explicitly since we need at each w_j only appropriate, unbiased, random samples. Based on insight into the physics of the problem, one can often construct recursion relationships for random-walk time-series simulations that provide the required sequences of stochastic samples without complete knowledge of the PDF, given only the initial conditions and sufficient data to determine the problem.*

For the trajectories outlined so far, we could devise several different types of recursion relationships; the exact form of each would depend on what type of additional meteorological inputs we chose to use. Generally, these inputs would have an integral, or time-averaged character; and the recursion relationships would contain key parameters to be fixed by requiring that the appropriate expected-value characteristics of the random walks match these integral data. (The larger the number of significant parameters and, hence, the body of basic data to which the model is normalized, the broader the inherent capability of the model.)

As discussed earlier, a principal goal of this effort is to model properly the dispersal of an airborne contaminant cloud as it is acted upon by realistic turbulence fields with a continuum of frequencies spanning many orders of magnitude. If the model is to have breadth of applicability commensurate with this capability, it should also be able to respond properly to different atmospheric turbulence structures. It therefore seems appropriate that the turbulence power spectrum should be an input for a given cloud simulation and that this input should constitute a basic class of data to which the model is normalized. This choice gives us the additional insight required to construct wind-velocity recursion relationships.

Later discussions identify the velocity autocovariance function $R_i(n)$ as a convenient means

for incorporating the atmospheric turbulence spectrum into our model, where

$$R_i(n) = \langle (u_i - \bar{u}_i) (u_{i+n} - \bar{u}_{i+n}) \rangle. \quad (3)$$

These functions will be obtained in a straightforward manner by a weighted Fourier transform of the input turbulence power spectrum. They measure correlations between velocity fluctuations (relative to the mean) at any step i and fluctuations at any other step $i + n$ in the trajectory. These functions allow us to relate the velocity at j to the velocity at preceding steps, which gives us a basis for determining the recursion relationships.

We can now write a velocity recursion relationship for u_j that has the properties outlined so far. It merely states that the deviation from the mean field of a velocity component at w_j consists of a weighted sum of the preceding deviations in the trajectory plus a current, random, small-scale contribution selected from the one-step PDF; that is,

$$(u_j - \bar{u}_j) = \sum_{i=1}^{j-1} \hat{e}_{j,i} (u_i - \bar{u}_i) + \Delta u_j. \quad (4)$$

This recursion relationship, in conjunction with an initial condition, gives u_j at w_j in terms of the mean wind field, the previous u 's in the trajectory, and the randomly selected elements Δu_j . It gives us a random independent sample, at w_j , from $f_{u-\bar{u}}(u_j - \bar{u}_j)$. As expected, it contains a set of parameters $\hat{e}_{j,i}$, plus the PDF for Δu_j , that must be fixed by input data.

An initial position w_0 is obtained from the starting cloud description and an initial velocity condition is implicit in the definition of the small-scale PDF; that is, for the first step in the random walk,

$$u_1 = \bar{u}_0 + \Delta u_1, \quad (5)$$

where Δu_1 is a sample from the small-scale PDF. If we assume*

* Recall that the cloud-simulation approach we are describing is an example of this technique. Each simulated trajectory is a sample from an unknown PDF.

*See footnote ** on p. 3.

$$\langle \Delta u_j \rangle = 0, \quad (6)$$

then, from Eqs. (4), (5), and (6), we have

$$\bar{u}_1 \equiv \langle u_1 \rangle = \langle \bar{u}_0 \rangle + \langle \Delta u_1 \rangle = \bar{u}_0,$$

$$\langle (u_2 - \bar{u}_2) \rangle = \langle u_2 \rangle - \bar{u}_2 = \beta_{2,1} [\langle u_1 \rangle - \bar{u}_1]$$

$$+ \langle \Delta u_2 \rangle = 0;$$

so that

$$\langle u_1 \rangle = \bar{u}_1,$$

$$\langle u_2 \rangle = \bar{u}_2,$$

$$\langle u_j \rangle = \bar{u}_j,$$

and Eq. (4) satisfies the condition in Eq. (1).

To complete the formal model, we need an explicit form for the small-scale PDF. A normal distribution appears adequate for this purpose. (Also see Sec. III-C.

$$p(\Delta u) = \frac{1}{\sigma_{\Delta u} \sqrt{2\pi}} \exp \left(-\frac{\Delta u^2}{2\sigma_{\Delta u}^2} \right) \equiv N(0, \sigma_{\Delta u}^2). * \quad (7)$$

Random samples are easily obtained from this distribution,⁵ so it is convenient for our purposes.

*Note that $\langle \Delta u \rangle = 0$ as assumed in Eq. (6).

The problem is now determined, since the $\beta_{j,i}$ can be obtained directly from the definition in Eq. (3). The recursion relationship gives $(u_j - \bar{u}_j)$ in terms of the preceding $(u_i - \bar{u}_i)$ in the trajectory through the correlation parameters $\beta_{j,i}$; and these, in turn, are fixed by the upstream autocovariance functions as follows. Multiplying Eq. (4) by $u_k - \bar{u}_k$, where $k < j$, and then taking the expected value of both sides, we get

$$\begin{aligned} & \langle (u_j - \bar{u}_j) (u_k - \bar{u}_k) \rangle \\ &= \sum_{i=1}^{j-1} \beta_{j,i} \langle (u_i - \bar{u}_i) (u_k - \bar{u}_k) \rangle \\ &+ \langle \Delta u_j (u_k - \bar{u}_k) \rangle; \end{aligned}$$

or, since

$$\langle \Delta u_j (u_k - \bar{u}_k) \rangle = \langle \Delta u_j \rangle \langle u_k - \bar{u}_k \rangle = 0, \text{ for } k < j,$$

we get

$$R_j(k-j) = \sum_{i=1}^{j-1} \beta_{j,i} R_i(k-i),$$

$$k = 1, 2, 3, \dots, j-1. \quad (8)$$

For a given j , there are $j-1$ of these linear equations in the $j-1$ unknowns $\beta_{j,i}$. These can be solved directly for the β s.

To illustrate, we use

$$R_j(-n) = \langle (u_j - \bar{u}_j) (u_{j-n} - \bar{u}_{j-n}) \rangle = R_{j-n}(n)^* \quad (9)$$

and consider the first four steps.

$$j=1$$

$$u_1 = \bar{u}_0 + \Delta u_1.$$

* Note, however, that the formulation used to derive $R_j(n)$ from the turbulence spectrum must also have this property; otherwise, an analogous property appropriate to the formulation used must be substituted for Eq. (9). An example of this is discussed later.

j = 2

$$u_2 = \beta_{2,1} (u_1 - \bar{u}_1) + \Delta u_2 + \bar{u}_2,$$

where $\beta_{2,1}$ is obtained from

$$a_1(1) = \beta_{2,1} a_1(0), \quad (k = 1).$$

j = 3

$$u_3 = \beta_{3,1} (u_1 - \bar{u}_1) + \beta_{3,2} (u_2 - \bar{u}_2) + \Delta u_3 + \bar{u}_3,$$

where $\beta_{3,1}$ and $\beta_{3,2}$ are obtained from

$$a_1(2) = \beta_{3,1} a_1(0) + \beta_{3,2} a_1(1), \quad (k = 1)$$

$$a_2(1) = \beta_{3,1} a_1(1) + \beta_{3,2} a_2(0), \quad (k = 2)$$

j = 4

$$u_4 = \beta_{4,1} (u_1 - \bar{u}_1) + \beta_{4,2} (u_2 - \bar{u}_2) + \beta_{4,3} (u_3 - \bar{u}_3) + \Delta u_4 + \bar{u}_4,$$

where the β s are obtained from

$$a_1(3) = \beta_{4,1} a_1(0) + \beta_{4,2} a_1(1) + \beta_{4,3} a_1(2) \quad (k = 1);$$

$$a_2(2) = \beta_{4,1} a_1(1) + \beta_{4,2} a_2(0) + \beta_{4,3} a_2(1), \quad (k = 2);$$

$$a_3(1) = \beta_{4,1} a_1(2) + \beta_{4,2} a_2(1) + \beta_{4,3} a_3(0), \quad (k = 3),$$

etc.

III. METEOROLOGICAL BASES FOR SPECIFICATION OF INPUT DATA

A. Background

Two things are required of a turbulent-diffusion

model. It must be sensitive to the primary forcing mechanism (fluid turbulence) and it must provide the mathematical vehicle for translating the inputs of source configuration and turbulence into air concentrations. A separate but related concept deals with the quality of the input data. These data may include time and space variations in the mean transport flow and turbulence, and details on the structure of turbulence, such as the probability density function of velocity fluctuations, anisotropy, and the spectral distribution of turbulence kinetic energy. These details represent a demanding set of observations for practical diffusion codes, but a goal for the diffusion model should be to see that the mathematical vehicle does not limit the specification of inputs. The model should be able to accept and use as much detail as the user can provide, whether from direct measurement, physical hypothesis, or climatology. Reducing the detail in the input variables is a simple logistical matter.

As presently formulated, our model requires probability density functions for the small-scale fluctuations of orthogonal velocity components. Also, the Lagrangian spectrum of turbulence kinetic energy provides a basic input from which the non-stationary (scale-dependent) diffusion inputs are derived. The need for artificially separating a long-range transport-diffusion problem into several separate time regimes is eliminated by providing a broad-enough energy spectrum at the outset. Contaminant travel time then becomes one of the fundamental time scales of the problem.

In the following sections, we describe techniques for deriving and estimating inputs for the large-scale mean transport winds, the small-scale PDF's of velocity fluctuations, and the scale-dependent diffusion parameters.

B. Mean Wind Fields

In broad terms the net transport of pollutant is ascribed to that part of the flow that can be specified deterministically, whereas the diffusion represents a stochastic spreading of material about the centroid. If the travel time is large, those scales of motion that are clearly transport components in early travel may become part of the stochastic field, but this situation should generally present no serious problem. The deterministic part

of the wind field may be derived on large scales from synoptic analyses and on local scales from local tower wind measurements. An important intermediate class of problem, particularly in regions of significant topographic variation, is mesoscale transport flow, which has recently gained attention because of many practical applications for plant siting and safety analysis. Efforts to determine the wind field for specific regions have centered on techniques for interpolating within networks of observing sites⁶⁻⁸ and on dynamic estimates of flows around terrain obstacles or thermally disturbed areas.⁹⁻¹¹

An important feature of the current model is that gradients in the mean wind field do not limit the model, a valuable property in the boundary layer where vertical gradients of the horizontal flow are a vital part of the flow structure. In applications to date, the transport flow has been derived by interpolation from an upper-level synoptic-scale data base. The data base and interpolation scheme are described in Appendix A.

