Transient Turbulence Theory. Part III: Bulk Dispersion Rate and Numerical Stability

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ABSTRACT

Even though a continuum of mixing parameters \( \gamma(t, z, \xi) \) is used in transient turbulence theory to describe the effects of many superimposed eddy sizes (\( \xi \)) on the mean field at height \( z \), the overall bulk dispersive rate at any height can be measured by one number, \( N_D(z) \). By utilizing second moment measures of dispersion, it is shown theoretically for various special cases that the variance of tracer position, \( \sigma_z^2 \), is given by \( \sigma_z^2(t, l) = N_D(z) \), where \( N_D(z) = \int \gamma^2(t, \xi) d\xi \). An analogous expression for \( N_D(z) \) is derived for the discrete version of transient theory, as can be used for grid point models. These bulk dispersive rates can easily be compared to eddy diffusivity, \( K(z) \), because the variance of tracer position for \( K \) theory is known to be \( \sigma_z^2(t, l) = 2K(z) \).

The discrete version of transient turbulence theory is shown to be absolutely numerically stable, regardless of the timestep size or the grid point spacing. In addition, it is shown how the values of the discrete transient coefficients are determined by two factors: 1) the physics governing the turbulence mixing, and 2) the nature of the discretization (i.e., size of timestep and grid spacing). Thus, it is possible to employ transient turbulence theory for both the diffusive and boundary layer parameterizations in a large-scale numerical forecast model that, by operational necessity, has coarse grid spacing and large timesteps.

1. Introduction and review

The difficulty of modeling atmospheric turbulence has stimulated the formation of a number of schools of thought regarding parameterization schemes. \( K \)-theory and mixing-length schools are local, first-order closure methods. The second and higher-order closure schools are also local in nature, but include equations for the higher turbulent moments. Large-eddy simulation schools make deterministic forecasts of the larger eddies with a very high resolution numerical model.

One of the growing schools of thought in atmospheric turbulence involves the transient turbulence theory. In this theory, eddies of varying sizes are parameterized by the rate of mixing that they produce between points separated in space. A mixing parameter is used for each size eddy; thus, the degrees of freedom (i.e., model parameters) is much larger than for \( K \) theory or second-order closure. Transient turbulence theory is thus a nonlocal, first-order technique to determine the ensemble-average effects of turbulence on the mean field.

Estoque (1968) and Blackadar (1979) were among the first to apply this scheme to model the heat transport away from the surface layer during free convection situations. Zhang and Anthes (1982) tested Blackadar's model, which is now the "high resolution boundary layer" option of the Anthes-NCAR-PSU (National Center for Atmospheric Research–Pennsylvania State University) mesoscale model. Fiedler (1984) showed that the spectral diffusivity concepts of Berkowitz and Prahl (1979, 1980) and Prahl et al. (1979) were identical to the transient turbulence theories. Fiedler also showed how the top-down, bottom-up diffusion model of Wyngaard and Brost (1984) could be simulated with transient theory. Fiedler and Moeng (1985) modeled transport of a conservative scalar in the convective boundary layer. Stull (1984; hereafter called Part 1) demonstrated that the transient mixing parameters could be modeled based on \textit{a priori} theories, or could be allowed to vary in response to mean flow characteristics. Stull and Hasgawa (1984; hereafter called Part 2) linked the turbulent adjustment scheme of Klemp and Lilly (1978) to transient mixing.

The one-dimensional transient dispersion model from Part 1 is

\[
\frac{dS(t, z)}{dt} = \int (S(t, z - \xi) - S(t, z))\gamma(t, z, \xi)d\xi, \quad (1)
\]

where \( \gamma \) is the transient coefficient that describes the rate of mixing of tracer from location \( z - \xi \) into location \( z \), and where \( \xi \) is a separation distance. Production and loss terms do not appear in (1), assuming a conservative tracer for simplicity. The corresponding discrete form in one dimension (see the Appendix) is

\[
S(t + \Delta t) = c(t, \Delta t)S(t), \quad (2a)
\]

where \( S \) is the column vector of tracer concentration at each of the grid points, and \( c \) is a square matrix of transient coefficients describing how much tracer from each grid point mixes with tracer from other grid points during a time step \( \Delta t \). Each element, \( S_i \), in \( S \) is found by

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where \( S_i(t + \Delta t) = \sum_j c_j(t, \Delta t) S_j(t) \), \( j \)

2. Review of the second moment as a bulk measure of dispersion

Although transient turbulence theory includes the effect of a whole spectrum of eddies on dispersion, it is possible to quantify a bulk measure of the dispersion. In the development of sections 3 and 4, second moments of the tracer concentration field will be used as a bulk dispersion descriptor for both transient theory and \( K \) theory. A brief review of the definitions and properties of moments is given here.

