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TURBULENT PENETRATIVE CONVECTION

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Nonlocal Transport of Passive Scalars in Turbulent Penetrative Convection

By

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We present and apply a Green-function-like method for quantifying the transport of a passive scalar (tracer) field for use in flows where local approximations such as turbulent diffusion break down. Here nonlocal transport is described by computing the flow's characteristic *transilient matrix*, whose elements contain the fractional tracer concentrations moving from one subvolume to another as a function of time. The approach was developed elsewhere for use initially with atmospheric flows, but here we extend the formalism and apply it in an astrophysical context – to three-dimensional simulations of turbulent, stratified convection with overshoot into convectively stable bounding regions. We emphasize the diagnostic capabilities of the matrix by computing from it matrix moments, transport coefficients, nonlocal fluxes and other measures. Results indicate that transport in both the vertical and horizontal directions is strongly influenced by the presence of coherent structures, resembling advection more than diffusion and dominated by scales comparable to the extent of the convection zone. This is especially the case at lower resolution. The technique is also applied to the problem of light element depletion in stars and it is found that the temporal scaling of the depletion rate can be more efficient than simple diffusive or even advective models suggest.

1. Introduction

The mixing of passive scalars in turbulent fluids is an important problem which occurs in many astrophysical and geophysical settings. The transport of light elements in stars is a prominent example.

In the simplest treatments of mixing, one prescribes a diffusion coefficient which is scaled by a characteristic size l and velocity amplitude v of the turbulence, and is typically much larger than the diffusivity arising from microscopic processes alone. The derivation of the turbulent diffusivity is based, among other things, on the assumption of *locality*, which means that a particle is carried only a very short distance by one eddy before being entrained in a different eddy which is completely uncorrelated with the first.

The local prescription fails if the velocity field displays long scale correlations or if the dynamics is governed by broad distribution functions (see Bouchaud & Georges 1990 for a review). This is just the situation which is now known to hold in many turbulent flows, including turbulent convection in stars. Recent simulations of convection (e.g. Brandenburg et al 1996; Rast 1995; Cattaneo et al. 1991) show coherent structures such as strong downward plumes, which extend over several scale heights. The validity of the diffusion approximation must be called into question in such systems. The main

question is what should replace it. The purpose of this paper is to explore one possible prescription: the *transilient matrix* approach first applied by Stull (1993) to atmospheric science problems. In the remainder of this introduction we place this approach in context.

A passive scalar field $c(\mathbf{r}, t)$ in a fluid flow $\mathbf{v}(\mathbf{r}, t)$ with negligibly small molecular diffusion evolves according to the advection equation

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = 0. \quad (1.1)$$

(The field is characterized as passive if c does not appear in any of the equations which determine $\mathbf{v}$). Equation (1.1) has the solution

$$c(\mathbf{r}, t) = c(\mathbf{r}_0(\mathbf{r}, t), t_0) \quad (1.2)$$

where $\mathbf{r}_0(\mathbf{r}, t)$ is the position at some initial time t_0 of a fluid particle which is at position $\mathbf{r}$ at time t . In turbulent flow, the particle paths are so complicated that this exact solution is not useful and not even readily computable from a simulation of the flow. Therefore, it is necessary to resort to an approximate solution of equation (1.1). All descriptions of turbulent transport are a compromise between the exact description given in equation (1.2) and a tractable simplification of it.

In the local picture, the turbulent diffusion term is the first member of a Taylor series, involving derivatives of c , in which the successive terms are ordered by powers of the mean free path (or correlation length) divided by the size of the system. Turbulent diffusion corresponds to the ∇^2 operator acting on c . Higher order terms have been calculated, for example by Rüdiger (1982), who calculated the ∇^4 term for turbulent viscosity and found good agreement with the measured profiles in channel flow. However, the convergence of the series itself is open to question, although in specific examples, such as the related problem of turbulent diffusion in a weakly turbulent medium driven by the Parker instability, Hasler, Kaisig, & Rüdiger (1994) found that the series does converge and the local approximation is adequate.

When the correlation lengths are large, a nonlocal description may be more accurate. The concentration c may be written in terms of a Green function for the initial value problem

$$c(\mathbf{r}, t, t_0) = \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}', t, t_0) c(\mathbf{r}', t_0). \quad (1.3)$$

(The solution 1.2 can be written in this manner, with the Green function given by an appropriate delta function). If the Green function is sharply peaked about $\mathbf{r} = \mathbf{r}'$ then the local approximation holds. More generally, Stull and collaborators (Stull 1993 and references therein) have demonstrated a method for computing a discretized analog of the Green function, which they term the *transilient matrix*, from a numerical simulation of turbulence. A variety of quantitative descriptors of nonlocal, nondiffusive transport can be obtained directly from this matrix, once it is computed for a given flow.

In this paper we develop a variant of Stull's technique and apply it to the three dimensional simulations of turbulence presented by Brandenburg et al (1996). These are fully compressible and include overshoot into a stable layer below the convectively unstable layer. We consider two different realizations of this turbulence; one with 63^3 and the other with $126^2 \times 105$ meshpoints, and either using static snapshots of the velocity field or solving the full, compressible MHD equations and thus evolving the velocity field in time after the tracer particles have been injected. The runs we have considered are summarized in Table 1. Section 2 describes the transilient matrix approach. In Section 3 we discuss several quantitative measures of transport and present them for these simulations, and we also apply the technique to the problem of light element depletion in

Case	Horizontal Resolution	Vertical Resolution	Aspect Ratio	Computational Domain	Stratification	Velocity Field
1	63	63	2	[0.00, 2.00]	11	snapshot
2	126	105	2	[-0.15, 1.50]	92	snapshot
3	126	105	2	[-0.15, 1.50]	92	evolving

TABLE 1. Descriptive Summary of the Simulations

stars. Section 4 is a summary and conclusion. A preliminary version of this work has appeared elsewhere (Miesch et al. 1995)

2. The Transilient Matrix

Our goal in this paper is to describe the nonlocal transport of a passive scalar field (i.e. a collection of tracer particles) in simulations of convective turbulence in a manner analogous to equation (1.3). When considering convection, it is natural to concentrate first on transport in the vertical (z) direction, parallel and antiparallel to the direction of the gravitational field, and thereby simplify the notation and the data storage requirements. So, we will begin with the horizontally averaged particle concentration, denoted by $\bar{c}(z, t)$, or rather, its discrete analogue, $\bar{c}_i(t)$, where i denotes a vertical level, or bin. Following equation (1.3) we can then express the temporal evolution of the mean concentration as

$$\bar{c}_i(t) = \sum G_{ij}(t, 0) \bar{c}_j(0), \quad (2.1)$$

where the subscripts i and j again refer to vertical bins and where, for convenience, we have chosen origin of our time coordinate to correspond to the instant at which tracer particles are injected. Although eqn. (2.1) is similar in form to eqn. (1.3), there are important differences between them. We return to this issue near the end of this section.