C. Small-Scale Probability Density Functions

A fundamental input requirement of the present model is the probability density function for each component of the turbulence fluctuations. Pasquill¹² offers empirical evidence that a Gaussian distribution of eddy velocities in the atmospheric boundary layer provides an adequate working basis for most practical problems. Dutton and Deaven¹³ and Frenkiel and Klebanoff¹⁴ have tested the validity of the Gaussian distribution and have suggested that small departures imply important interpretations of turbulence dynamics. For example, the intermittency of small-scale clear-air turbulence gives rise to extended periods of relatively calm air and a few sudden accelerations. This tends to sharpen the peak of the distribution function slightly.

The present application doesn't call for new insights into the dynamics but does require a reasonable approximation to the distribution for kinetic purposes. That is, we are sampling for fluctuations about a mean trajectory primarily to estimate the dispersion of trajectories. We are less interested in isolated bursts of intense small-scale turbulence than in more continuous meandering of the wind vector due to low-intensity

variations over a wide range of scales in the free atmosphere and in the boundary layer. Data on these variations are somewhat scarce, but three sets of records have been analyzed. Trajectories of constant-density balloons at about 10-km altitude were analyzed by Mantis,¹⁵ and a series of trajectories at about 1-km altitude was run by the Air Resources Laboratory, NOAA.¹⁶ Kao and Woods¹⁷ present aircraft data in the vicinity of the jet stream that are adequate to estimate the distribution of longitudinal and lateral mesoscale velocity fluctuations. Figure 1 is a plot of the probability density functions derived from the above three sources. All three satisfy the Gaussian relation between the 95 to 98% tails. From these results, it is reasonable to select a Gaussian function for the distribution of velocity fluctuations in components parallel and transverse to the mean flow.

An important complication develops in regions of strong velocity gradients, such as the lower boundary layer, namely, the existence of joint PDFs between components, or Reynolds stresses. These correlations between orthogonal velocity fluctuations account for momentum transfer and will also produce distortions in an expanding cloud of contaminant. Well away from a bounding surface, however, the Reynolds stresses are expected to be very small. Also, the existence of correlated components does not necessarily introduce serious problems in a diffusion estimation scheme. It is necessary to study the relative scales of motions contributing to the momentum flux and to the dispersion. Close to the ground in neutral or stable

Fig. 1. Composite cumulative frequency distribution for mesoscale, free-atmosphere, turbulent velocity fluctuations.

thermal stratification, small-scale motions dominate the Reynolds stresses. If the dispersing cloud is large compared with this scale, these eddies will be ineffective in the diffusion process. Therefore, the distortions they produce will be insignificant. However, if the cloud dimension and the correlated eddies are of similar scale, any dispersion formulation that neglects the correlation will be in error. The extent of this error must be determined by explicit sensitivity analyses.

D. Scale-Dependent Inputs in the Intermediate Regime

One very important aspect of atmospheric turbulent diffusion is the broad range of eddy sizes present to work on the diffusing cloud of tracer material. The kinetic energy of the wind is distributed over all scales from global to microscale, though not uniformly, nor is it equipartitioned among the directional components. Specifying the amount of turbulent energy in various eddy-size ranges and among the components, as functions of location and time, constitutes a major part of the problem of estimating turbulent diffusion. The other main aspect of the problem is to determine how the specified turbulence field acts on a cluster of tracer particles.

First, we'll discuss the structure of atmospheric turbulence in very general terms. The atmosphere is bounded laterally by the circumference of the earth, but its vertical dimension is only

a few tens of kilometers. A motion system will thus become predominantly horizontal in structure as its size exceeds this vertical dimension. The directional components of velocity are not actually independent, so the restrictions imposed on the vertical scales are reflected to some extent in the horizontal components.

One very useful way to present and interpret data on atmospheric turbulence structure is with the power spectrum, which is essentially a Fourier-transformed statistical wind field describing kinetic energy as a function of frequency or wave number. Figure 2 shows a typical spectrum, after Panofsky.¹⁸ The dynamics of global circulation determine significant wind variations on the so-called synoptic scale of several days. Another significant input to kinetic-energy variations occurs at periods of several minutes because of shear-induced (mechanical) and thermally generated convective turbulence. There has been considerable speculation about the relative minimum in energy for periods between several minutes and a few hours. For many applications, the assumption of a "meso-scale gap" is a useful and important concept. In estimating transport, however, weak eddies or those with a low probability of occurrence can introduce significant errors if not taken into account. Figure 2 shows us that we must consider eddies of all scales in problems involving several hours of transport in the free atmosphere.

It will be useful here to discuss the effects of various averaging procedures as spectral filters in wave-number space. (We often find that mathematical procedures are similar for different manifestations of spectral influence, but interpretations may be very different.) The relevant problems here are (1) averaging of directly observed wind velocity fluctuations, (2) diffusion of an infinitely long sequence of particles released from a point, and (3) diffusion of a finite cluster of tracer particles.

Pasquill¹² discusses the effects on velocity variance of total observation time T_2 and resolution time T_1 = the time over which individual observations are averaged. He presents the expression

Fig. 2. Turbulent-energy spectrum over a wide range of frequencies (after Panofsky,¹⁸ 1969).

$$\sigma_{T_1, T_2}^2 =$$

$$\sigma_{0, \infty}^2 \int_0^\infty F(v) \left[1 - \left(\frac{\sin \pi v T_1}{\pi v T_1} \right)^2 \right] \left(\frac{\sin \pi v T_2}{\pi v T_2} \right)^2 dv, \quad (10)$$

where σ_{T_1, T_2}^2 is the velocity variance, $F(v)$ is the power spectral density at frequency v , and v is in cycles per second. A similar effect on the autocovariance function, due to a sampling time T_2 , is expressed by

$$R_{T_2}(\tau) = \frac{2}{\pi} \int_0^\infty F(v) \left[\frac{\sin \pi v T_2}{\pi v T_2} \right]^2 \cos 2\pi v \tau dv, \quad (11)$$

where τ is lag time.

Equation (10) suggests that, as the total observation time increases, the observed variance will increase. This relation is logical, since a longer observation time allows us to observe the inputs of larger and larger eddies. Similarly, as the basic resolution time T_1 gets large, we reject eddies with periods smaller than T_1 , so the measured variance decreases.

A classical analysis¹⁹ applied to an ensemble of particle displacements x gives insight into the role of turbulence structure on the second moment of the particle distribution. The results, elegantly extended by Kempe de Fariet,²⁰ give the spectral dependence of the second moment in one-dimensional, homogeneous turbulence.

$$\langle x^2 \rangle = u^2 T_2^2 \int_0^\infty F_L(v) \left[\frac{\sin \pi v T_2}{\pi v T_2} \right]^2 dv, \quad (12)$$

where u is velocity and the subscript L refers to the Lagrangian measurement frame. The second term in the integrand is a filter on the spectrum in the same sense as the last term in Eq. (10). For small T_2 (time from release), all scales of motion contribute to the growth of $\langle x^2 \rangle$; but, as T_2 grows, larger and larger eddies dominate the process. An important difference between Eqs. (10) and (12) is that the formulation leading to Eq. (12) is based on following tracer particles through a flow and therefore is a Lagrangian measurement, whereas Eq. (10) represents an Eulerian measurement. Pasquill¹² suggested a simple scale transformation between the Eulerian and Lagrangian

spectra that would yield the second moment in terms of the Eulerian measurements.

$$\langle x^2 \rangle = u^2 T_2^2 \int_0^\infty F_E(v) \left[\frac{\sin \frac{\pi v T_2}{\beta}}{\frac{\pi v T_2}{\beta}} \right]^2 dv, \quad (13)$$

where β is now the ratio of Lagrangian to Eulerian time scales of turbulence.

A cluster of particles released into the turbulence field described by Fig. 2 will not utilize all scales of motion at all times for its growth. Rather, the cloud behaves as a filter on the spectrum, using only certain scales for its dispersive growth. Large eddies (compared with the particle separation distance) tend to transport particles coherently rather than dispersing them. Small eddies produce small-scale motions that cancel one another, leading to no net dispersion. Therefore, only turbulent motions on the scale of the separation distance of the particles will serve to increase the relative separation. As the cluster grows, however, it will "see" larger scales of motion, and its growth will be time dependent. Figure 3, adapted from Corrsin,²¹ demonstrates schematically the filtering effect as a cluster of tracer particles expands in a turbulent field. Corrsin introduced the concept of dispersion efficiency to account for the fact that large eddies cotransport the cluster. Hence, the efficiency rises sharply in the range of the cluster size (Fig. 3). In the portion of the spectrum of interest to us, however, the energy decreases in going from large to small scales. The net spectral contribution is a product of the energy and efficiency and is expected to peak at about the cluster dimension.

The quantitative expression of Fig. 3 is difficult because the relative diffusion process is basically nonstationary. For guidance in the specification of functional forms for the efficiency we depend on Taylor's¹⁹ analysis of single-particle diffusion, which is a stationary process. Following a similar logic, Pasquill arrives at the expression

$$\langle x^2 \rangle = u^2 T_2^2 \int_0^\infty F_L(v) \left[1 - \left(\frac{\sin \pi v t}{\pi v t} \right)^2 \right] \left(\frac{\sin \pi v T_2}{\pi v T_2} \right)^2 dv, \quad (14)$$

Fig. 3. Schematic diagram showing spectral efficiency of cluster dispersal (after Corssin,²¹ 1963).

where t is a time-scale characteristic of source size, and T_2 is travel time.

The spectral filtering effect introduced by a finite but growing cloud, in a domain characterized by a fundamental resolution time T_1 , is reflected in the autocovariance function through

$$R_{T_1, T_2}(\tau) =$$

$$\frac{2}{\pi} \int_0^{\infty} F_L(v) \left[1 - \left(\frac{\sin \pi v T_1}{\pi v T_1} \right)^2 \right] \left(\frac{\sin \pi v T_2}{\pi v T_2} \right)^2 \cos 2\pi v T dv, \quad (15)$$

where T_2 is the travel time. Equation (15) can be interpreted as the autocovariance function generated by a particle trajectory with a resolution T_1 and travel time T_2 . Equation (15) provides the basic inputs required to generate a trajectory from the Eq. (4) recursion relationships, where we note that the parameters in Eq. (15) are identified in terms of the random walk parameters as follows.

T_1 = time resolution of the model = Δt .

T_2 = travel time = t_j .

τ = lag time = $n\Delta t$.

$$R_{T_1, T_2}^{(T)} = R_{\Delta t, t_j}(n\Delta t) \approx R_j(n).$$

In closing this discussion, we should note a subtle but important characteristic of Eq. (15);

namely, that it does not have the commutative property of Eq. (9). This is a direct result of the fact that Eq. (15) is not exact. Although our diffusion model gives a detailed description of the non-stationary diffusion process, Eq. (15) is derived on the basis of quasi-stationary meteorological data and has the stationary property

$$R_j(-n) = R_j(n). \quad (16)$$

Equation (16) must therefore be substituted for Eq. (9) if Eq. (15) is used to evaluate the $\beta_{j,i}$ for Eq. (4). Otherwise, an inconsistency between Eqs. (8) and (15) is introduced that can lead to singularities in the β s, and the trajectories can "blow up."