Define the zero through second moments of tracer concentration by

\[
\begin{bmatrix}
M_0(t) \\
M_1(t) \\
M_2(t)
\end{bmatrix} = \int \begin{bmatrix} 1 \\
z \\
z^2 \end{bmatrix} S(t, z) dz,
\]

(3a)

where \( z \) is height and \( S \) is the lineal concentration (number of particles per length) of a passive conservative tracer. For a discretized representation of the tracer concentration field, the moment definitions can be written as

\[
\begin{bmatrix}
M_0(t) \\
M_1(t) \\
M_2(t)
\end{bmatrix} = \sum_i \begin{bmatrix} 1 \\
(i \Delta z) \\
(i \Delta z)^2 \end{bmatrix} S_i(t),
\]

(3b)

where \( S_i \) is the concentration (number of particles) at grid point \( i \), and \( \Delta z \) is the spacing between grid points.

Moments for the continuous form of the transient coefficients are similarly given by

\[
\begin{bmatrix}
N_0(t, z) \\
N_1(t, z) \\
N_2(t, z)
\end{bmatrix} = \int \begin{bmatrix} 1 \\
\xi \\
\xi^2 \end{bmatrix} \gamma(t, z, \xi) d\xi.
\]

(4)

Because of its complexity, the second moment, \( N_2 \), of the discrete transient coefficients is introduced later, in section 4.

By utilizing the definitions that \( \bar{z}^2 = \sigma_z^2 = \int (z - \bar{z})^2 n(t) dz \) and the particle count, \( n(t) \), is given by \( S = dn(t)/dz \), it is easy to express our usual definition of dispersion, \( \sigma_z^2 \), in terms of the above moments:

\[
\sigma_z^2(t) = \frac{M_2(t)}{M_0(t)} - \left( \frac{M_1(t)}{M_0(t)} \right)^2,
\]

(5)

where \( t \) is time. The last term in (5) is equal to \( \bar{z}^2 \), and thus accounts for the location of the centroid of the tracer cloud. Stated another way, this last term removes advective effects from the first term on the right, leaving a second moment about the mean as the measure of dispersion.

For the general case of an arbitrary tracer distribution with height, the rate of dispersion is given by the change of \( \sigma_z^2 \) over time. If there is no mean vertical transport, then

\[
\sigma_z^2(t) - \sigma_z^2(0) = \frac{M_2(t)}{M_0(t)} - \frac{M_2(0)}{M_0(0)}.
\]

(6)

For the special case of a one-dimensional “puff” initiated as a point source, this reduces to \( \sigma_z^2(t) = M_2(t)/M_0(t) \). By using (6), we will not only be able to quantify transient dispersion, but we will be able to compare it to \( K \) theory. Also, the bulk rate of tracer dispersal leading to the \( \sigma_z^2 \) change described by (6) will be shown to equal \( N_2 \).

3. Bulk dispersion of continuous tracer fields

a. Derivation

To derive the bulk dispersion rate applicable to the special case of homogeneous, stationary, isotropic turbulence within an unbounded domain, start with the continuous form of transient theory, (1), and multiply by \( z^2 \). After integrating over height and rearranging, this becomes

\[
\frac{d}{dt} \int z^2 S(t, z) dz \approx \int \int z^2 S(t, z - \xi) \gamma(t, z, \xi) d\xi dz
\]

\[
- \int \int z^2 S(t, z) \gamma(t, z, \xi) d\xi dz,
\]

(7)

where \( \gamma \) is independent of height under the homogeneous turbulence assumption.

The first term on the right is the second moment of the convolution of \( S \) with \( \gamma \), and can be shown to equal \( M_0 N_2 + 2 M_1 N_1 + M_2 N_0 \). The second term on the right of (7) reduces to \( M_2 N_0 \). Also, the term on the left becomes \( dM_2/dt \). After combining these intermediate results, we find that

\[
\frac{dM_2}{dt} = M_0 N_2 + 2 M_1 N_1.
\]

(8)

For isotropic turbulence, \( N_1 = 0 \) because \( \gamma(\xi) = \gamma(-\xi) \) (i.e., symmetry). Upon using this in the equation above and rearranging, we find

\[
\frac{d}{dt} \left( \frac{M_2}{M_0} \right) = N_2 - \frac{M_2}{M_0} \frac{dM_0}{dt}.
\]

(9a)

However, \( dM_0/dt = 0 \) because of conservation of state (i.e., of tracer amount). By integrating the above equation over time and employing the stationarity hypothesis, the bulk dispersion for the transient turbulence theory becomes

\[
\frac{M_2(t) - M_2(0)}{M_0(t) - M_0(0)} = N_2 t.
\]

(9b)
where $\gamma$ and $N_2$ are not a function of $z$ or $t$ because of the assumptions of homogeneity and stationarity.