If the fluid is vertically stratified, the particle concentration will tend to trace the density stratification, and so, in that case, it is convenient to define vertical levels of constant fluid mass, where the spatial extent of the levels decreases as the density increases toward the bottom of the computational domain. It is also useful in some cases to introduce vertical levels of constant volume (with equal thickness) when physical length scales are desired, as in the computation of nonlocal fluxes in section 3.3 below. Unless otherwise noted, however, constant mass bins are used for the present work. The number of mass bins to consider is to some extent arbitrary, but here we choose it to be equal to the number of grid points in the vertical direction, so the width of a bin is larger than a grid spacing near the top of the computational domain, where the density is low, and smaller near the bottom. Following Stull (1993 and references therein), we call the discrete analogue of the Green function, G_{ij} , the transilient matrix for the flow. The elements of the transilient matrix give the fraction of tracer particles moving from one subvolume (in the above case, one vertical bin) to another as a function of time. Although the system is actually deterministic, it might be useful to think of the matrix G_{ij} as a set of transition probabilities between the source levels j and the destination levels i .

For convenience, we will often refer to the Green function in continuous space, $G(z, z', t, t')$, which is approximated by the transilient matrix as follows:

$$G(z_i, z'_j, t, t') = G_{ij}(t, t') \quad (2.2)$$

where z_i and z_j are the depths about which the source and destination bins, i and j , are centered.

In principle, the transilient matrix for a flow can be computed by a series of numerical experiments, each measuring the response of the system to different initial conditions (usually resembling δ functions). However, this becomes impractical for turbulence simulations because of the computational expense. Alternatively, a set of differential equations (one for each level), each describing the time evolution of a passive scalar field with different δ function-like initial conditions could be solved simultaneously in a single run. This is the procedure originally used by Stull and colleagues in their large-eddy simulation models (see, e.g., Ebert et al. 1989). We adopt here a less rigorous, but more computationally efficient way of calculating the transilient matrix, G_{ij} , which involves injecting a large number of passive tracer particles, initially uniformly distributed among the levels, advecting them with the flow, and then computing the matrix directly from their statistical behavior. This approach is only valid if microscopic (sub-grid scale) diffusion can be neglected, which is a good approximation for large Reynolds numbers, although large gradients can develop in small regions of the fluid where the approximation breaks down. Such effects are not strictly captured by this procedure. However, this is not a severe problem, because in practice we consider flows that are solutions of the full diffusive equations. Furthermore, the tracer particles will still give a good description of the evolution of c in those regions where diffusion is weak.

The temporal evolution of the transilient matrix (plotted as $G(z, z', t, 0)$; see eqn. 2.2) for one of the simulation runs (case 2) is exhibited in Figure 1 as a series of contour plots, and Figure 2 shows a cross section along a particular source level (the other two cases are qualitatively similar). These plots were made using bins of constant mass. The dotted lines in the figures delineate the convectively unstable region, which is bounded above and below by regions of stable stratification. Note that the z coordinate (depth) increases downward. If the mixing occurred via classical diffusion in an infinite domain, cross sections through the matrix would yield Gaussians which would progressively decrease in amplitude and increase in dispersion with time. Note in the simulations the asymmetric spread away from the diagonal, which is the initial state. Although the peak concentration arising from a source level is typically advected upward, the downward moving particles tend to propagate away from the diagonal more rapidly, characteristic of the broad upflows and relatively strong, narrow downflows typically seen in compressible, stratified convection. We will return to this issue later.

As alluded to in the introduction and Table 1, when computing the transilient matrix for a flow, one has the option of either using a single, time-independent snapshot of the velocity field to advect particles (as in Figs 1 and 2) or to continue solving the full MHD equations and thus evolve the fluid in time while the particles are being advected. If the fluid has reached a statistically steady state then there will be little difference between the two approaches (although, as pointed out by Vincent et al 1996, a frozen velocity field can produce too coherent an advection and thus overestimate the transport). We find that there is indeed only a minor difference for the convective turbulence simulations presented here, as illustrated in Figure 3. There we show the temporal evolution of corresponding cross sections through two transilient matrices of the higher resolution data, the first obtained using a time-evolving velocity field (case 3; dotted line) and the second an analogous run obtained by using only a single, instantaneous snapshot of the velocity field (case 2; solid line). There is a very close correspondence between the two, which indicates that the use of a single snapshot in order to ameliorate the computational requirements does not significantly alter the results and the subsequent conclusions. In what follows, therefore, we present results primarily obtained with the time-independent

FIGURE 1. The transient matrix, $G(z, z', t)$, for Case 2 at several times, which are labeled on each frame, using bins of constant mass as described in the text (a convective timescale is roughly 20 in dimensionless temporal units). The boundaries of the convectively unstable region are marked with dotted lines. The source and destination axes indicate depth, which increases downward, in the direction of the gravitational force. The contour levels are 0.001, 0.003, 0.006, 0.01, 0.03, 0.06, 0.1, 0.3, 0.6, and 1.0.

velocity field snapshot, case 2, with the understanding that the results for case 3, with the evolving velocity field, are very similar. Results for the lower resolution run, case 1, are also obtained with a time-independent snapshot of the velocity field.