IV. MODEL IMPLEMENTATION

A. Model Summary

For reference purposes, it will be useful to summarize the overall approach.

Fundamental assumptions:

- Particle-particle interactions can be ignored.
- Particle volumes can be ignored.

Other assumptions:

- Statistical fluctuations of the wind components about their respective means are mutually independent.
- PDFs for the small-scale fluctuations (on the time scale of Δt) are normal, with mean zero.

Inputs:

1. Large-scale wind field giving $\bar{u}(\omega)$, $\bar{v}(\omega)$, and $\bar{w}(\omega)$ for all $\omega_j = (x_j, y_j, z_j, t_j)$.
2. Turbulence power spectrum $F(v)$, spanning the frequency range of interest.*
3. $\sigma_{\Delta u}^2$, $\sigma_{\Delta v}^2$, $\sigma_{\Delta z}^2$ **
4. t_0 = starting time, $\bar{r}_{oc}$ = location of cloud at t_0 .
5. $f(\bar{r}_0)$ = initial cloud (source) configuration.
6. M = number of trajectories to be calculated.
7. N = number of steps in each trajectory.

*Typically, we have used $v = 40 \text{ h}^{-1}$ to 0.02 h^{-1} for our problems.

**Alternatively, these could be calculated from the input power spectrum. We have generally preferred to estimate these parameters independently.

Trajectory simulation:

1. Calculate the required β_k values for Eq. (8) from Eq. (15).
2. Solve Eq. (8) for the required $\beta_{j,1}$.
3. Get (x_0, y_0, z_0) by random sampling from $f(\vec{r}_0)$.
4. Get $\bar{u}_0 = \bar{u}(\omega_0)$, $\bar{v}_0 = \bar{v}(\omega_0)$, $\bar{w}_0 = \bar{w}(\omega_0)$ from the input data base.
5. Pick random samples $\Delta u_1, \Delta v_1, \Delta w_1$ from $N(0, \sigma_{\Delta u}^2)$, $N(0, \sigma_{\Delta v}^2)$, $N(0, \sigma_{\Delta w}^2)$, respectively.
6. $u_1 = \bar{u}_0 + \Delta u_1$
 $v_1 = \bar{v}_0 + \Delta v_1$
 $w_1 = \bar{w}_0 + \Delta w_1$
7. Get $\omega_1 = (x_1, y_1, z_1, t_1)$, where*
 $x_1 = x_0 + \Delta x_1 = x_0 + v_1 \Delta t$
 $y_1 = y_0 + \Delta y_1 = y_0 + u_1 \Delta t$
 $z_1 = z_0 + \Delta z_1 = z_0 + w_1 \Delta t$
 $t_1 = t_0 + \Delta t$

Iteration ($n - 1$ times) of the following then produces a series of steps in the ω -space; that is, a random-walk trajectory.

8. Get $\bar{u}_{j+1} = \bar{u}(\omega_{j+1})$, $\bar{v}_{j+1} = \bar{v}(\omega_{j+1})$, $\bar{w}_{j+1} = \bar{w}(\omega_{j+1})$ from the data base.

Note: $(\bar{u}, \bar{v}, \bar{w})$ for preceding steps are, of course, still available.

9. Pick $\Delta u_{j+1}, \Delta v_{j+1}, \Delta w_{j+1}$ from $N(0, \sigma_{\Delta u}^2)$, $N(0, \sigma_{\Delta v}^2)$, $N(0, \sigma_{\Delta w}^2)$.

10. Calculate $u_{j+1}, v_{j+1}, w_{j+1}$ from the Eq. (4) recursion relationships.

11. Get ω_{j+1} by advancing the trajectory by*

$$\begin{aligned} x_{j+1} &= x_j + v_{j+1} \Delta t, \\ y_{j+1} &= y_j + u_{j+1} \Delta t, \\ z_{j+1} &= z_j + w_{j+1} \Delta t, \\ t_{j+1} &= t_j + \Delta t. \end{aligned}$$

12. Repeat steps 8 through 11 ($n - 1$ times for the complete trajectory).

To review, we input an atmospheric turbulence energy spectrum, the one-step σ_{Δ} parameters, a

large-scale mean wind field, and the source conditions. The model then calculates appropriate covariance functions from the turbulence spectrum, solves for the step-by-step $\beta_{j,1}$, and then generates M random-walk particle trajectories by using the velocity recursion relationships and the large-scale wind-field data base.

B. Illustrative Ensemble-Property Estimators

A variety of statistical relationships are implicit in the model. For example,

$$\sigma_{u_j}^2 \equiv \langle (u_j - \bar{u}_j)^2 \rangle = \langle u_j^2 \rangle - \langle u_j \rangle^2 =$$

$$\sum_{i=1}^{j-1} \beta_{j,i} \langle (u_i - \bar{u}_i) (u_j - \bar{u}_j) \rangle + \langle \Delta u_j (u_j - \bar{u}_j) \rangle;$$

or,

$$\sigma_{u_j}^2 = \sum_{i=1}^{j-1} \beta_{j,i} R_i (j-i) + \sigma_{\Delta u_j}^2, \quad (17)$$

where we have used

$$\langle \Delta u_j (u_j - \bar{u}_j) \rangle = \langle \Delta u_j^2 \rangle = \sigma_{\Delta u_j}^2. \quad (18)$$

Cloud-ensemble properties are also directly available; for example,

$$\langle y_j \rangle = \langle y_0 + \Delta t \sum_{i=1}^j u_i \rangle = y_0 + \Delta t \sum_{i=1}^j \langle u_i \rangle,$$

or

$$\langle y_j \rangle = y_0 + \Delta t \sum_{i=1}^j \bar{u}_i = y_0 + \sum_{i=1}^j \Delta \bar{y}_i, \quad (19)$$

that is, the expected-value path of the cloud centroid is the mean path determined by the large-scale mean wind field.*

In general, the cloud-ensemble properties are too complex to be obtained by such simple procedures (otherwise, the random-walk simulation would not be necessary). Such properties are, however, implicit

*See the SPOOR footnote on p. 24.

*See last paragraph of Appendix A, however.

in the set of particle trajectories and are readily available through simple tallying techniques using the particle state variables generated in the calculation. For example, the variance $\sigma_{r_j}^2$ of the

particle distribution about the cloud centroid (at any step j) is a parameter of basic interest. Let

M = number of trajectories generated,

m = trajectory index = 1, 2, 3, ... M ,

(x_{jm}, y_{jm}, z_{jm}) = position of particle m at step j (time t_j).

The position of the cloud centroid at t_j is (x_{jc}, y_{jc}, z_{jc}) , where

$$x_{jc} = \frac{1}{M} \sum_{m=1}^M x_{jm}, \quad (20a)$$

$$y_{jc} = \frac{1}{M} \sum_{m=1}^M y_{jm}, \quad (20b)$$

$$z_{jc} = \frac{1}{M} \sum_{m=1}^M z_{jm}. \quad (20c)$$

The radial position of particle m from the centroid at t_j is

$$\vec{r}_{jm} = (x_{jm} - x_{jc}, y_{jm} - y_{jc}, z_{jm} - z_{jc}),$$

with magnitude

$$r_{jm} = [(x_{jm} - x_{jc})^2 + (y_{jm} - y_{jc})^2 + (z_{jm} - z_{jc})^2]^{1/2}. \quad (21)$$

The parameter $\sigma_{r_j}^2$ is then estimated by

$$\sigma_{r_j}^2 = \langle r_j^2 \rangle - \langle r_j \rangle^2 = \frac{1}{M} \sum_{m=1}^M r_{jm}^2 - \left(\frac{1}{M} \sum_{m=1}^M r_{jm} \right)^2, \quad (22)$$

where the sums are taken over all the particle trajectories in the calculation. Appendix B discusses another example.

C. The SPOOR Code

We have implemented this diffusion model in a FORTRAN IV CDC-7600 code system called SPOOR.* The code is based on modular programming concepts and emphasizes flexibility and versatility. For example, we can input mean wind-field data from a climatological data base or by means of real-time analyses, or from a separate, subjectively defined data base. The code will accept these data in either geographic (latitude-longitude) coordinates or in the National Meteorological Center's (I,J) coordinates.** This flexibility aids parameter and sensitivity studies; for example, the user can specify his own wind field or storm system for preselected portions of the position-time phase space.

The most important advantage of the code's modular structure is that we can easily change or replace the modules that make up the code. Upgrading is thus easily accomplished as we feed back (into the code) new data and insight gained into the physics of the simulation. This feature also makes extensions to different classes of transport problems or to other phase-space regimes much easier.

We have also developed a "chain" capability that allows us to increase the time step Δt systematically as a function of travel time throughout a simulation. The user can decrease the time resolution of the calculation as travel time increases, consistent with the decreasing resolution required as larger and larger scales of motion dominate the diffusion process. This flexibility can markedly reduce the number of time steps in a given calculation to effect large savings in computer costs for long transport times. The practical range of cloud travel times that can be simulated is extended correspondingly.

The present version of SPOOR assumes u and v velocity-component correlations between a given time step and the three preceding time steps [$i = j - 3, j - 2, j - 1$ in Eq.(4)]. This seems

* SPOOR is the work of R. Allenson, LASL; a detailed report is in preparation.

** Appendix A gives transformations between the (x,y) and the NMC (I,J) coordinate systems.

to be sufficient for the problems we have addressed so far* (Δt of 0.1 h, travel times of up to a few hours, middle troposphere) and is consistent with the correlations implicit in the turbulence data we have used. Longer travel times (or smaller Δt) would require more terms in Eq. (4). We can easily incorporate such extensions into SPOOR, and plan to do so. Computing times should be relatively insensitive to the number of terms included. We have not yet explored these topics in detail, however.

The present SPOOR also uses only one correlated term for the vertical velocity component w , that is,

$$(w_j - \bar{w}_j) = \beta_w (w_{j-1} - \bar{w}_{j-1}) + \Delta w_j, \quad (23)$$

where $\gamma_w = 1 - \beta_w$ is an input constant. This simplified treatment is a holdover from an earlier version of the code and is an indication of its evolving character. Equation (23) also illustrates a point about our overall modeling approach, an approach designed to allow continuing, orderly evolution of the physics embodied in the code. A key element in this evolution is reliance on user feedback based on the calculated results--feedback of improved understanding incorporated through simple, routine, code-module modifications. This approach places a premium on exhaustive verification of the overall code framework, and we have devoted much effort to such verification. For illustration, Appendix B gives an example of such a process, one that, in this instance, is possible only because of the simplified form of Eq. (23).