This general answer, when applied to the special case of a nonadvecting one-dimensional puff that started as a point source, becomes

$$
\sigma_z(t) = N_2 t. \tag{10}
$$

This increase of $\sigma_z$ with the square root of time was also observed in the one-dimensional puff simulation of Part 1. The puff half-width measured out to the point where $S/S_{\text{max}} = 10\%$, however, varies with time depending on the relationship between puff size and maximum eddy size. One must remember that (10) was developed using homogeneity and stationarity assumptions to allow a simple analytic solution. Real atmospheres are rarely homogeneous and isotropic, particularly for the larger eddy sizes.

b. Comparison of transient and $K$-theories

Using $K$-theory, the dispersion equation can be written as

$$
\frac{\partial S(t, z)}{\partial t} = \frac{1}{\partial z} \left[ K(t, z) \frac{\partial S(t, z)}{\partial z} \right], \tag{11}
$$

where $K$ is the eddy diffusivity. We know a priori that $K$-theory yields $\sigma_z(t) = 2Kt$ for a one-dimensional puff in stationary, homogeneous turbulence with constant $K$ (Pasquill, 1974). This fact can be used to verify that (6) produces the same answer, even for an arbitrary initial concentration distribution. The following approach is fairly standard, so we will just outline the steps.

For an arbitrary initial tracer distribution $S(0, z)$, the solution $S(t, z)$ to (11) can be written in terms of a Green’s function (Morse and Feshbach, 1953):

$$
S(t, z) = \int G(t, z - Z)S(0, Z) dZ, \tag{12}
$$

where $G(t, z - Z) = (4\pi Kt)^{1/2} \exp[-(z - Z)^2/4Kt]H(t)$, and where $H(t)$ is the Heaviside step function [$H(t) = 0$ for $t < 0$, and $H(t) = 1$ for $t > 0$]. $Z$ is a dummy height of integration, distinct from location $z$.

To find the second moment of this tracer cloud, multiply (12) by $z^2$ and integrate over $z$ to give, after some manipulation:

$$
M_2(t) = G_2(t)M_0(0) + M_2(0)G_0(t),
$$

where $G_2(t) = 2Kt$ and $G_0(t) = 1$ are the second and zeroth moments of the Green’s function. Thus, the above equation can be rearranged to be in the form of (6):

$$
\frac{M_2(t)}{M_0(t)} - \frac{M_2(0)}{M_0(0)} = 2Kt, \tag{13}
$$

where conservation of state (i.e., of total tracer amount) was used to substitute $M_0(t) = M_0(0)$ in (13).

This answer is certainly no surprise, in light of the second sentence of this subsection. However, it puts us on solid ground for using (6) as the basis of comparison of transient theory to $K$ theory. In a bulk sense, the dispersion associated with transient theory equals that of $K$-theory when $N_2 = 2K$. Although the bulk dispersion rates can be compared, this in no way implies that the tracer concentration fields are the same. In fact, $K$-theory dispersion from a point source yields a Gaussian tracer distribution, while a variety of distributions are possible using transient theory.

4. Bulk dispersion of discrete tracer field representations

a. Derivation

First, the zeroth and second moments can be calculated. When (2b) is used in (3b) to find the zeroth moment, we confirm that tracer amount is conserved and the zeroth moment is not a function of time:

$$
M_0(t = \Delta t) = \sum_i S_i = \sum_i S_j = M_0(t = 0). \tag{14}
$$

Conservation of state (i.e., tracer conservation) $\sum_j c_{ij}$ = 1, is used in the derivation of (14).

The second moment initially is $(\Delta z)^2 \sum_j j^2 S_j$, but becomes $(\Delta z)^2 \sum_i i^2S_i$ after timestep $\Delta t$. Combining these relationships into our usual second moment definition of dispersion gives

$$
\frac{M_2(\Delta t)}{M_0(\Delta t)} - \frac{M_2(0)}{M_0(0)} = (\Delta z)^2 \left[ \sum_i \left( \sum_j i^2S_j \right) \right. - \left. \sum_j j^2S_j \right] / \sum_j S_j. \tag{15}
$$

By employing the conservation of state and performing a little manipulation, the general form of the dispersion rate is given by

$$
\frac{M_2(\Delta t)}{M_0(\Delta t)} - \frac{M_2(0)}{M_0(0)} = (\Delta z)^2 \left[ \sum_j \left[ \sum_i \left( i - j \right)^2 c_{ij}(\Delta t) \right] \right] / \sum_j S_j. \tag{16}
$$