The transient matrix, by its nature, must satisfy certain constraints (see Stull 1993). Among them, G_{ij} must lie between zero and unity, since it is a fractional measure. Also, particle conservation requires that the sum over each column (i.e. over all destinations for a particular source level) equal unity unless tracer particles are allowed to escape the computational domain. In the work of Stull and colleagues (e.g. Ebert et al. 1989), the matrix rows were also restricted to sum to unity, but the reason for this lies in their assumption of a Boussinesq fluid in which no accumulation of tracer particles on a given level is possible if those particles do indeed accurately trace the fluid mass. When compressibility (in particular, stratification) is taken into account, there is nothing in principle preventing the accumulation of tracer particles on any given level, and in fact, they will tend to trace the density stratification as mentioned above. Thus, in the present work, the matrix rows do not in general sum to unity (although they come very close if bins of constant mass are used; see Fig. 5 below)

We now discuss the consequences of horizontal averaging. First of all, although eqn. (1.3) is an exact solution of eqn. (1.1), eqn. (2.1) is not the solution of the horizontal average of eqn. (1.1), nor is it the horizontal average of eqn. (1.3) (the fact that eqn. (1.3)

FIGURE 2. A cross section through the transient matrix for Case 2 at the same times that are shown in Figure 1. The concentration begins as a delta function at the source depth, marked with a dotted line, and the progressively more disperse curves correspond to later times. Again, dotted lines mark the boundaries of the convection zone.

FIGURE 3. Shown are transient matrix cross sections for a given source level, $z' = 0.25$, for both cases 2 (solid line) and 3 (dashed line). The results for several different times are included (plotted left to right), and note that the horizontal axes cover only a fraction of the total computational domain. Bins of constant volume have been used to compute both matrices.

is in continuous form and eqn. (2.1) in discrete form is irrelevant to this conclusion). The fact that the average Green function we compute is not a Green function for the averaged dynamics means that the Green function cannot be “restarted”. Consider two times t_1 and t_2 , with $0 < t_1 < t_2$. According to eqn. (2.1)

$$\bar{c}_i(t_2) = \sum_j G_{ij}(t_2, 0) \bar{c}_j(0) = \sum_j G_{ij}(t_2, t_1) \bar{c}_j(t_1), \quad (2.3)$$

where the final equality treats $c_j(t)$ as an initial condition. But, since $\bar{c}_j(t_1) = G_{jk}(t_1, 0) \bar{c}_k(0)$ (c.f. eqn 2.1), we should have

$$G_{ij}(t_2, 0) = \sum_k G_{ik}(t_2, t_1) G_{kj}(t_1, 0) \quad (2.4)$$

In fact, equations (2.3) and (2.4) are not, in general, satisfied for our computations. They do hold if the flow is statistically homogeneous in the horizontal directions, and if

the initial concentration c is independent of horizontal position. However, the horizontal averaging represents a loss of information about horizontal particle positions, so if significant inhomogeneities are present, such as those due to coherent structures, equations (2.3) and (2.4) break down. In this context, it is important to point out that transilient matrices do not provide a turbulence model in the usual sense, although they were introduced and have been used for this purpose (cf. Stull 1984; Stull 1993). Instead, such matrices provide an *a posteriori* description of average properties of the flow (since the full three-dimensional dependence of particle trajectories is followed, the transilient matrices in this sense are exact, provided microscopic diffusion can be neglected and the initial conditions are uniform in the horizontal directions. This latter restriction, however, can be relaxed somewhat when horizontal transport is taken into account; see below). The main power of the transilient matrix approach is that it allows answers to the question of how structures of different scale and shape evolve in time. Thus, instead of carrying out new full three-dimensional simulations for each initial profile, we can obtain the evolution of arbitrary profiles by simple matrix multiplications.

A more general Green function which depends on six spatial dimensions $x, y, z, x', y',$ and z' , can be derived in principle, but computer memory storage and visualization requirements become prohibitively large at high resolutions unless some “coarse graining” is implemented. However, we can generalize the matrix to study horizontal transport without too much trouble if we include the average horizontal displacement as an extra dimension, i.e. if we consider $G_{\mu ij}(t)$, where μ is the root-mean-square horizontal displacement of a particle which begins on level j and ends up on level i after a time t . In practice, however, even this reduced matrix can become prohibitively large, so here we select only particular source levels, j , and use a more coarse binning for the destination levels (typically the destination bins for the horizontal matrix, $G_{\mu ij}$, contain 11 of the mass or volume levels used for the G_{ij} matrices, with one of the larger bins always centered around the source level, j).

Finally, it is straightforward to generalize the transilient matrix approach to study the passive advection of vector fields for which the flux through a material area element is conserved (see Brandenburg et al 1996??). Applications include the transport and amplification of weak magnetic fields in an infinitely conducting medium, which could have relevance for convective dynamos and associated flux transport.

3. Applications

3.1. Matrix Moments

Once the transilient matrix is known for a given flow, a number of quantitative measures of transport can be obtained from it directly. The most straightforward are its various moments, with respect to either the source or destination indices:

$$\mathcal{M}_j^{(d;n)} = \sum_i (j - i)^n G_{ij} \quad (3.1)$$

and

$$\mathcal{M}_i^{(s;n)} = \sum_j (j - i)^n G_{ij}. \quad (3.2)$$

We will restrict attention to the mean, variance, and kurtosis, which are simply the first, second, and normalized fourth moments respectively,

$$\mu_i^p = M_i^{(p;1)}, \quad \sigma_i^p = M_i^{(p;2)}, \quad \text{and} \quad \kappa_i^p = M_i^{(p;4)} / (\sigma_i^p)^2 \quad (3.3)$$

where $p = s$ or d . For classical diffusion in an infinite domain, $\mu_i^p = 0$, $\kappa_i^p = 3$, and σ_i^p increases linearly with time.

In many other physical systems as well, the variance is found to scale with time as $\sigma_i^p \propto t^\beta$, and the scaling exponent, β , is often used as a quantitative measure for anomalous diffusion. Again, a value $\beta = 1$ corresponds to classical diffusion, while $\beta > 1$ holds for the superdiffusive, or *ballistic* case, and $\beta < 1$ holds for the subdiffusive, or *stagnant* case (see, e.g. Wang & Hu 1993). In practice, the value of β can vary significantly between flows, with turbulent transport being generally superdiffusive. For incompressible, three-dimensional, isotropic, homogeneous turbulence, for example, *Richardson's law* predicts $\beta = 3$ while $\beta = 1/3$ has been predicted and experimentally verified for laminar convective rolls (Pomeau et al 1989; Cardoso & Tabeling 1988). Laminar advection at a constant velocity, from, say, a divergent source, is also superdiffusive, characterized by $\beta = 2$. Bohr & Pikovsky (1993) found less extreme superdiffusive behavior, $\beta = 1.38$, for the Kuramoto-Sivashinsky equation, which is a simple, nonlinear field equation exhibiting spatiotemporal chaos. On the other hand, for observations of concentrations of magnetic flux in the solar photosphere, Lawrence & Schrijver (1993) found subdiffusive transport, with $\beta = 0.89 \pm 0.19 / -0.14$. Our results for the convection simulations presented here indicate superdiffusive transport in both the vertical and horizontal directions, which likely arises primarily from larger-scale, non-turbulent flow structures. These results will be presented and discussed later in this section.