We have not yet used this code to explore vertical-transport phenomena to any substantial extent, although the mechanics of the system are all operational. So far, we have incorporated only one set of vertical boundary conditions: a simple specular reflection of w_j at $z = z_{\max}$ and at $z = z_{\min}$, where $z_{\max}$ and $z_{\min}$ are input numbers. Later we will show a sample calculation illustrating vertical transport and shear effects.

*An early version of SPOOR included correlations with only one immediately preceding time step. Cloud-ensemble properties were generally within a few tens of percent of those from the present code, and computer running times were essentially the same.

Two source geometries are now available in the SPOOR package: a point source and a cylindrical source (axis in the z -direction) with arbitrary radius, height, and vertical position in the atmosphere. The cylinder can have either a uniform or a Gaussian initial particle distribution in either the axial or radial direction (or both). Other source geometries and distributions can also be readily incorporated, of course.

The code uses slightly over 47 000 words of fast core storage and about 37 000 words of slow storage, the latter being primarily for the built-in mean-wind data base (Appendix A). These figures also include buffer blocks for accumulation and output of complete descriptions of all variables in all trajectories.

SPOOR output consists of a data tape containing state variables ($\vec{p}_j, \vec{x}_j, t_j$) for all time steps and all trajectories. We can also list intermediate data ($\vec{p}_j, \Delta \vec{p}_j, \Delta \vec{x}_j$) for each trajectory as the calculation proceeds. Modules to make this listing and to calculate and list the means and variances of the state-variable components are integral parts of the code. This second listing also gives input data and calculated β s automatically.

An important adjunct to the development of SPOOR has been the development of computer graphics codes for displaying SPOOR results.* These codes use specially prepared subsets of the SPOOR output tapes to generate a variety of particle and cloud-ensemble displays. These displays include two- and three-dimensional (perspective) snapshots and motion pictures of particle ensembles, in either black and white or color, plus running displays of differential and integral ensemble characteristics. The displays provide valuable information about the statistical and physical behavior of the "clouds."

We have run over 100 cloud simulations, both real cases to compare our cloud data with those in the literature and fictionalized cases to learn more about the details of statistical and ensemble behavior and the intricacies of transport phenomena in the transient regime between $t = 0$ and $t = 1$ to 10 h. We also have examined the sensitivity of results to internal model details and to wide variations in the input data. We find the code and

*Primarily the work of W. Rich, LASL.

```

*****
* SAMPLE CALCULATION WITH MEDIUM ENERGY SPECTRUM OF 3-27-75
*****
***** SPOOR INPUT PARAMETERS *****
YEAR = 1966  LON = 9.67496  SIGMAU = 1.6000  TYPE = 12  ZTYPE = 0  N = 51  KAN = 0  YIELD = 0.0000E+00
MONTH = 9  LAT = 50.73932  SIGMAV = 1.6000  RC = 0.50000  ZMAX = 12.00000  M = 5000  YESHUMP = 0
DAY = 17  I = 35.12983  SIGMAW = 0.7200  SIGMAR = 0.00000  ZMIN = 0.00000  DT = 0.10000  SNOPT = 0
HOUR = 0  J = 25.93686  GAMMA = 0.9400  DELTAZ = 0.10000
MINUTE = 7  ALT = 2.98874  WBAR = 0.00000  SIGMAZ = 0.05000

TI (HOURS) = 1.0000E+00

      NU      NU=PHI-NU
ENTR:  ARRAY      ARRAY
1  .00000E+01  .25000E+02
2  .00000E+01  .20000E+03
3  .00000E+01  .12000E+03
4  .00000E+01  .70000E+02
5  .00000E+01  .00000E+02
6  .00000E+01  .25000E+01
7  .00000E+01  .10000E+02
8  .00000E+01  .10000E+02
9  .00000E+01  .70000E+01
10 .00000E+02  .25000E+02
11 .00000E+02  .70000E+02

```

Fig. 4. Sample problem: input data.

model to be well behaved; ensemble statistical information accumulates so rapidly that we feel no urge to incorporate any of the standard Monte Carlo variance-reducing techniques (importance sampling, for example) into the code. We typically run between 1000 and 10 000 5-h trajectories (5×10^4 to 5×10^5 time steps) for a given problem at the rate of 1000 trajectories (5×10^4 steps) in about 35 to 40 s.

D. Sample Calculations

Figures 4-8 show the results from an illustrative calculation.

Figure 4 gives the problem-description input. The source (TYPE = 12) is a cylinder with uniform (in area) radial particle distribution and Gaussian vertical distribution. It has a radius (RC) of 0.5 km, a half thickness (DELTAZ) of 0.1 km, and a total source-strength normalization factor (YIELD) of 0.4.* The initial phase-space location (see Appendix A) of the center of the cylinder is height (ALT) = 2.98874 mb, $I_0 = 35.12983$, $J_0 = 25.93686$ (or latitude = 50.73932, longitude = 9.67496), and $t_0 = 0007$ h, 17 September 1966. Vertical boundary conditions (ZTYPE) are those described on p. 14, with ZMAX = 12 km and ZMIN = 0. Other input parameters are N = number of time steps per trajectory = 51, M = number of trajectories to be calculated = 5000, $DT = \Delta t = 0.1$ h, $GW/MW = \gamma_w = 0.94$, $SIGMAU = \sigma_{\Delta u_j}$ and $SIGMAV = \sigma_{\Delta v_j}$ (both = 1.6 km/h), $SIGMAW = \sigma_{\Delta w_j} = 0.72$ km/h, $SIGMAR =$ standard deviation

of Gaussian radial source distribution (not used in this case) = 0, $SIGMAZ =$ standard deviation for Gaussian axial source distribution = 0.05 km, and $WBAR =$ mean vertical wind field = $\bar{w}_j = 0$. The input turbulence spectrum is also given in Fig. 4, where NU is in cycles per hour and NU-PHI-NU has units of km^2/h^2 .

Figure 5 lists the resultant β_s calculated by SPOOR, Fig. 6 shows the step-to-step means and variances of the state variables,* and Fig. 7 gives the covariance of I and J at each step. Figure 8 is a time (t) plot of σ_r , the standard deviation of the particle radii about the cloud centroid.

Figure 9 shows computer-generated displays of vertical slices along the I-axis through the particle ensemble at several trajectory travel times. A pronounced vertical shear is evident, resulting from variations in the horizontal wind speed as a function of altitude. These shear effects are three-dimensional, of course, because the horizontal wind vectors have direction and magnitude gradients in both time and altitude.

V. RESULTS AND DISCUSSION

A. Illustrative Cloud Simulations

The novel and somewhat revolutionary character of this atmospheric diffusion model places a special burden on the interpretation of results. First, specific features and behavior of our results should be discussed, including sensitivities and asymptotic behavior. Second, certain key input variables should

*This is not used in SPOOR but is part of the output tape to be used by a subsequent output-processing code.

*The u, v, w, z and r variables are in kilometers and hours; one (I,J) unit = 362 km for this case.

TIME STEP	***** (1)	RETA ARRAY (2)	***** (3)
1	0.	0.	0.
2	0.	0.	.58957E-01
3	0.	-.74395E-02	.25109E+00
4	-.49725E-02	-.10632E-02	.38903E+00
5	-.43281E-02	.13177E-01	.46933E+00
6	-.15693E-02	.23083E-01	.52669E+00
7	.19028E-02	.29551E-01	.56870E+00
8	.49040E-02	.34262E-01	.60097E+00
9	.74443E-02	.37960E-01	.62589E+00
10	.10039E-01	.39980E-01	.64652E+00
11	.12591E-01	.42728E-01	.66158E+00
12	.14869E-01	.45003E-01	.67430E+00
13	.16820E-01	.47631E-01	.68424E+00
14	.18545E-01	.48872E-01	.69513E+00
15	.20308E-01	.49556E-01	.70282E+00
16	.22077E-01	.50752E-01	.70949E+00
17	.23428E-01	.52057E-01	.71543E+00
18	.24417E-01	.53201E-01	.72096E+00
19	.25249E-01	.54010E-01	.72612E+00
20	.26064E-01	.54656E-01	.73069E+00
21	.26728E-01	.55856E-01	.73411E+00
22	.27479E-01	.55695E-01	.73842E+00
23	.27811E-01	.54838E-01	.74364E+00
24	.28472E-01	.56781E-01	.74454E+00
25	.29430E-01	.56869E-01	.74697E+00
26	.29875E-01	.57069E-01	.74958E+00
27	.31019E-01	.57357E-01	.75092E+00
28	.31171E-01	.59124E-01	.75168E+00
29	.32057E-01	.58239E-01	.75428E+00
30	.32669E-01	.58720E-01	.75554E+00
31	.33162E-01	.59061E-01	.75688E+00
32	.33493E-01	.59478E-01	.75817E+00
33	.33685E-01	.59093E-01	.76044E+00
34	.33792E-01	.60344E-01	.76066E+00
35	.34467E-01	.59847E-01	.76213E+00
36	.34373E-01	.58494E-01	.76532E+00
37	.34563E-01	.60833E-01	.76386E+00
38	.34587E-01	.59460E-01	.76677E+00
39	.36515E-01	.61346E-01	.76398E+00
40	.32982E-01	.43554E-01	.78894E+00
41	.32442E-01	.71390E-01	.75925E+00
42	.37640E-01	.58026E-01	.76900E+00
43	.34851E-01	.62812E-01	.76760E+00
44	.35540E-01	.61597E-01	.76904E+00
45	.35278E-01	.61821E-01	.76961E+00
46	.36058E-01	.59271E-01	.77206E+00
47	.36018E-01	.61071E-01	.77068E+00
48	.35345E-01	.61594E-01	.77116E+00
49	.34525E-01	.56116E-01	.77883E+00
50	.34827E-01	.62300E-01	.77162E+00
51	.35820E-01	.60855E-01	.77232E+00

Fig. 5. Sample problem: calculated β_s .

be compared with the inputs of other, more standard models. Third, it is necessary to show that bulk features of our calculated clouds compare with available data.

Figures 10 through 13 show calculated cluster-growth curves as a function of travel time t for three different input spectra and for various source sizes. The ordinate in these figures is the standard deviation σ_r of the tracer-particle radial

distribution about the cloud centroid. Figure 14 is the set of three turbulent-energy spectra used for these test calculations. The spectra are derived from a composite diagram offered by Vinnechenko and Dutton.²² The designations low, medium, and high spectrum respectively identify the lower bound, median, and upper bound of the composite.

Figure 10 shows σ_r vs t for the three input spectra with separate, characteristic σ_Δ parameters for the small-scale fluctuations. The source is a 1-km diam, vertically oriented disk (no vertical transport is included) with uniform area distribution of material. Figure 11 demonstrates the effect of changing source size with a point source and disk sources of 0.2-, 1-, and 6-km diam. Figure 12, a counterpart of Fig. 10, uses the same three spectra but a common σ_Δ . Figure 13 demonstrates the role of correlated velocity fluctuations by comparing point-source calculations for the three spectra with completely uncorrelated random walks. We discuss each of these figures in detail below.