The special case of homogeneous, isotropic turbulence in an unbounded domain implies $c_{ij} = c_{ji}$, which is identical to the exchange hypothesis discussed in Part 1. When this is used in (15), we find that the dispersion is

$$
\frac{M_2(\Delta t)}{M_0(\Delta t)} - \frac{M_2(0)}{M_0(0)} = (\Delta z)^2 \sum_{i=\text{const}} (i - j)^2 c_{ij}(\Delta t). \tag{16}
$$
The index $j$ is a free index—any value can be used. The reason is that $c_{ij}$ and $(i-j)^2$ are both symmetric about $i-j$. Thus, we get the same value of $\sum_i (i-j)^2 c_{ij}(\Delta t)$ regardless of which one row or one column of the $c_{ij}$ array we use in our sum, assuming that we are not near a boundary of the turbulent domain. This conclusion is consistent with the work of Part 1, where one row of the transient matrix was all that was needed for the a priori model of puff dispersion.

The right-hand side of (16) is valid for any one time-step. To step forward $n$ timesteps, multiply the right-hand side by $n$. The final dispersion, $\sigma_z^2(t) - \sigma_z^2(0)$, at time $t = n\Delta t$ is

$$\frac{M_2(t) - M_2(0)}{M_2(0)} = \left[ \frac{(\Delta z)^2}{\Delta t} \sum_{(j=\text{const})} (i-j)^2 c_{ij}(\Delta t) \right] t,$$

$$= N_2 t.$$  \hspace{1cm} (17a)

We see that the bulk dispersion, $\sigma_z$, increases with the square root of time, even at small times. As discussed earlier, we note that this differs from the linear-with-time increase predicted with statistical theory for small times. However, as was discovered in Part 1, puff width does not exhibit such square-root-with-time growth, except in the special case of the puff being larger than the largest eddy. The spectral diffusivity theory of Prahm et al. (1979) also predicts that puff width grows at a different rate than $\sigma_z$ when the puff is smaller than the largest eddies. Prahm et al. (1979) showed that the predicted puff growth compared well with many observations.

The dependence of bulk dispersion rate on $\Delta t$ and $(\Delta z)^2$ marks a significant difference of (17) from (9). Namely, the dispersive effect of a particular choice of $c_{ij}$ depends on the $\Delta z$ resolution and the $\Delta t$ increment. If one changes $\Delta z$ without changing $[c_{ij}]$, then the only way that the bulk dispersive characteristics can be preserved is by altering $\Delta t$ such that the ratio $(\Delta z)^2/\Delta t$ remains constant (Ames, 1969). An alternate view is that the $c_{ij}$ elements are determined by two factors: 1) the physics governing the diffusion, and 2) the nature of the discretization (i.e., $\Delta t$ and $\Delta z$). As was shown in Part 1, a change in timestep must be accompanied by a change in $[c_{ij}]$ to preserve the physics. The bulk diffusion rate given by (17) is one measure of the physics.

b. Comparison of transient and $K$-theories

Starting with a brief review, the forward-in-time difference approximation to the one-dimensional dispersion equation (11) using $K$-theory is (Haltiner and Williams, 1980):

$$S_j(t + \Delta t) - S_j(t) = K \frac{S_{j+1}(t) - 2S_j(t) + S_{j-1}(t)}{(\Delta z)^2}.$$  \hspace{1cm} (18)

This can be expressed in matrix form (2a) by using the following matrix form for $[c_{ij}]$:

$$[c_{ij}(t, \Delta t)]$$

$$= \begin{bmatrix}
  0 & 0.5\tilde{K} & 1 - \tilde{K} & 0.5\tilde{K} & 0 \\
  0 & 0.5\tilde{K} & 1 - \tilde{K} & 0.5\tilde{K} & 0 \\
  0 & 0.5\tilde{K} & 1 - \tilde{K} & 0.5\tilde{K} & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots \\
  \vdots & \vdots & \vdots & \vdots & \vdots 
\end{bmatrix}$$  \hspace{1cm} (19)

and $\tilde{K} = 2K\Delta t/(\Delta z)^2$.

Substituting the array values from (19) into (17) and performing the indicated sum gives

$$\frac{M_2(t) - M_2(0)}{M_2(0)} = 2K t.$$  \hspace{1cm} (20)

Again, this is no surprise. The value of $K$ which would yield the same bulk dispersion as transient theory is

$$K = \frac{(\Delta z)^2}{2\Delta t} \sum_{(j=\text{const})} (i-j)^2 c_{ij}(\Delta t),$$

which, as before, is given by $N_2 = 2K$.