Because of the inherent anisotropy of the vertical transport, we generally split the moments into upward ($i < j$) and downward ($i > j$) components and consider them separately. Furthermore, equation (3.1) can be generalized in a straightforward way to the transilient matrix for horizontal transport, $G_{\mu ij}(t)$ discussed in the previous section to yield moments with respect to the destination shells: $\mathcal{M}_{ij}^{(h,n)} = \sum_\mu \mu^n G_{\mu ij}$. In what follows, when computing the horizontal moments and similar quantities, we only consider several selected injection levels for particles, i , and for each only consider destination levels within 5 mass bins of the source ($|i - j| \leq 5$), which we then combine to yield a matrix that is in effect only a function of horizontal displacement, μ , source level, i , and time, t .

The destination means for a collection of tracer particles initially uniformly distributed among mass bins are exhibited in Figure 4 as a function of depth and time for cases 1 and 2. The leftmost plots include both upwardly and downwardly directed particles, while the center and rightmost plots only include those moving upward ($i < j$), and those moving downward ($i > j$) respectively. Consider first the second row of plots, corresponding to the lower resolution run, Case 1. The apparent difference in upward and downward transport can be attributed to the effects of stratification on the velocity field. Large-scale horizontal converging flows near the top of the convection zone sweep particles into strong downflows which persist over several scale heights and transport particles to the base of the convection zone, where the more turbulent conditions and less efficient large-scale vertical transport make a rapid return trip unlikely. Upward moving particles, on the other hand, upon nearing the top of the convection zone, will quickly be swept into strong downdrafts and rapidly reverse direction in roughly half the turnover timescale (depending on their initial height). These tendencies are evident in Figure 4 and, together with the intersections and subsequent crossings of the curves (also evident in the Figure), suggest that the tracer particle transport for Case 1 is dominated by large-scale, overturning motions. This is contrast to the results for the run with higher resolution, Case 2 (upper plots), which show a more homogeneous, less efficient transport which is instead suggestive of smaller-scale eddies. In fact, there seems to

FIGURE 4. The destination means μ_i^d as a function of depth and time for Cases 1 (lower plots) and 2 (upper plots). The left plots include both upward and downward moving particles, while the center and right plots only include particles that come and go from a particular direction (upward and downward, respectively). The initial ($t = 0$) injection of particles is distributed equally among mass shells (not all shells are shown). Recall that the convection zone lies in the range $0 \leq z \leq 1$ in both cases.

be a convergence point for particles in Case 2 just below the middle of the convection zone. However, if we calculate the total number of particles in each level for late times (beginning with a uniform initial distribution) as shown in Figure 5, we see that there is no significant accumulation on this or any level (with the exception of the topmost), so the convergence instead suggests the displacement of particles by incoming ones, and therefore strong mixing. The accumulation and the inefficient mixing for the topmost level (see Figures 4 and 5) imply that once particles are advected into the stably stratified region above the convection zone, they tend to remain there.

The square root of the variance is another measure of the typical particle displacement, or mixing length, measured in *mass bins* if the transilient matrix is so constructed. The upward, downward, and horizontal variances as a function of time at several depths for cases 1 and 2 are shown in Figure 6. The axes are logarithmic so the linear behavior (at least over some time interval) apparent in the plots implies a power law relationship of the form $\sigma^2 \sim t^\beta$. A similar power-law behavior is found for most levels, and the value of

FIGURE 5. Shown is the particle concentration, $\bar{c}_i(t) = \sum_j G_{ij}$, with uniform initial conditions ($\bar{c}_i(0) = 1$) for case 2 at time $t = 21.0$. Notice that it remains close to unity, implying no significant accumulation of particles on any level with the exception of the topmost one.

the best-fit exponents, β , as a function of depth are shown in Figure 7. The fits typically yield a value close to two, with the notable exception of the vertical transport in upper half of the convection zone. As discussed near the beginning of this section, this indicates superdiffusive behavior – “anomalous” diffusion which resembles pure advection in the temporal scaling of the variances.

The relatively large value of β for the downward variance near the top of the layer can be understood if the top layers are modeled as horizontal flows which converge into downward plumes. To see this, note that the downward variance for a collection of tracer particles is given by

$$\sigma_d^2 = \int_0^\infty \zeta^2 N_p(\zeta, t) d\zeta / N_o$$

, where $\zeta = z - z'$, N_o is the (initial or steady state) number of particles in the source level ($\zeta = 0$), and $N_p(\zeta, t)$ is the number of particles located a distance ζ below the source level. If the downflow has a characteristic, approximately constant velocity w_o , then $N_p(\zeta, t)$ will vanish for $\zeta > w_o t$ and will equal $R(t - \zeta/w_o)$ for $\zeta \leq w_o t$, where $R(t)$ is the rate at which particles enter the downflow at $\zeta = 0$. This rate is given by the time derivative of the total number of particles which have entered the downflow after a time t has elapsed, which in turn is given by the (initial or steady state) particle concentration in the source level, c_o , multiplied by the volume of fluid swept up by the downflow, $\pi(u_o t)^2 \Delta z$, where u_o is a typical horizontal velocity scale of the converging flow and Δz is the thickness of the source layer. So, putting this all together, we have, $R(t) = 2\pi u_o^2 \Delta z c_o t$, and

$$\sigma_d^2(t) = 2\pi u_o^2 \Delta z c_o \int_0^{w_o t} \zeta^2 (t - \zeta/w_o) d\zeta \quad (3.4)$$

$$= \frac{1}{6} \pi u_o^2 w_o^3 \Delta z c_o t^4, \quad (3.5)$$

which implies a β of 4. So, converging flows could be responsible for the tendency for β to increase for downward moving particles near the top of the convection zone, where

FIGURE 6. The upward (dotted lines), downward (dashed lines), and horizontal (solid lines) variances, or mean square particle displacements, are shown for cases 1 and 2 as functions of time for a layer within the convection zone, another in the stable region below it, and another at their interface (note that the vertical displacements are measured in mass levels, which vary with depth but are comparable to the vertical grid spacing, while the horizontal variances are in terms of the horizontal grid spacing).