B. Cloud Growth vs Input Spectrum

One very useful model output is the growth rate of the particle ensemble. For the free atmosphere, this growth rate is virtually the only quantity we can test empirically. The parameter selected to describe the cloud size is σ_r , the radial standard deviation of the particle distribution.

Figure 10 is a display of σ_r vs time out to 10 h for the three spectra described above. The small-scale eddy kinetic energy in each instance is characterized by a σ_Δ specified independently and consistently for each spectral input. The key features of interest in this figure are the relative positions and characteristic shapes of the curves. The ensemble dimension σ_r is greatest for the high spectrum and smallest for the low spectrum, with the median spectrum between. The curves have slopes that increase monotonically with travel time for several hours. In the low-spectrum case, the early slope is very shallow, giving rise to a relatively sharp knee in the curve at 0.3 to 0.7 h. This characteristic shape depends on both the initial source size and the small-scale energy available for early growth. A sharp knee for the low-energy spectrum results from the fact that the accumulated random displacements become comparable to the initial source size only after several tenths of an

FIRST MOMENT/SECOND MOMENT

	N	I	J	Z	U	V	W	R
1	.351298E+02	.259369E+02	.298A12E+01	.898631E+01	-.35A55AF+01	-.4A8A45E-03	.332451E+00	.445052E-06
	.445052E-06	.475848E-06	.194000E-02	.260343E+01	.249419F+01	.809699E+00	.139830E-01	.351323E+02
2	.351323E+02	.259359E+02	.298A07E+01	.913883E+01	-.35724E+01	.517148E-01	.389436E+00	.675129E-06
	.675129E-06	.662025F-06	.707105E-02	.252774E+01	.268270F+01	.515084E+00	.291946E-01	.351348E+02
3	.351348E+02	.259349F+02	.298A59E+01	.919475F+01	-.361445E+01	.252187E-02	.433829E+00	.888867E-06
	.888867E-06	.892756F-06	.129404E-01	.272744E+01	.278021E+01	.517223E-01	.439710E-01	.351374E+02
4	.351374E+02	.259339E+02	.298A84E+01	.927718F+01	-.361878E+01	.154523E+00	.504668E+00	.120540F-05
	.120540F-05	.123743E-05	.186642E-01	.310208E+01	.306745E+01	.532797E+00	.648916E-01	.351399E+02
5	.351399E+02	.259329E+02	.299000E+01	.931531F+01	-.369287E+01	.129368E-01	.587945E+00	.164175E-05
	.164175E-05	.171125F-05	.246806E-01	.339963E+01	.353717F+01	.531193E-00	.926069F+00	.351425E+02
6	.351425E+02	.259319E+02	.299168E+01	.938911E+01	-.372466E+01	.114520E-02	.686356E+00	.223459E-05
	.223459E-05	.235434F-05	.307004E-01	.385544E+01	.368946F+01	.543316E-01	.129241E+00	.351451E+02
7	.351451E+02	.259304E+02	.299179E+01	.947437F+01	-.374534E+01	.708379F-02	.797442E+00	.302606F-05
	.302606F-05	.317327E-05	.371977E-01	.407570E-01	.404629F+01	.526742E+00	.175677F+00	.351477E+02
8	.351477E+02	.259294E+02	.299100E+01	.952138F+01	-.377845E+01	-.878039E-02	.919079E+00	.400191F-05
	.400191F-05	.422015E-05	.433001E-01	.427958E+01	.441348E+01	.518266E+00	.231939E+00	.351503E+02
9	.351503E+02	.259284E+02	.299021F+01	.952892E+01	-.384337E+01	.936258E-02	.106695E+01	.518592F-05
	.518592F-05	.549128E-05	.488898E-01	.458742E+01	.460776E+01	.519436E+00	.392410F+00	.351539E+02
10	.351539E+02	.259277E+02	.299115F+01	.958839F+01	-.391432E+01	.427004E-02	.118166E+01	.661505E-05
	.661505E-05	.700723E-05	.553040E-01	.93424E+01	.500182F+01	.506651E+00	.388188F+00	.351558E+02
11	.351558E+02	.259266E+02	.299157E+01	.962334F+01	-.396012E+01	.131165E-01	.132461E+01	.830062E-05
	.830062E-05	.877897F-05	.605305E-01	.505148E+01	.514777F+01	.545807E+00	.403031F+00	.351583E+02
12	.351583E+02	.259255E+02	.299020F+01	.966678F+01	-.399095E+01	.2260033E-02	.147296E+01	.102680F-04
	.102680F-04	.108157E-04	.652987E-01	.555513E+01	.546130F+01	.524057E+00	.592603F+00	.351609E+02
13	.351609E+02	.259244E+02	.299049E+01	.970269F+01	-.407254E+01	.176610F-01	.162753E+01	.125701F-04
	.125701F-04	.131473E-04	.718364E-01	.565611E+01	.562476E+01	.458783E+00	.720376E+00	.351636E+02
14	.351636E+02	.259233E+02	.298972F+01	.972563F+01	-.417457E+01	.437107E-02	.178025E+01	.151144F-04
	.151144F-04	.157100F-04	.780115E-01	.601110E+01	.581182F+01	.492641E+00	.868898E+00	.351663E+02
15	.351663E+02	.259221E+02	.298892E+01	.975490E+01	-.424081E+01	.174070E-02	.193884E+01	.180525F-04
	.180525F-04	.185578E-04	.825917E-01	.593499E+01	.603076F+01	.510807E+00	.103685E+01	.351690E+02
16	.351690E+02	.259210E+02	.298846E+01	.978947F+01	-.422788E+01	.154522E-02	.209933E+01	.211488E-04
	.211488E-04	.217807E-04	.881946E-01	.627507E+01	.658022F+01	.513389E+00	.121621E+01	.351717E+02
17	.351717E+02	.259198E+02	.298833F+01	.980060F+01	-.433959E+01	.928442E-02	.226783E+01	.246937F-04
	.246937F-04	.254596E-04	.931147E-01	.651273E+01	.660788F+01	.517263E+00	.142570E+01	.351744E+02
18	.351744E+02	.259188F+02	.298923E+01	.983886F+01	-.440888E+01	.836400E-02	.243819E+01	.284229E-04
	.284229E-04	.296144E-04	.981474E-01	.660299E+01	.702961F+01	.820065E+00	.165671E+01	.351771E+02
19	.351771E+02	.259173E+02	.299007E+01	.987573F+01	-.445484E+01	.699271E-02	.260939E+01	.324103F-04
	.324103F-04	.341292F-04	.104504E+00	.705738E+01	.718009F+01	.518941E+00	.190518E+01	.351799E+02
20	.351799E+02	.259161F+02	.298937E+01	.990071F+01	-.465368E+01	.144512E-02	.278099E+01	.368365E-04
	.368365E-04	.389017E-04	.110404E+00	.746580E+01	.759472E+01	.533280E+00	.218386E+01	.351826E+02
21	.351826E+02	.259148E+02	.298920E+01	.990330F+01	-.477742E+01	.147685F-01	.295672E+01	.415971E-04
	.415971E-04	.441049E-04	.115140E+00	.768171E+01	.766855E+01	.518252E+00	.247927E+01	.351854E+02
22	.351854E+02	.259135E+02	.299008E+01	.996670F+01	-.486611E+01	.610658E-02	.313205E+01	.465969F-04
	.465969F-04	.494604E-04	.119799E+00	.767525E+01	.800492F+01	.519484E+00	.279366E+01	.351881E+02
23	.351881E+02	.259121E+02	.299007E+01	.998898F+01	-.491976E+01	.124469E-01	.331217E+01	.520340F-04
	.520340F-04	.557621F-04	.124378E+00	.777397E+01	.809976F+01	.529905E+00	.314117E+01	.351908E+02
24	.351908E+02	.259108E+02	.299130E+01	.992939F+01	-.506242E+01	.675408F-02	.349447E+01	.577315E-04
	.577315E-04	.623728F-04	.131933E+00	.801547E+01	.847249F+01	.503361E+00	.350997F+01	.351936E+02
25	.351936E+02	.259094E+02	.299109E+01	.993435F+01	-.515125E+01	.777700E-02	.367819E+01	.638058E-04
	.638058E-04	.669404E-04	.136343E+00	.817387E+01	.841625F+01	.531588E+00	.390594E+01	.351963E+02
26	.351963E+02	.259079E+02	.299274E+01	.997057F+01	-.522571E+01	.884367E-02	.386652E+01	.703045E-04
	.703045E-04	.769184E-04	.141498E+00	.840768E+01	.884080F+01	.520802E-01	.431715E+01	.351991E+02
27	.351991E+02	.259065E+02	.299330E+01	.100004F+02	-.531448E+01	.444885E-02	.405433E+01	.772618F-04
	.772618F-04	.847854F-04	.146493E+00	.856986E+01	.886693E+01	.510158E+00	.475451E+01	.352001E+02
28	.352001E+02	.259050E+02	.299404E+01	.100521F+02	-.539197E+01	.152878E-01	.424403E+01	.845454E-04
	.845454E-04	.928539E-04	.151980E+00	.885649E+01	.946623E+01	.524246E+00	.519967E+01	.352046E+02
29	.352046E+02	.259035E+02	.299556E+01	.100827F+02	-.545761E+01	.318667E-02	.443568E+01	.922547E-04
	.922547E-04	.101024E-03	.157140E+00	.896732F+01	.917837E+01	.412584E+00	.560965E+01	.352074E+02
30	.352074E+02	.259020E+02	.299598E+01	.100724F+02	-.555188E+01	.352736E-02	.462414E+01	.100267E-03
	.100267E-03	.110054F-03	.163294E+00	.909599E+01	.917365E+01	.529373E+00	.619037E+01	.352102E+02
31	.352102E+02	.259005E+02	.299557E+01	.101376E+02	-.567302E+01	.469017E-03	.481727E+01	.108697E-03
	.108697E-03	.120806E-03	.168459E+00	.917136E+01	.947782F+01	.511592E+00	.670917E+01	.352130E+02
32	.352130E+02	.258990E+02	.299558E+01	.101804F+02	-.577671E+01	.557640E-02	.501064E+01	.117436E-03
	.117436E-03	.129984F-03	.174742E+00	.952078E+01	.950144F+01	.511787E+00	.725240E+01	.352158E+02
33	.352158E+02	.258973E+02	.299617E+01	.101914F+02	-.589132E+01	.140885E-02	.520340E+01	.126567E-03
	.126567E-03	.140827E-03	.180690E+00	.967500E+01	.973351E+01	.521023E+00	.781908E+01	.352186E+02
34	.352186E+02	.258957E+02	.299594E+01	.102255E+02	-.595724E+01	.148615E-01	.539606E+01	.135829E-03
	.135829E-03	.151157F-03	.188396E+00	.938801E+01	.989222F+01	.513153E+00	.846701E+01	

Fig. 6. Sample problem: step-to-step means and variances of the state variables.