Table 1 gives values of $\sigma_z^2$ and $N_2$ as a function of time for the one-dimensional puff dispersion example from Part 1. This numerical example uses $c_{ij}$ determined from the inertial subrange envelope up to a maximum eddy rise of 100 m. The initial timestep increment is $\Delta t = 0.073$ s, and the resolution is $\Delta z = 10$ m. For this case, we see that $\sigma_z$ increases with the square root of time, as theoretically predicted from (17). The $N_2$ values found from the numerical forecast are constant with time, even though the tracer distribution profile (Part 1, Fig. 7) varies far from Gaussian at initial

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>$0.5 \sum_i (i-j)^2 c_{ij}$</th>
<th>$\sigma_z^2$ (m$^2$)</th>
<th>$N_2$ (m$^2$/s)</th>
</tr>
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<td>1.17 s</td>
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<td>7.932</td>
<td>6.76</td>
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<tr>
<td>1.25 min</td>
<td>2.538</td>
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<td>10.14</td>
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<td>6.76</td>
</tr>
<tr>
<td>10.0 min</td>
<td>20.31</td>
<td>4061</td>
<td>6.76</td>
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<tr>
<td>20.0 min</td>
<td>40.64</td>
<td>8128</td>
<td>6.78</td>
</tr>
</tbody>
</table>
times, and the puff width (Part 1, Fig. 8) changes from one power-law growth to another.

5. Local instantaneous dispersive characteristics

In this section, we turn away from the bulk overall view of dispersion, and focus on the local effects. Transient turbulence theory allows, but is not limited to, strong local mixing. Such local mixing can be caused by the subset of small-size eddies present in a turbulent field. The nature of local mixing can be explored by utilizing Taylor series expansion techniques, in the limit as eddy size becomes small. The result can easily be compared to K-theory, because K-theory is intrinsically local in nature.

For transient theory, start with (1), and expand both \( S(t, z + \xi) \) and \( \gamma(t, z, \xi) \) in Taylor’s series about \( \xi = 0 \). The former series is straight-forward, because \( S \) is usually a smooth and continuous function of height for real atmospheric tracers. The latter series is written here. It must be expanded in two parts because the transient curves might have a kink at \( \xi = 0 \) (see Figs. 4 and 7 of Part 1):

\[
\gamma(z, \xi)|_{\xi=0} = \gamma(z, 0) + \xi \frac{\partial \gamma}{\partial \xi}|_{\xi=0} + \frac{\xi^2}{2!} \frac{\partial^2 \gamma}{\partial \xi^2}|_{\xi=0} + \cdots, \]

\[
\gamma(z, \xi)|_{\xi<0} = \gamma(z, 0) + \frac{\partial \gamma}{\partial \xi}|_{\xi=0} + \frac{\xi^2}{2!} \frac{\partial^2 \gamma}{\partial \xi^2}|_{\xi=0} + \cdots. \]

Inserting these into (1) yields

\[
\frac{dS}{dt} = \frac{\partial S}{\partial z} \frac{\partial \gamma}{\partial \xi}|_{\xi=0} \int_0^\beta \xi^2 d\xi + \frac{\partial S}{\partial \xi} \frac{\partial \gamma}{\partial z}|_{\xi=0} \int_0^\beta \xi^2 d\xi \]

\[
+ \frac{\partial^2 S}{\partial \xi^2} \int_0^\beta \xi^2 d\xi + \cdots. \]

This integration is performed between \( \xi = \pm \beta \), where \( \beta \) represents a value close to zero.

For the case of asymmetric \( \gamma \), the transient approach results in

\[
\frac{dS}{dt} = \frac{\beta^3}{3} \left[ \gamma \frac{\partial^2 S}{\partial \xi^2} + \frac{\partial \gamma}{\partial \xi}|_{\xi=0} + \frac{\partial \gamma}{\partial \xi}|_{\xi=0} \right] \frac{dS}{d\xi} + \cdots, \tag{21} \]

where the limit as \( \beta \rightarrow 0 \) allows us to drop the higher-order \( \xi \) terms to study the local nature of dispersion. Usually, \( \partial \gamma/\partial \xi|_{\xi=0} \) and \( \partial \gamma/\partial \xi|_{\xi=0} \) are of opposite sign but differing magnitude, thus the sum of these two terms in the right side of the above equation give us information about the change of \( \gamma \) about \( \xi = 0 \). Note the similarity of the above equation with the general form of K-theory, which can be written as

\[
\frac{dS}{dt} = K \frac{\partial^2 S}{\partial z^2} + \frac{\partial K}{\partial z} \frac{dS}{dz}. \]

The residuals in the series expansions for the case above are on the order of \( \beta^4 \), assuming a relatively smooth shape for \( \gamma \). Thus, the portion of the \( \gamma \) curve near \( \xi = 0 \) describes K-theory-like behavior, while contributions to turbulence for \( \xi \neq 0 \) (i.e., larger eddies) are not captured by K theory.