FIGURE 7. Best-fit power law exponents which satisfy $\sigma^2 \propto t^\beta$ as a function of depth. A β value of two corresponds to advective behavior, while $\beta = 1$ implies classical diffusion.

such flows may dominate the horizontal transport. The small values of β for the upward variance near the top can be attributed to the flattening of the $\sigma^2(t)$ curve as particles reach the top of the convection zone and turn around (see Fig. 6).

The kurtosis is a good quantitative measure of the shape of the distribution function, and its upward, downward, and horizontal components are exhibited as a function of depth and time in Figures 8 and 9. The kurtosis values, especially those in the horizontal and upward directions, are found to be relatively independent of time. The mid

FIGURE 8. Plots analogous to Figure 5, showing the kurtosis in the upward, downward, and horizontal directions, κ , represented by dotted, dashed, and solid lines respectively, for cases 1 and 2 at three selected levels in the computational domain. The cutoffs at early times are imposed because there are initially too few levels populated (< 5) to give a reliable result. Classical diffusion yields $\kappa = 3$.

FIGURE 9. The kurtosis in the upward (dotted lines), downward (dashed lines), and horizontal (solid lines) directions are shown as a function of depth for cases 1 and 2 at a time $t = 16.8$. The cutoffs for the upward kurtosis near the top of the convection zone and the downward near the base, again, are imposed because at levels closer to the boundaries, there are too few data points to give a reliable value.

convection zone for the higher resolution data, for example, shows a variation of the kurtoses of less than 25% (see Fig. 8), over a time interval in which the variances increase by three or four orders of magnitude (see Fig. 6). The kurtoses therefore provide a useful quantitative measure for the shape of the transient matrix as it evolves away from the diagonal. The value $\kappa = 3$ is expected for diffusive processes and $\kappa = 1$ characterizes pure advection at a specific velocity. The large downward kurtoses just below the base of the convection zone indicate the relative importance of extreme events, wherein

relatively few particles go on long excursions into the stable region below and enhance the tails of the distribution functions relative to the cores (and similarly for the peaks in the upward kurtosis just below the convection zone). Note that the maximum in the downward kurtosis tends to lie slightly below the base of the convection zone for case 1 and slightly above the base for case 2, which has higher stratification and a smaller penetrative region. These results may have important implications for the problem of light element depletion in the Sun and other stars (see §3.4).

3.2. A Generalized Diffusion Equation

As mentioned above, a common approach to the study of transport in fluids centers around a Taylor expansion of equation (1.3), which yields turbulent diffusion and advection together with terms involving higher order derivatives of the tracer concentration, c . If the correlation length l of the velocity field is small compared to the gradient lengthscale D of the system, the magnitude of these terms will in general decrease with increasing order as powers of l/D . One must still compute the coefficients of the Taylor expansion up to the order at which they become insignificant. The information with which to do this is captured in the transilient matrix and can be extracted by following Van Beijeren (1982). The first step is to write the Fourier transform of the Green function (here we use the continuous version, $G(z, z', t, t')$, for simplicity) as

$$\tilde{G}(k, z', t) = \int e^{-ik\zeta} G(\zeta, z', t) d\zeta = \langle e^{-ik\zeta} \rangle, \quad (3.6)$$

where z' and z are again the source and destination depths (corresponding to levels i and j in the transilient matrix; see eqn 2.2), $\zeta = z - z'$ and the angular brackets denote an average over all particles. The Green function can then be expanded in the Taylor series for eqn. 3.4 and written as follows:

$$\tilde{G}(k, z', t, t') = \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \langle \zeta^n \rangle \quad (3.7)$$

$$= \exp\left(\sum_1^{\infty} (ik)^n \chi_n / n!\right), \quad (3.8)$$

where the χ_n are cumulative moments, which can be found by equating like powers of k in the two series (3.5) and (3.6) (see Van Beijeren 1982):

$$\chi_1 = -\langle \zeta \rangle \quad (3.9)$$

$$\chi_2 = \langle \zeta^2 \rangle - \langle \zeta \rangle^2 \quad (3.10)$$

$$\chi_3 = -\langle \zeta^3 \rangle + 3\langle \zeta \rangle \langle \zeta^2 \rangle - 3\langle \zeta \rangle^3 \quad (3.11)$$

$$\dots \quad (3.12)$$

Taking a time derivative and applying an inverse Fourier transformation to eqn. (3.6) then yields:

$$\frac{\partial G(z, z', t, t')}{\partial t} = \sum_{n=1}^{\infty} T_n(z', t, t') \frac{\partial^n G(z, z', t, t')}{\partial z^n}, \quad (3.13)$$

where the transport coefficients are given by

$$T_n = \frac{1}{n!} \frac{\partial \chi_n}{\partial t}. \quad (3.14)$$

Again, in the spirit of the Green function formalism, an expansion in terms of these transport coefficients yields the particle fluxes that would arise in terms of local deriva-

tives of the concentration if the initial concentration were a delta function at level z' . Thus, the time derivative of the concentration for an arbitrary initial condition is again a sum over all the individual contributions:

$$\frac{\partial \bar{c}(z, t)}{\partial t} = \int \sum_{n=1}^{\infty} T_n(z', t) \frac{\partial^n G(z, z', t) \bar{c}(z', 0)}{\partial z^n} dz', \quad (3.15)$$

and if the T_n are independent of depth (which means that the flow is statistically uniform with depth, this reduces to the more familiar, but less general equation,

$$\frac{\partial \bar{c}(z, t)}{\partial t} = \sum_{n=1}^{\infty} T_n(t) \frac{\partial^n \bar{c}(z, t)}{\partial z^n}. \quad (3.16)$$

Whether the transport coefficients can be taken outside the integral or not, the right hand side of eqn. (3.15) is in the form of the divergence of a generalized flux, as expected for a conservation law. Similar relations also hold for horizontal transport, but note that the assumption of isotropy inherent in our approach implies that the only nonzero horizontal transport coefficients are those with n even.