35 .352214E+02 .258941E+02 .299458E+01 .102229F+02 -.607225E+01 -.795859E-02 .558972E+01
 .145527E-03 .162454E-03 .192415E+00 .955606E+01 .989172F+01 .516358E+00 .902095F+01
 36 .352243E+02 .258924E+02 .299376E+01 .102036E+02 -.020167E+01 .155910F-02 .578345E+01
 .155574F-03 .174261E-03 .198807E+00 .963146E+01 .101004F+02 .515279E+00 .966995F+01
 37 .352271F+02 .258907F+02 .299384F+01 .102411F+02 -.629520E+01 -.413240F-02 .597693E+01
 .165847F-03 .184431F-03 .203739E+00 .994537E+01 .102327F+02 .523990E+00 .103235F+02
 38 .352299F+02 .258889E+02 .299345E+01 .102547F+02 -.643370F+01 .150212F-01 .617454F+01
 .176755F-03 .190869F-03 .209844E+00 .100355E+02 .104231F+02 .566002F+00 .109934F+02
 39 .352327F+02 .258871F+02 .299504E+01 .102959F+02 -.044305F+01 -.113123F-01 .637351F+01
 .188007F-03 .212393E-03 .214146E+00 .101177E+02 .104244F+02 .531500E+00 .117033E+02
 40 .352356E+02 .258853E+02 .299391F+01 .102760F+02 -.662907E+01 .123322F-01 .647062F+01
 .199339F-03 .226062E-03 .219773E+00 .101741E+02 .106544E+02 .510183E+00 .124127F+02
 41 .352384E+02 .258835E+02 .299514E+01 .102944F+02 -.673700F+01 .131062E-01 .676569E+01
 .210791F-03 .240331E-03 .224954E+00 .103276E+02 .109949F+02 .522625E+00 .131654F+02
 42 .352413E+02 .258816E+02 .299645E+01 .103049F+02 -.684494E+01 -.649840F-02 .696400E+01
 .222635F-03 .255245E-03 .232328E+00 .103153E+02 .109074F+02 .540331E+00 .139312F+02
 43 .352441E+02 .258797E+02 .299586F+01 .103611F+02 -.698834E+01 .173007E-01 .716007E+01
 .234892F-03 .270474F-03 .238902E+00 .105384E+02 .110472F+02 .518895E+00 .147450F+02
 44 .352470F+02 .258778F+02 .299753E+01 .104173F+02 -.713030E+01 -.600884E-02 .736097E+01
 .247659E-03 .286253F-03 .245478E+00 .105341E+02 .114550F+02 .533726E+00 .155483F+02
 45 .352499E+02 .258758F+02 .299693F+01 .104147F+02 -.726298E+01 -.750056E-02 .756477E+01
 .261253F-03 .302329E-03 .251456E+00 .105873E+02 .111825F+02 .512145E+00 .163729F+02
 46 .352528E+02 .258738E+02 .299618E+01 .104183E+02 -.736526E+01 -.896002F-03 .777089F+01
 .274965E-03 .319280E-03 .257117E+00 .109129E+02 .114583F+02 .531401E+00 .172070F+02
 47 .352556E+02 .258718E+02 .299609E+01 .104211E+02 -.745892E+01 -.502728E-02 .797501E+01
 .288974E-03 .336518E-03 .261658E+00 .107862E+02 .112883F+02 .567992E+00 .180617F+02
 48 .352585E+02 .258697E+02 .299559E+01 .104447E+02 -.758428E+01 .608771E-02 .817602E+01
 .303184E-03 .354082F-03 .267043E+00 .107526E+02 .114800E+02 .540618E+00 .189455E+02
 49 .352614E+02 .258676E+02 .299628E+01 .104716F+02 -.772783E+01 .177690E-01 .837879E+01
 .317707E-03 .371932E-03 .272547E+00 .110194E+02 .118799F+02 .510008E+00 .198138E+02
 50 .352643E+02 .258655E+02 .299797F+01 .104650F+02 -.785169E+01 .891778E-02 .858021E+01
 .332398E-03 .390612E-03 .276363E+00 .110105E+02 .120418F+02 .529201E+00 .207425E+02
 51 .352672E+02 .258633E+02 .299886E+01 .105152F+02 -.804060E+01 -.115314E-01 .878319E+01
 .347885E-03 .410032E-03 .282280E+00 .109746E+02 .120655E+02 .514080E+00 .217623F+02

Fig. 6. (cont)

hour. Larger random fluctuations, however, give rise to an earlier "loss of memory" of the original cluster dimension, and thus shallower knees. Each curve of Fig. 10 shows a characteristic knee at about the same travel time, with a slight shift to longer travel times for lower values of σ_Δ .

Batchelor²³ formalizes the roles of turbulence energy and source size for the particular case of eddies governed by similarity theory. The integrated form of Batchelor's expression for early times is

$$\sigma^2(t) = \sigma_0^2 + 1.33c(\epsilon\sigma_0)^{2/3}t^2, \quad (24)$$

where σ_0 is the standard deviation of the initial cluster, c is a constant (~ 1), ϵ is the turbulent dissipation rate, and t is travel time.

Equation (24) exhibits a knee at about the time the second term on the right-hand side of the equation becomes comparable to the first term on the right. Estimates place the knee at less than 0.1 h for high turbulence levels to a few tenths of an hour for low turbulence levels. Table I compares the fundamental input parameter σ_Δ of the present

model to ϵ , the basic turbulence parameter of the similarity theory. These estimates were derived by assuming a -5/3 power-law turbulence spectrum from $\omega = 10 \text{ h}^{-1}$ to very high frequencies.

TABLE I
PARAMETER ESTIMATES

$\epsilon \left[\frac{\text{cm}^2}{\text{s}^3} \right]$	$\sigma_\Delta \text{ (km/h)}$	Subjective Pilot Descriptions
0.01	0.2	No turbulence
0.1	0.4	No turbulence
1	0.8	No turbulence
10	1.6	Light turbulence (clear air)
100	3.6	Moderate turbulence
1000	7.6	Severe turbulence
10^4	16.6	Thunderstorm turbulence

The slopes of the curves in Fig. 10 for travel times between about 1 and 10 h are in the range of 1.1 to 1.2. Batchelor's theory suggests that, if eddies with periods greater than 0.1 h satisfy a similarity relationship, the slopes of the growth curves should be 1.5. The input spectra for the

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N	RHO
1	.624641E-08
2	-.134642E-07
3	-.134241E-07
4	-.123946E-07
5	-.993532E-08
6	-.177242E-07
7	-.171312E-07
8	-.256405E-07
9	-.417094E-07
10	-.927284E-07
11	-.165070E-06
12	-.305303E-06
13	-.524396E-06
14	-.741682E-06
15	-.100664E-05
16	-.136105E-05
17	-.182125E-05
18	-.232716E-05
19	-.292184E-05
20	-.364169E-05
21	-.449194E-05
22	-.536341E-05
23	-.640404E-05
24	-.767296E-05
25	-.902150E-05
26	-.104327E-04
27	-.119724E-04
28	-.135793E-04
29	-.152676E-04
30	-.171024E-04
31	-.189765E-04
32	-.210955E-04
33	-.234145E-04
34	-.258327E-04
35	-.284459E-04
36	-.313809E-04
37	-.345046E-04
38	-.379266E-04
39	-.415768E-04
40	-.452606E-04
41	-.493081E-04
42	-.536009E-04
43	-.578494E-04
44	-.625117E-04
45	-.674699E-04
46	-.725333E-04
47	-.776692E-04
48	-.830235E-04
49	-.887560E-04
50	-.945234E-04
51	-.100456E-03

COMPLETE REAWINDUL 3

Fig. 7. Sample problem: step-to-step covariance of I and J.

curves of Fig. 10, however, were not constrained to satisfy a similarity condition. An interesting feature is the greater-than-linear growth for travel times where the diffusion is dominated by eddies in a steeply rising part of the turbulence spectrum.

Fig. 8. Sample problem: growth curve of radial standard deviation for particle ensemble.

C. Effect of Changing Source Size

Figure 11 shows results from a series of calculations in which four source sizes were run for the medium spectrum with $\sigma_\Delta = 1.6$ km/h. At long travel times, the curves asymptotically approach the cluster-growth curve for a point source. Each finite-sized source exhibits the characteristic knee described above; and the knee tends to be sharper and to occur later as the initial source becomes larger. Hence, for a cylindrical source of 3-km radius, the first rapid growth begins at a travel time of about 1 h, whereas, for a 0.1-km cloud, the knee is not discernible within the time resolution of the problem; that is, it occurs at less than 0.1 h. If an objective measure of the position of the knee is taken to be the time t_* at which $\sigma_r = 2\sigma_\Delta$, Eq. (24) suggests that t_* is proportional to $\sigma_\Delta^{2/3}$. Estimating this relation from Fig. 11 gives $t_* \propto \sigma_\Delta^{0.9}$.

D. Spectral Effects on Correlated Velocity Components

Figure 12 represents a computational experiment that does not give a practical result but which gives considerable insight into the relative roles of the random and correlated velocity fluctuations. Calculations were performed for the three input spectra but with a single σ_Δ . Although this procedure is unrealistic because higher energy in the mesoscale range is expected to be associated with increased small-scale turbulence, it does help us focus on the role of mesoscale fluctuations.

The most obvious result is that the relative positions of the curves are reversed compared with

(Each Division = 2 km)

Fig. 9. Sample problem: vertical distribution of particle ensemble along I-axis.

those in Fig. 10 because at early times (<1 h) the random component of the velocity fluctuations is dominant. Because a lower energy spectrum offers less coherent interference to this random growth than a higher energy spectrum, the lower energy curve rises more quickly in the first hour. Because of the large-eddy structure, however, lower energy coherent spreading would be expected to reduce the slope of the low-spectrum curve continuously with respect to the high-spectrum curve as travel time increases, leading to eventual crossing of the curves

Fig. 10. Growth curves, three energy spectra with consistent subgrid-scale energy inputs.

of Fig. 12. Although Fig. 12 gives evidence of slight trends in this direction, any crossing point is well beyond the time-range of the calculations (10 h), which suggests that details of mesoscale turbulence structure may not become important in cloud growth until at least a few tens of hours of travel time have elapsed. If this is true, simpler

Fig. 11. Growth curves, medium spectrum with four different source sizes.

Fig. 12. Growth curves, three energy spectra with a single subgrid-scale energy input.

models may be adequate for typical transport distances of a few hundred kilometers. Requirements for detailed turbulence structure in the diffusion model will be much more severe, of course, for regional-scale problems.