The last term in (21) represents the dispersion that can occur in a linear concentration gradient, when the flow is represented by asymmetric transient coefficient functions. Such asymmetry allows greater mixing in one direction (e.g., up) than the other (e.g., down), resulting in a net turbulent flux divergence and associated change of concentration \( S \) with time.

6. Numerical stability

a. Derivation

As is derived here, transient dispersion is absolutely stable for forward time differences, given that the entropy and continuity constraints are not violated. This stability exists regardless of the magnitude of the timestep, grid spacing, or bulk dispersion rate \( N_2 \).

If the eigenvalues, \( \lambda \), of the transient matrix, \([c]\), satisfy the condition that

\[
|\lambda| \leq 1 \quad \text{for all} \quad \lambda, \]

then numerical stability is insured (Haltiner and Williams, 1980). Gershgorin’s theorem (Pearson, 1974) states that the largest eigenvalue-modulus, \(|\lambda|\), of matrix \([c]\) does not exceed \(|c|\), nor \(|c|\), where these norms are defined by

\[
||c||_\infty = \max_i \sum_j |c_{ij}|, \]

\[
||c||_1 = \max_i \sum_j |c_{ij}|. \]

If the transient matrix satisfies the entropy constraint (i.e., all elements are non-negative, see Part 2), and satisfies mass continuity and continuity of state (i.e., each row and each column sums to 1; see Part 1), then we see that each of the above norms is identically equal to unity. Thus, \(|\lambda| \leq 1\), completing our proof that transient mixing is always numerically stable for forward time differences.

The significance of this conclusion is far-reaching. It holds for any transient matrix that satisfies the above constraints. Assumptions of homogeneity and isotropy were not made in the above derivation. Therefore, even the matrices for convective overturning, and the responsive matrices used to simulate Wangara Years 33–34 in Part 1, are numerically stable. Also, it was shown in Part 2 that turbulent adjustment can be expressed in transient form; thus, it too is numerically stable.

b. Comparison with K-theory

To compare this result to that for K-theory, Haltiner and Williams (1980) point out that the forward-in-time difference equation for K-theory dispersion (18) is numerically unstable whenever \( K > 1 \). If \( K > 1 \) is used
in (19), then it is obvious that the elements on the main diagonal are negative. Negative array elements violate the entropy constraint. Namely, fluid becomes unmixed and discontinuities sharpen when negative array elements are used, which is contrary to our concepts of turbulent mixing.

By using the Green's function approach to the dispersion equation, however, it is well known that a matrix representation of \(K\)-theory in a grid point model can be formed that is not limited by the magnitudes of \(K\) or \(\Delta t\). For example, start with (6) and approximate the integral by a sum of the form

\[
S(z, t) = A \sum_{Z} \left\{ \frac{\exp[-(z - Z)^2/4Kt]}{(4\pi Kt)^{1/2}} S(Z, 0) \right\}
\]

(22)

where \(A\) is a normalization factor, discussed later. By making the substitutions that \(z = i\Delta z, Z = j\Delta z, \) and choosing the time step such that \(t = \Delta t\), (22) can be rewritten in the matrix (transient) form of (2a) with

\[
S_i = A \sum_j S_j \left[ \frac{(\Delta z)^2}{4\pi K \Delta t} \right]^{1/2} \exp \left[ -\frac{(i-j)^2(\Delta z)^2}{4K \Delta t} \right].
\]

The resulting transient coefficients that correspond to \(K\)-theory dispersion over the finite time \(\Delta t\) are given by

\[
c_{ij}(\Delta t) = (2\pi K)^{-1/2} A \exp[-(i-j)^2/2K].
\]

(23)

The transient curve given by these coefficients is plotted in Fig. 1. The Gaussian shape is typical of "small eddy" diffusion; namely, an idealization where all scales of turbulent motion are assumed to be smaller than the size of the tracer cloud. Compared to the transient curves in Part 1, it is obvious that \(K\)-theory dispersion is just one of many different representations that can be described under the transient framework.

If the discretization of the original Green's function is performed at coarse resolution, then the resulting \(c_{ij}\) coefficients will not sum to unity as required by conservation of state. Thus, the normalization factor, \(A\), in (23) is found from \(\sum_i c_{ij} = 1\) for any \(i\).