FIGURE 10. The transfer coefficients T_1 , T_2 , and T_3 (solid, dotted, and dashed lines respectively) describing vertical transport as a function of depth are shown in the upper plots for cases 1 and 2 at a time $t = 3.36$. All are normalized with respect to their maximum values. The lower plots show the normalized values of T_2 , T_4 , and T_6 (solid, dotted, and dashed lines) corresponding to horizontal transport for the same data sets and time.

The first three nonzero transport coefficients in both the vertical and horizontal directions for cases 1 and 2 are exhibited in Figure 10 as a function of source depth at time $t = 3.36$. Note that, for the horizontal transport, only 13 and 14 depths were chosen respectively out of the 63 and 105 available for the two different runs, so the curves are not complete, but do show a definite tendency for the coefficients, especially those of higher order, to decrease with depth. This decrease is expected because the characteristic horizontal velocity decreases with increasing density, although the relative decrease of the higher order coefficients is not a priori obvious and indicates a relatively more diffusive behavior for the larger depths. The first vertical coefficient can be regarded as a typical advection velocity, and shows positive and negative values in the upper and lower regions

FIGURE 11. The magnitude of the transfer coefficients, $|T_n|$, averaged over depth for both resolutions at time $t = 3.36$, as a function of order, n (plotted on log-linear axes). Results are shown for both vertical (asterisks) and horizontal (diamonds) transport. Recall that $T_n = 0$ by assumption for n odd in the horizontal case.

of the convection zone. Note that the secondary peaks in several of the coefficients just below the interface with the stable region indicates a typical scale at which downward plumes penetrate, then turn around and transport particles back upward. This is also apparent in the mean plots above (Figure 4). The typical magnitude for the transfer coefficients, $|T_n|$, averaged over depth for the same times as shown in Figure 10, are plotted in Figure 11 (log-linear) as a function of order, n . For both vertical and horizontal transport, the expansion of equation (3.15) is found to converge exponentially with increasing n . The relative dominance of the T_1 coefficient indicates that the vertical transport is more advective than diffusive, as we showed in Figure 6.

3.3. Nonlocal Fluxes and other Measures

Other useful non-local transport measures are obtained from the transilient matrix by summing the total particle fluxes across particular levels which arise from particle displacements of a specified length Stull (1993). Thus, we define upward and downward “eddy fluxes” as follows:

$$F_{k\ell}^{up}(t, t') = \sum_{i=k}^{N_z} \sum_{j=0}^k G_{ij}(t, t') \delta_{\ell(i-j)} \quad (3.17)$$

and

$$F_{k\ell}^{dn}(t, t') = \sum_{i=0}^k \sum_{j=k}^{N_z} G_{ij}(t, t') \delta_{\ell(j-i)}. \quad (3.18)$$

These fluxes can be roughly associated with the scale, ℓ , of eddies that transport particles through the level k , although that identification is somewhat ambiguous because “eddies” of a given size would contribute to eddy fluxes at all smaller scales at time intervals which are not nearly multiples of the turnover time of that particular eddy. Still, they can give some useful information on the typical scale of mixing across a given level. We are interested in associating ℓ with a real physical length scale, so in calculating equations (3.17) and (3.18) from the simulation data, we use layers of constant volume rather than constant mass. It is therefore necessary to evolve the particles to a statistically steady state before initializing the matrices to avoid the transient initial large downward flux of particles that occurs with stratified flows when volume shells are used. From the above quantities, we can also define the net upward flux,

$$F_{k\ell}^{net}(t, t') = F_{k\ell}^{up}(t, t') - F_{k\ell}^{dn}(t, t'), \quad (3.19)$$

and the mixing intensity,

$$I_{k\ell}(t, t') = F_{k\ell}^{up}(t, t') + F_{k\ell}^{dn}(t, t'). \quad (3.20)$$

FIGURE 12. Shown are the upward, downward, and net particle flux (dotted, dashed, and solid lines respectively) after the particle concentration has reached a roughly steady state ($t = 78.9$) for layers within, below, and at the base of the convection zone for Case 2. The abscissa is the “eddy size”, ℓ , as defined in equations (3.17) and (3.18)

Figure 12 shows the upward, downward, and net particle flux for several layers (using the lower resolution data, Case 1) as a function of “eddy size”, ℓ , as defined in equations (3.17) and (3.18). Note that the upward flux tends to peak at somewhat smaller values of ℓ relative to the downward flux, leading to a net upward flux which is positive (negative) for small (large) particle displacements. There is virtually no upward flux carried by eddies which exceed the size of the convection zone, $\ell \gtrsim 1$, although a significant amount of downward transport occurs on these scales. In other words, particles beginning in the convection zone often end up in the stable layer, but rarely does the converse happen.

The mixing intensity (not shown in the figure) peaks at fairly large eddies, typically about 70 - 80% of the depth of the convection zone.

FIGURE 13. The curves in each frame represent the fraction of particles which travel upward (dotted line), those which travel downward (dashed line), and those which stay at the same level (solid line) as a function of depth after a steady state has been reached ($t = 17.64$). Both cases 1 and 2 are shown.

We can also use the transient matrix to answer a simpler question about the nature of particle transport; upon injecting particles at a particular source level, what fraction of them are transported upward and downward as a function of time (here we return to the use of mass levels for vertical binning)? Denoting the fraction of particles which go upward, downward, and stay on the same vertical level, i , as $f_i^{up}(t, t')$, $f_i^{dn}(t, t')$, and $f_i^{sm}(t, t')$ respectively, we have

$$f_i^{(up)}(t, t') = \sum_{j=1}^{i-1} G_{ij}(t, t'), \quad (3.21)$$

$$f_i^{(dn)}(t, t') = \sum_{j=i+1}^N G_{ij}(t, t'), \quad (3.22)$$

and

$$f_i^{(sm)}(t, t') = G_{ii}(t, t') = 1 - f_i^{up}(t, t') - f_i^{dn}(t, t'). \quad (3.23)$$

These quantities tend to reach a steady state by about half the convective turnover time and the steady state values are plotted in Figure 13 as a function of depth. In both cases 1 and 2, the level in the convection zone which separates generally upward moving particles from downward moving ones lies below the middle, and is actually at a slightly larger depth for Case 1, which has a lower resolution and lower stratification, but a larger penetrative layer. The relative proximity of the lower boundary, aided possibly by the higher stratification, for Case 2 also seem to suppress the secondary peak in f^{dn} seen in case 1 below the base of the convection zone (this downward transport is also discernible in the mean plots, Fig. 4). Thus, it seems that the influence of the lower boundary (likely due to the reflection of gravity waves) extends deep into the computational domain and a realistic study of mixing near the base of the convection zone requires a relatively large penetrative region (at least as deep as the convection zone itself). However, this required extent should decrease with increasing stratification.