E. Relative Roles of Random and Correlated Velocity Components

For characterizing dispersion, the current model considers the turbulence spectrum to be divided into two regimes--the subtime-step regime, made up of eddies that produce random velocity fluctuations, and the larger scale regime that produces correlated velocities affecting many time steps. To observe the relative roles of these two spectral regimes, we ran a series of calculations for instantaneous point sources, and in one set of computations the correlated part of the wind field was turned off by setting the $\beta_{j,1}$ matrix [Eq. (4)] equal to zero. Figure 13 shows these completely random curves and their counterparts that include the full spectrum. The slopes of the random curves are independent of σ_Δ and are estimated to be about 0.57. The relative displacements of the curves (the values of σ_r at 1 h, for example) are approximately proportional to σ_Δ .

Sutton²⁴ analyzes a one-dimensional random-walk diffusion process that results in $\sigma_x \propto t^{1/2}$. The small difference between the 0.57 slope of σ_r vs t observed in Fig. 13 and the 0.50 slope suggested by Sutton could result from the difference in the spatial variables being considered (x vs r), or from numerical uncertainties, or from both.

Fig. 13. Effect of intermediate-scale spectral energy on growth curves.

The correlated portion of the wind velocity has a major influence. After the first 0.1 h, all correlated values of σ_r are systematically higher than their random counterparts. (The model initialization assures the identity, in each case, of the two curves for the first time step.) After an hour's travel, the correlated trajectories have produced a σ_r that is 1-1/2 to 2 times larger than that for the purely random walk.

F. Comparisons With Cloud Growth Data

Figure 15 shows representative SPOOR-calculated growth curves overlaid on a composite diagram of

Fig. 14. Three selected input power spectra.

observations from Hage and Chruch.²⁵ (A detailed summary of the experimental data is also given by Crawford.²⁶) The empirical data in the figure represent sources widely diverse in elevation, size, and function time, and, without the relevant source parameters, specific quantitative interpretation of the data is seriously compromised. However, some of the broader aspects of model-data comparisons are enlightening. First, calculated cluster dimensions and growth rates are consistent with the observations. The only observations that fall consistently outside the range of our model estimates (for reasonable turbulence levels and comparable source sizes) are referenced as experiment No. 10, which is a continuous-boundary-layer source and is thus not comparable. In these comparisons, one must remember that the calculations in Fig. 15 are derived solely from free-atmosphere turbulence spectra and include no feedback from, or normalizations to, cloud-size measurements.

The present model is intended more as a tool for appreciating atmospheric physics than as a cloud-size predictor,* but we have briefly explored some of the reasons for the good agreement between calculated and observed cloud sizes. Atmospheric diffusion is fundamentally an integrating process. The properties (size, shape, mass distribution, etc.) of a particle cluster after some given travel time depend on the integrated effects of turbulence encountered up to that point. For this reason, the demands for detail in the turbulence structure are less stringent than in some other turbulence dynamics problems. Also, for travel times up to 10 h or so, small-scale turbulence plays a dominant role in cloud dispersion; and parameters for the smaller scales of motion are established more successfully than for the intermediate mesoscale. Both the mechanics and the statistics favor the modeler of small-scale influences.

VI. SOME STRAIGHTFORWARD MODEL EXTENSIONS

We have described a basic, broadly applicable, computational tool for atmospheric transport problems even though our current interest is in a free

*Certainly, for example, the present model is not the only one that attains the favorable agreement in Fig. 15.

Fig. 15. Demonstration growth curves for three input spectra and three source sizes, plotted on an empirical composite of observed cluster sizes (after Hage et al. 1967).

atmosphere for transport times up to ~10 h. A logical extension, requiring minimum alteration to the present code, is to longer travel times. For example, the SPOOR code should be an ideal tool for regional-scale transport simulation; that is, for travel times on the order of 100 h. An expanding time step must be used for computational efficiency, but larger time steps at longer travel times merely transfer the parameter description of slightly larger eddies from the intermediate to the random field.

Another consequence of longer travel times is the fundamental requirement for a longer history or memory in the correlated velocity components. Our selection of three 0.1-h steps is consistent for travel times of less than a few hours, since empirical evidence suggests that the autocovariance functions drop rapidly to near zero in that lag time. However, as Fig. 16 indicates, the autocovariance at longer travel times T_2 takes on a different character, requiring correlations over longer lag times. This correlation can be accommodated both by adding more correlated time steps and, because time resolution is less critical for longer T_2 , by using larger time steps.

We can anticipate the behavior of the growth curves beyond the present 10-h runs. The energy spectrum peaks at synoptic-scale periods of around 100 h; corresponding spatial scales approach global

Fig. 16. Evolution of the effective autocovariance function with travel time.

dimensions. The continuously larger eddies that are available for relative dispersion, and which characterize the intermediate regime, change to an asymptotic regime with a bounded energy supply at the global scale. We must thus expect the cluster growth rates to become smaller beyond about 100-h travel time, as indicated in the empirical data in Fig. 15.

Another extension of the model is to applications in the boundary layer. Many air-pollution problems require that such a flexible model be used for transport estimates in the range of tens of hours. Boundary conditions both at the ground and at internally bounded mixing layers must be assessed carefully when setting up boundary-layer problems.

For medium- to long-range problems, diurnal variations in basic input parameters also become important.

Many computational experiments must be done to test the properties of the code and to examine the physics of atmospheric dispersion. We can initiate such calculations with the model in its present form, although we expect the results will lead to a natural evolution in the computational scheme. Included in these experiments would be testing responses to specially designed input spectra, such as selected power laws or a spectrum with a micro-scale peak and a distinct mesoscale energy gap.

Also, because the present model takes gradients in the mean transport wind completely in stride, it becomes a valuable tool for estimating dispersion in time- and space-varying flow fields, such as occur in areas near terrain or urban influences. Introducing selected mean-wind properties, including shear or curvature, and assessing cluster responses to these properties are natural extensions of the existing analytical base. Other fundamental and straightforward alterations to the basic model would extend the utility of the approach to cover a much wider range of applications. For example, introducing a body force, such as gravity, would require only a simple extension of the basic velocity-recursion relationships but would make the model appropriate to large-particle transport where gravitational settling is important. Also, we could easily incorporate velocity-dependent forces, such as drag, in the same manner. The buoyancy of thermally affected particles or a source in a water medium might be handled similarly.

APPENDIX A

THE NCAR WIND DATA BASE AND SPOOR INTERPOLATION SCHEMES

The built-in mean-wind data we use in SPOOR came from data tapes compiled by the National Center for Atmospheric Research (NCAR), Boulder, Colorado.²⁷ The NCAR compilations contain worldwide historical wind data translated to the National Meteorological Center (NMC) octagonal grid system.²⁸ Figure A-1 shows the northern hemisphere of this system, which is a regularly spaced rectangular grid laid out on a

polar stereographic projection of the earth's surface. We later give the transformations between NMC (I,J) coordinates and geographic (latitude-longitude) coordinates. We have written codes* to read the NCAR tapes, process and print the data in various ways, tally and print statistical features of the data, and produce a SPOOR wind-data tape.

*This was the work of W. Rich and R. Allenson, LASL.

Fig. A-1. NMC 47 x 51 grid. There are 1977 data points in the octagon. The pole point is $I, J = 24, 26$.

The SPOOR code is part of a larger code system LASL is developing to study collateral damage from postulated defensive nuclear engagements in NATO Europe and other parts of the world. For this reason, the specific data base now in SPOOR covers only a 42-point, Western Europe subset ($I = 33, 34, 35, 36, 37, 38; J = 23, 24, 25, 26, 27, 28, 29$) of the NMC grid. Figure A-2 shows this subset.

The NCAR data are given in (I, J) space and consist of orthogonal wind components, $\bar{u}$ in the I -direction and $\bar{v}$ in the J -direction. For each of the 42 (I, J) grid points shown in Fig. A-2, the specific data set extracted for SPOOR gives these components at six pressure altitudes (850, 700, 500, 400, 300, and 250 mb) for each 12-h interval from September 1963 to December 1967.*

Because SPOOR operates in a continuous phase space, we used an interpolation scheme to supply $\bar{u}$ and $\bar{v}$ values between the data-base points; and we developed a generalized code module for this purpose.²⁹ When called by SPOOR, this module generates biquadratic or bicubic least-square fits of the appropriate data-base winds vs I and J for any of the

six altitudes and 12-h time points in the data base. Linear interpolations in altitude and time then provide the required $\bar{u}_j$ and $\bar{v}_j$.

To illustrate, consider a trajectory step beginning at $\omega_j = (I_j, J_j, z_j, t_j)$, which defines bounding altitudes z_k and z_{k+1} and times t_i and t_{i+1} in the data base, so that

$$z_k \leq z_j \leq z_{k+1},$$

$$t_i \leq t_j \leq t_{i+1}$$

We then make separate least-square fits vs I and J over the 42-point grid of Fig. A-2 for altitudes k and $k + 1$ at times i and $i + 1$. Linear interpolations in z and t between these surfaces then give $\bar{u}_j = \bar{u}(\omega_j)$ and $\bar{v}_j = \bar{v}(\omega_j)$.

It is convenient to do these calculations in the (I, J) space, whereas the SPOOR tracking module operates more conveniently in the horizontal (x, y) space defined at each step by the tangent plane to the earth's surface at ω_j . A transformation between the (I, J) and (x, y) spaces is thus required. We avoid some complications by using instead the transformation between (I, J) coordinates and geographic coordinates.²⁸ As an example, for step j at ω_j , let the displacements in (x, y) space be $(\Delta x_j, \Delta y_j)$, where

$$(\Delta x_j, \Delta y_j) = (v_j \Delta t, u_j \Delta t).^*$$

The corresponding displacements in (I, J) space are

$$(\Delta I_j, \Delta J_j) = (\Delta y_j / \Delta E_j, \Delta x_j / \Delta E_j),$$

where

$$\Delta E_j = 381/k_j,$$

$$k_j = \frac{1 + \sin 60^\circ}{1 + \sin \theta_j},$$

*Many of these data are not actually available. We have used simple linear extrapolations and interpolations to infer missing data-base entries when required.

*In SPOOR, we arbitrarily take the positive x -direction along the positive J -axis and the positive y -direction along the positive I -axis.

Fig. A-2. WMC grid from SPOOR overlaid on map of Western Europe.

β_j = latitude of the point
(I_j , J_j).

$$\sin \beta_j = \frac{4a^2 - R_j^2}{4a^2 + R_j^2},$$

$$R_j^2 = (I_j - 24)^2 + (J_j - 26)^2,$$

$$4a^2 = 973.712023868.$$

Substituting the (I,J)-to-geographical transformation for the (I,J)-to-(x,y) transformation introduces a small bias in the trajectories, but, at latitudes of usual interest to us, this bias is small for track lengths up to several thousand kilometers.