It can be seen from Fig. 1 that if \(K\) or \(\Delta t\) are large, then the number of grid points used in the dispersion calculation increases above the three that are used in (19). In other words, the dispersion given by (2a) and (23) has an order-in-space that is automatically adjusted to accommodate large values of \(K\) and \(\Delta t\), and is therefore always numerically stable by the arguments in the first part of this section.

7. Summary and conclusions

In transient turbulence theory, the mixing rate for each size eddy in a whole spectrum of sizes must be specified at each point in space. This large number of degrees of freedom makes it difficult to compare directly to \(K\)-theory, which has one degree of freedom at any one point in space. One way to compare these two theories is via their second moments. In other words, we can compare the theoretical bulk dispersion rate of each approach.

Regardless of whether the diffusion equation is expressed in differential or difference form, \(K\)-theory exhibits a dispersion rate of \(\sigma_z^2(t) - \sigma_z^2(0) = 2Kt\). For the special case of homogeneous and isotropic turbulence, the bulk dispersive effects of transient theory are given by \(\sigma_z^2(t) - \sigma_z^2(0) = N_2t\), where

\[
N_2 = \begin{cases} \int \xi^2 \gamma(\xi) d\xi, & \text{continuous form} \\ \frac{(\Delta z)^2}{\Delta t} \sum_{i} (i-j)^2 c_{ij}(\Delta t), & \text{discrete form}. \end{cases}
\]

These theoretical equations confirm the numerical forecast results of Parts 1 and 2.

The square root of time dependence of \(\sigma_z\) in transient theory occurs at all times. This differs from the statistical theory of dispersion, which predicts a linear dependence initially, followed by a square root of time dependence at longer times. However, the distribution of tracer concentration within a puff need not be Gaussian under transient theory. Therefore, the puff width can grow at rates different from those of \(\sigma_z\), depending on the spectrum of mixing coefficients used (see Part 1).

We see that the discrete transient coefficients are dependent not only on the underlying physics, but also on \(\Delta z\) and \(\Delta t\). As a practical consequence, any changes made to \(\Delta z\) during a numerical forecast must be accompanied by compensating changes to \(\Delta t\) or \(c_{ij}\), otherwise the bulk dispersion rate, \(N_2\), will change.

Transient turbulence forecasts are always numer-
ically stable, as can be shown using Gershgorin's theorem with the matrix eigenvector stability analysis method. This stability not only applies to mundane mixing between neighboring layers, but also applies to extremes such as complete convective overturning. Anisotropic and nonhomogeneous flows are also numerically stable.

By using a Green's function solution to the \( K \) theory diffusion equation, \( K \) theory can be posed in a matrix fashion that is also numerically stable for all values of \( K \) and \( \Delta t \). This differs from the simpler forward-in-time, centered-in-space difference form of the diffusion equation \((18)\), which is numerically unstable whenever \( K > (\Delta z)^2/2\Delta t \).

Focusing on the local dispersion near one point, a Taylor's series expansion is used to show that transient theory includes the small-eddy dispersion characteristics of \( K \)-theory as well as the larger-eddy effects that \( K \)-theory cannot model.

Transient turbulence theory is closely tied with spectral diffusivity theory and with the turbulent adjustment method. Taken together, this body of theories represents a growing school of thought regarding the parameterization of atmospheric turbulence. It is a parameterization that allows a spectrum of eddy sizes to transport matter across finite distances in a manner that has many physically realistic qualities. By helping to define the nature of transient theory, as was done in this paper, it is hoped that more investigators will be able to apply the theory to practical situations such as pollutant dispersion and numerical weather prediction.

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APPENDIX

Conversion Between the Discrete and Continuous Forms of Transient Turbulence Theory

Physical reasoning was used in Part I to convert the discrete form of transient turbulence theory \((2b)\) into the continuous form \((1)\). By reader request, more of the mathematical details concerning this conversion are given below. In particular, the relationship between \( \gamma(t, z, \xi) \) and \( c_{ij}(t, \Delta t) \) will be addressed.

Start with the continuous form given by \((1)\). Employ the Dirac delta function, \( \delta^D(\xi) \), to write an alternative continuous form as

\[
\frac{\partial S}{\partial t}(t, z) = \int \alpha(t, z, \xi) S(t, z + \xi) d\xi; \tag{A1}
\]

where

\[
\alpha(t, z, \xi) = \gamma(t, z, \xi) - \delta^D(\xi) \int \gamma(t, z, \xi') d\xi' \tag{A2}
\]

with \( \xi' \) being a dummy of integration.