3.4. The Evolution of Structures

Since the transient matrix is in effect a Green function, then the temporal evolution of an arbitrary initial concentration can be followed by applying the simple matrix multi-

plication described by eqn (2.1). If we wish to use the continuous version of the matrix, $G(z, z', t, t')$ (see eqn 2.2 and the corresponding discussion), then we can rewrite that equation as

$$\bar{c}(z, t) = \int G(z, z', t, t') \bar{c}(z', t') dz'. \quad (3.24)$$

Now we wish to consider in a similar manner the temporal evolution of axisymmetric structures using the modified transilient matrix described above, $G_{\mu ij}(t, t')$ (recall that this matrix represents the fraction of particles which begin at time t' on the level j and end up on the level i at time t , after having traveled a horizontal distance μ). Again, for simplicity, we will consider the continuous analogue of the matrix, which we denote as $G(r, z, z', t, t')$, and we wish to obtain from this a related function, $\hat{G}(r, r', z, z', t, t')$, such that

$$\hat{c}(r, z, t) = \int \int \hat{G}(r, r', z, z', t, t') \hat{c}(r', z', t') dr' dz', \quad (3.25)$$

where $\hat{c}(r, z, t)$ is the three dimensional concentration, $c(x, y, z, t)$, in cylindrical coordinates (with an arbitrary origin for r), integrated over rings of infinitesimal thickness: $\hat{c}(r, z, t) = \int_0^{2\pi} c(r, \theta, z, t) r d\theta$. To this end, we first note that the distance between two arbitrary points on the same horizontal plane, one a distance r from the axis of symmetry ($r = 0$), the other a distance r' is just $\sqrt{r^2 + (r')^2 - 2rr' \cos \theta}$, where θ is the angle between the vectors $\mathbf{r}$ and $\mathbf{r}'$. So the total contribution from an axisymmetric impulsive source, $\delta(r')$, is obtained by a superposition of the contributions from all differential volume elements at the source radius, r' , given the original matrix, $G(r, z, z', t, t')$, and again assuming horizontal homogeneity:

$$\hat{G}(r, r', z, z', t, t') = \int_0^{2\pi} G(\sqrt{r^2 + (r')^2 - 2rr' \cos \theta}, z, z', t, t') d\theta. \quad (3.26)$$

For classical diffusion in two unbounded dimensions,

$$\hat{G}(r, r', z, z', t) = (\pi \sigma_D)^{-2} \exp(-(r^2 + (r')^2)/\sigma_D^2) I_0\left(\frac{2rr'}{\sigma_D^2}\right). \quad (3.27)$$

where I_0 denotes a modified Bessel function of the first kind (Abramowitz & Stegun 1972), $\sigma_D = \sqrt{4Dt}$, and D is the diffusion coefficient. In practical applications, to spare computer memory and to make the computation of equation (3.26) more efficient, we often consider only destination levels close to the source level so that $|z - z'|$ is small (or, in terms of the mass level indices introduced in Section 2, $|i - j|$ is small. Typically, we include 11 levels, centered around the source level; see section 2). The temporal evolution of slices through several source levels of the modified Green function, $\hat{G}$ is shown in Figure 14 for both Case 2 (Case 1 is similar) and for classical diffusion, the latter being obtained from equation (3.27). At source shells near the origin, the simulations tend to resemble advection rather than diffusion, although the opposite is the case for source shells at larger radii.

An alternative way to describe the time evolution of vertical structures (in a rectangular geometry) which can potentially provide insight into the scale properties of the transport is by introducing a Green function in Fourier spaces, $\tilde{G}(k, k', t, t')$, which is obtained from the Green function $G(z, z', t, t')$ in physical space and which describes the decay and mixing of different Fourier components such that

$$\bar{c}(k, t) = \int \tilde{G}(k, k', t) \bar{c}(k', 0) dk'. \quad (3.28)$$

The transformed Green function can be obtained from the original one by first multiplying

FIGURE 14. Several cross sections through the horizontal Green function, $\tilde{G}(r, r', t)$ for different source shells, r' . The upper plots show the result for classical diffusion, obtained from equation (3.27), while the lower plots show the data for Case 2 at a representative source level within the convection zone ($z' = 0.480$), computed using the transient matrix via equation (3.26). Each frame includes the following snapshots: $t = 0.21, 0.42, 0.63, 1.05, 1.89, 3.57, 6.93$, and 13.65 (the initial, $t = 0$, profile is a delta function at $r = r'$). Progressively more disperse curves correspond to later times.

both sides of eqn (3.24) by $\exp(ikz)$, integrating over z , and introducing the equations which define the Fourier Transformation:

$$\bar{c}(k, t) = \int_{-\infty}^{\infty} \bar{c}(z, t) e^{ikz} dz \quad (3.29)$$

and

$$\bar{c}(z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{c}(k, t) e^{-ikz} dk. \quad (3.30)$$

The result is

$$\tilde{G}(k, k', t, t') = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(z, z', t, t') e^{ik(z-z')} dz dz'. \quad (3.31)$$

So, the Green function describing the evolution of Fourier components through equation (3.28), $\tilde{G}(k, k', t, t')$, is given by applying a Fourier transformation with respect to the destination (first) index of the original Green function, $G(z, z', t)$, and an inverse transformation with respect to the source (second) index. The real (imaginary) diagonal terms, where $k = k'$, describe the decay of individual cosine (sine) modes, the imaginary (real) diagonal terms describe phase shifts, and the off-diagonal terms, where $k \neq k'$, describe mode mixing.

This approach is most useful when the system to be described is periodic in the z (in this case, the vertical) direction. This does not apply the simulations presented here, however, because the stratification and the transition between convectively stable and

unstable regions break the symmetry and therefore limit the utility of the analysis in terms of Fourier modes. We therefore present the method here only for its potential interest. Similar eigenfunction expansions are also possible for other geometries.