APPENDIX B

VERIFICATION OF σ_z CALCULATION FOR THE VERTICAL-TRANSPORT MODULE OF SPOOR.

AN ILLUSTRATION

The simple form of Eq. (23) lets us calculate, in closed form, the expected value of the standard deviation σ_z for net vertical displacements of a set

of particle trajectories at any travel time t . We can then compare our results with numerical SPOOR results as a code-verification technique. We proceed as follows.

Assume a point source at vertical position z_0 , a constant time-step width Δt , and a mean vertical velocity $\bar{w} = 0$. Equation (23) for the z-velocity at step j becomes

$$w_j = \beta_w w_{j-1} + \Delta w_j, \quad (B-1)$$

where β_w is an input constant, Δw_j is a random independent sample from $N(0, \sigma_{\Delta w}^2)$, and $w_0 = 0$. The general term w_k of the sequence of w's is then

$$w_k = \sum_{i=1}^k \beta_w^{k-i} \Delta w_i. \quad (B-2)$$

The net z-displacement at step j is the sum of the individual displacements Δz_k up to j, so that

$$z_j - z_0 = \sum_{k=1}^j \Delta z_k = \sum_{k=1}^j \Delta t w_k = \Delta t \sum_{k=1}^j w_k$$

or, substituting Eq. (B-2),

$$z - z_0 = \Delta t \sum_{k=1}^j \sum_{i=1}^k \beta_w^{k-i} \Delta w_i, \quad (B-3)$$

and

$$\begin{aligned} (z_j - z_0)^2 &= \Delta t^2 \left(\sum_{k=1}^j \sum_{i=1}^k \beta_w^{k-i} \Delta w_i \right)^2 \\ &= \Delta t^2 [\Delta w_1 (1 + \beta_w + \beta_w^2 + \beta_w^3 + \dots \\ &\quad + \beta_w^{j-1} + \Delta w_2 (1 + \beta_w + \beta_w^2 + \dots \\ &\quad + \beta_w^{j-2}) + \Delta w_3 (1 + \beta_w + \dots + \beta_w^{j-3}) \\ &\quad \cdot \\ &\quad \cdot \\ &\quad \cdot \\ &\quad + \Delta w_j]^2, \end{aligned}$$

or,

$$(z_j - z_0)^2 = \Delta t^2 \left(\sum_{k=1}^j \Delta w_k \sum_{i=0}^{j-k} \beta_w^i \right)^2. \quad (B-4)$$

Let

$$y_{jk} = \sum_{i=0}^{j-k} \beta_w^i = \frac{\beta_w^k - \beta_w^{j+1}}{\beta_w^k (1 - \beta_w)}. \quad (B-5)$$

From Eqs. (B-4) and (B-5), the variance $\sigma_{z_j}^2$ of the net z-displacement at step j, which is the expected value $\langle (z_j - z_0)^2 \rangle$, is

$$\begin{aligned} \sigma_{z_j}^2 &= \langle (z_j - z_0)^2 \rangle = \Delta t^2 \left\langle \left(\sum_{k=1}^j y_{jk} \Delta w_k \right)^2 \right\rangle \\ &= \Delta t^2 \langle (y_{j1}^2 \Delta w_1^2 + y_{j2}^2 \Delta w_2^2 + y_{j3}^2 \Delta w_3^2 \\ &\quad + \dots + y_{jj}^2 \Delta w_j^2 + y_{j1} y_{j2} \Delta w_1 \Delta w_2 + y_{j1} \\ &\quad y_{j3} \Delta w_1 \Delta w_3 + \dots) \rangle. \end{aligned} \quad (B-6)$$

We now recall that the Δw 's are random independent samples from $N(0, \sigma_{\Delta w}^2)$ so that

$$\begin{aligned} \langle \Delta w_i \Delta w_\ell \rangle &= 0, \text{ if } i \neq \ell; \\ &= \sigma_{\Delta w_i}^2 = \sigma_{\Delta w}^2, \text{ if } i = \ell. \end{aligned}$$

Equation (B-6) thus gives

$$\sigma_{z_j}^2 = \Delta t^2 \sigma_{\Delta w}^2 \sum_{k=1}^j y_{ik}^2. \quad (B-7)$$

Finally, noting that

$$\sum_{k=1}^j \frac{1}{\beta_w^k} = \frac{1 - \beta_w^j}{\beta_w^j (1 - \beta_w)}$$

and

$$\sum_{k=1}^j \frac{1}{\beta_w^{2k}} = \frac{1 - \beta_w^{2j}}{\beta_w^{2j}(1 - \beta_w^2)},$$

$$+ \frac{\beta_w^2(1 - \beta_w^{2j})}{(1 - \beta_w^2)^2} \Big]. \quad (B-8)$$

Eqs. (B-5) and (B-7) give

$$\sigma_{z_j}^2 = \frac{\Delta t \sigma_{\Delta w}^2}{(1 - \beta_w)^2} \left[j - \frac{2\beta_w(1 - \beta_w^j)}{(1 - \beta_w)} \right]$$

Table B-1 compares σ_{z_j} from Eq. (B-8) and σ_{z_j} calculated by SPOOR for a point-source version of the sample calculation described earlier.

TABLE B-1
COMPARISON OF ANALYTIC AND SPOOR-CALCULATED σ_{z_j} vs t_j

j	t_j (h)	σ_{z_j}		
		Eq. (B-8)	SPOOR	Ratio
1	0.05	0.072	0.071	1.01
2	0.15	0.105	0.105	1.00
3	0.25	0.130	0.130	1.00
4	0.35	0.151	0.151	1.00
5	0.45	0.169	0.170	1.00
10	0.95	0.241	0.243	0.99
15	1.45	0.295	0.294	1.00
20	1.95	0.342	0.337	1.01
25	2.45	0.382	0.374	1.02
30	2.95	0.419	0.409	1.02
35	3.45	0.452	0.445	1.02
40	3.95	0.484	0.473	1.02
45	4.45	0.513	0.506	1.01
50	4.95	0.541	0.531	1.02

REFERENCES

1. J. von Neumann, S. Ulam, and R. D. Richtmyer, "Statistical Methods in Neutron Diffusion," Los Alamos Scientific Laboratory report LAMS-551 (1947).
2. E. D. Cashwell and C. J. Everett, A Practical Manual on the Monte Carlo Method for Random Walk Problems (Pergamon Press, New York, NY, 1959).
3. C. W. Watson and E. D. Cashwell, "Monte Carlo Development and Applications in the Los Alamos Nuclear Rocket Program," Proceedings of the Fourth International Conference on Reactor Shielding, Vol. 1, Paris (Oct. 1972).
4. G. E. P. Box and G. M. Jenkins, Time Series Analysis, Forecasting and Control (Holden-Day, Inc., San Francisco, CA, 1970).
5. C. J. Everett and E. D. Cashwell, "A Monte Carlo Sampler," Los Alamos Scientific Laboratory report LA-5061-MS (1972).
6. L. L. Wendell, "Mesoscale Wind Fields and Transport Estimates Determined from a Network of Wind Towers," Mon. Weather Rev. 100, 565-578 (1972).
7. M. H. Dickerson, "Summary of Research Related to Mass-Consistent Wind Field Analysis for the San Francisco Bay Area," Lawrence Livermore Laboratory report UCRL-74265 (1972).
8. S. K. Kao, University of Utah, Private communication (1973).
9. D. Raymond, "Calculation of Airflow Over an Arbitrary Ridge Including Diabatic Heating and Cooling," J. Atmos. Sci. 29, 837-843 (1972).

10. B. Nichols and C. W. Hirt, "Calculating Three-Dimensional Free Surface Flows in the Vicinity of Submerged and Exposed Structures," *J. Comput. Phys.* 12, 234-246 (1973).
11. J. Vukovich, "Theoretical Analysis of the Effect of Mean Wind and Stability on a Heat Island Circulation Characteristic of an Urban Complex," *Mon. Weather Rev.* 99, 919-926 (1971).
12. F. Pasquill, *Atmospheric Diffusion* (D. Van Nostrand Co., Ltd., London, 1962).
13. J. Dutton and D. Deaven, "A Self-Similar View of Atmospheric Turbulence," *Radio Sci.* 4, 1341-1349 (1969).
14. F. Frenkiel and T. S. Klebanoff, "Higher Order Correlations in a Turbulent Fluid," *Phys. Fluids* 10, 507-520 (1967).
15. H. T. Hantis, "The Structure of Winds of the Upper Troposphere at Mesoscale," *J. Atmos. Sci.* 20, 94-106 (1963).
16. Air Resources Laboratory, "A Catalog of Radar-Positioned Constant Volume Balloon (Tetron) Flights," Tech. Paper No. 58 (1966).
17. S. K. Kao and H. D. Woods, "Energy Spectra of Mesoscale Turbulence Along and Across the Jet Stream," *J. Atmos. Sci.* 21, 513-516 (1964).
18. H. A. Panofsky, "Spectra of Atmospheric Variables in the Boundary Layer," *Radio Sci.* 4, 1101-1109 (1969). (Copyrighted by American Geophysical Union).
19. G. I. Taylor, "Diffusion by Continuous Movements," *Proc. London Math. Soc.*, A, 20, 196-211 (1921).
20. J. Kempe de Fariet, "Les Fonctions Aleatoires Stationnaires et la Theorie Statistique de la Turbulence Homogene," *Ann. Soc. Sci. de Brux.* 59, 145 (1939).
21. S. Corrsin, "Theories of Turbulent Dispersion," *Proc. Int. Colloq. on Turbulence* (Univ. d'Aix-Marseille), *Centr. Nat. Rech. Sci.*, pp 28-51 (1963).
22. N. K. Vinnechenko and J. A. Dutton, "Empirical Studies of Atmospheric Structure and Spectra in the Free Atmosphere," *Radio Sci.* 4, 1115-1126 (1969).
23. G. K. Batchelor, "The Application of the Similarity Theory of Turbulence to Atmospheric Diffusion," *Quant. J. Roy. Met. Soc.* 76, 133-146 (1950).
24. O. G. Sutton, *Micrometeorology* (McGraw-Hill, New York, NY, 1953).
25. K. D. Hage and H. W. Church, "A Computer Model for Calculation of Fall and Dispersion of Particles in the Atmosphere," *Proc. (SAEC Met. Inform. Meeting, AECL-2787, p. 320 (1967).*
26. T. V. Crawford, "A Computer Program for Calculating the Atmospheric Dispersion of Large Clouds," Lawrence Livermore Laboratory report UCRL-50179 (1966), p. 56.
27. D. H. Joseph, National Center for Atmospheric Research, personal communication (October 1972).
28. R. L. Jenne, "The NMC Octagonal Grid," National Center for Atmospheric Research informal report, Boulder, CO (1970).
29. K. Fong and L. Rathmann, Los Alamos Scientific Laboratory, unpublished work (1973).