Let location \( Z \) be distance \( \xi \) from location \( z \); namely, \( Z = z + \xi \). This leaves

\[
\frac{\partial S}{\partial t}(t, z) = \int \alpha(t, Z, Z - z) S(t, Z) dZ. \tag{A3}
\]

Split the integral of \((A3)\) into the sum of smaller integrals, each of subdomain size \( \Delta z \). If \( j \) is the index of each subdomain (i.e., a grid point index), then it can be shown that

\[
\frac{\partial S_j(t)}{\partial t} = \sum_j \alpha_{ij}(t) S_j(t) \Delta z \tag{A4}
\]

where

\[
\alpha_{ij}(t) \Delta z = \int_{Z_{j-1}}^{Z_{j+1}} \alpha(t, Z, Z - z) dZ,
\]

\[
S_j(t) \Delta z = \int_{Z_{j-1}}^{Z_{j+1}} S(t, Z) dZ
\]

and \( Z_{j+1} = Z_j + \Delta z \). \( S_j(t) \) is defined analogously to \( S_j(t) \), with \( z \) becoming \( z_j \) and \( Z \) becoming \( Z_j \).

For an infinitesimal time step, \( \delta t \), one finds via series expansion that to good approximation:

\[
S_j(t + \delta t) = S_j(t) + \frac{\partial S_j(t)}{\partial t} \delta t. \tag{A5}
\]

Substituting \((A4)\) into \((A5)\) yields, after some rearrangement:

\[
S_j(t + \delta t) = \sum_j [\Delta z \delta t \alpha_{ij}(t) + \delta_{ij}] S_j(t), \tag{A6}
\]

where \( \delta_{ij} \) is the Kronecker delta. Thus, if one defines

\[
c_{ij}(t, \delta t) = \Delta z \delta t \alpha_{ij}(t) + \delta_{ij}, \tag{A7}
\]

then the desired discrete form of transient turbulence theory \((2b)\) is obtained.

At this point, \((A2)\) and \((A7)\) can be combined to yield a relationship between \( c_{ij} \) and \( \gamma \):

\[
c_{ij}(t, \delta t) = \Delta z \delta t \tilde{\gamma}(t, z_i, z_j - z_i) A
\]

\[+ \delta_{ij}[1 - \Delta z \delta t \sum_k \tilde{\gamma}(t, z_i, z_i - z_k)] \tag{A8}
\]

\[B\]
for any fixed $i$, where $\bar{\gamma}$ is the average of $\gamma$ between $\xi = z_i - z_j - \frac{1}{2}\Delta z$ and $\xi = z_i - z_j + \frac{1}{2}\Delta z$, and $k$ is a dummy index of summation. Also, the Dirac delta function was integrated over $\Delta z$ to give the Kronecker delta: $\Delta z\delta_{\xi}(z_i - z_j) = \delta_{i,j}$. The repeated $i$ in term B of (A8) does not imply a sum.

Term A shows that $c_{ij}$ is proportional to $\gamma$ when $i \neq j$, for infinitesimal time increment $\delta t$. Stated another way, the plot of $c_{ij}$ vs $(j - i)$ follows the same shape, or same envelope, as $\gamma$ vs $\xi$. This equivalence of shapes was assumed in Part I to convert from $\gamma$ to $c_{ij}$. Term B insures that tracer conservation is satisfied. For example, by summing (A8) over all $j$, one finds that $\sum_{j} c_{ij} = 1$.

Although the value of $\gamma$ at $\xi = 0$ is not known, or even needed in (1), the value of $c_{ij}$ for $i = j$ is important because it specifies how much fluid in a grid cell is not mixed out by turbulence. Term B shows that if all the $c_{ij}$ values for $i \neq j$ are determined by the shape of $\gamma$, then $c_{ij}$ for $i = j$ is uniquely determined by the tracer conservation requirement.

Given $c_{ij}$ for an infinitesimal $\delta t$, it is still necessary to use the change in timestep procedures to find $c_{ij}$ for a finite $\Delta t$. For all practical purposes, a small but non-zero value for $\delta t$ can be used based on physical arguments, such as the viscous-subrange timescale used in Part I. The timestep conversion is then $[c(t, \Delta t)] = [c(t, \delta t)]^n$, where $n = \Delta t/\delta t$ and $c$ represents the matrix of $c_{ij}$ transient coefficients. The selection of $\delta t$ is critical to the outcome, and unfortunately is somewhat ad hoc. Although a better approach might be to employ a Green’s function to get $c_{ij}$ from $\gamma$, attempts to find this Green’s function have been challenging, and unsuccessful, to date.

REFERENCES