3.5. Transport with Sinks: Light Element Depletion in Stars

It is well established that the abundances of light elements (Li, Be, and B) in the photospheres of stars with convective envelopes are reduced below interstellar abundances (e.g. Zahn 1994; Schatzmann & Baglin 1991). This deficiency is often addressed by invoking mixing processes which occur during the star's main sequence lifetime and which transport light elements from the envelope to the interior, where they are efficiently burned. The layer at which this burning occurs typically lies at least several pressure scale heights below the base of the convection zone, and the depletion therefore occurs on timescales longer than convection timescales, although convective overshoot may play a significant role, at least in stars of solar and earlier type (Straus, Blake, & Schramm 1976; Christensen-Dalsgaard, Gough, & Thompson 1992). Light element depletion therefore provides an important diagnostic tool for studying mixing properties in the interiors of main sequence stars.

If we identify light elements as passive tracer particles, which is well justified by their low abundance, then the transilient matrix framework is directly applicable to the depletion problem. In this context, we are especially interested in transport in the stable, penetration region below the convection zone. As noted above (section 2.1), the kurtosis associated with the downward transport of tracers near the base of the convection zone is very large, which indicates a relatively large number of extreme events - that is, it is relatively common for particles to be sent deep into the radiative interior, where light elements would be burned. The peak in the fraction of particles moving downward for the run with the larger penetrative region, Case 1, (see Fig. 13) also suggest that penetrative convection can efficiently transport particles into the stable region. Thus, the transport of elements from the convection zone to the deep interior through convective overshoot and the gravity waves it generates could be much more efficient than naively expected based on diffusive or other simple models.

FIGURE 15. Depletion, D , in Case 1, as a function of time for several chosen burning layers; $l = 1.09, 1.27, 1.42, 1.55, 1.67, 1.78, 1.88$, and 1.96 (recall that the base of the convection zone lies at a depth of 1.0). Curves with lower depletion values correspond to lower burning layers (i.e. those at larger depths, z). Also shown are the scaling results predicted for Depletion by classical diffusion ($D \sim t^{1/2}$) and by pure advection ($D \sim t$).

The problem of light element depletion can be treated in a more quantitative manner using the transilient matrix as follows. Since reaction rates are very sensitive to tem-

FIGURE 16. The logarithmic Derivative, $\partial \ln(\mathcal{D})/\partial \ln(t)$, of the depletion with respect to time for case 1 for several different choices of the burning layer, z_λ . The results expected for simple advection and diffusion are overplotted with dashed and dotted lines respectively.

perature, we can approximate the burning layer as a discontinuity, so that particles are destroyed the moment they cross some fiducial level below the convection zone, and the tracer concentration below that level is zero for all time. A first approximation to the depletion rate, for an initial concentration of particles uniformly distributed among mass bins above the burning layer is then just given by the probability that particles initially above the burning layer, λ , are found below it at time t :

$$\mathcal{I}_\lambda(t) = \sum_{i=\lambda+1}^N \sum_{j=1}^{\lambda} G_{ij}(t). \quad (3.32)$$

Recall that the subscripts i and j represent vertical levels, which increase downward, and range between 1 and the total number of levels, N . The tracer concentration drops to zero below the burning level, where $i, j > \lambda$. Equation (3.32) only represents a lower limit to the depletion rate because it does not take into account those particles whose trajectories took them below the burning layer and then back, so that they are again above the layer at time t . These particles would also have been destroyed, so we must include them also in the depletion rate. The probability of such a trajectory is given by

$$\mathcal{J}_\lambda(t) = \int_0^t \sum_{i=\lambda+1}^N \sum_{j=1}^{\lambda} \sum_{k=1}^{\lambda} G_{ij}(t') G_{ki}(t-t') dt'. \quad (3.33)$$

Of course, there may also be particles which have crossed the burning layer more than twice, repeatedly dipping into the burning region and then back out, and these should strictly be accounted for as well. However, provided the time interval isn't too long, such trajectories are relatively improbable and can be neglected as a first approximation. The

total depletion rate as a function of time and the location of the burning layer is therefore

$$\mathcal{D}_\lambda(t) = \frac{\mathcal{I}_\lambda(t) + \mathcal{J}_\lambda(t)}{\sum_{i=1}^N \sum_{j=1}^\lambda G_{ij}}. \quad (3.34)$$

The normalization by the denominator in equation (3.34) (which is independent of time if particles are conserved) ensures that the depletion lies between zero and unity (with some extra care in implementation to ensure probabilities do not exceed unity), and is therefore a fractional measure. Figure 15 shows the total depletion rate as a function of time in Case 2, for several different burning layer locations. The temporal scaling of the depletion expected for simple advection and classical diffusion are also shown in the picture and indicate that the simulation results give more rapid depletion than either model. This is shown more clearly in Figure 16, where the quantity $\partial \ln(\mathcal{D})/\partial \ln(t)$ is plotted as a function of time for burning layers at several different locations below the convection zone.

The transport of particles into the penetrative region is likely due to the presense of gravity waves. Knobloch & Merryfield have shown that particle trapping in traveling gravity waves and the buildup of large gradients in standing waves (which may be present in the simulations because of the reflective boundary conditions) can lead to enhanced transport. A better understanding of the role of gravity waves and of transport in penetrative convection in general would benefit from further simulations that vary the depth of the penetrative region, or with boundary conditions that allow for the radiation of gravity waves. Several models for light element depletion by the action of internal waves have already been proposed (Montalbán 1994; Schatzmann 1993).

Although our results seem promising for shedding some light on the problem of light element depletion in stars, their importance should not be overemphasized. Numerical simulations of convection such as these are limited by the resolution attainable in practice, so the Reynolds numbers are necessarily too small (molecular viscosities relatively too large) to correspond directly to the situation in stars, and this could tend to overestimate the importance of convective overshoot (Zahn 1994). Furthermore the pressure scale height, which increases with depth, has a value at the base of the convection zone, in the dimensionless units used here, of 0.62 for case 1 and 0.50 for case 2. This is far larger relative to the extent of the convection zone than is the case in actual stars. A larger stratification would likely lead to relatively stronger horizontal turbulence, which could in turn inhibit particle transport (Vincent et al 1996).

Still, our results suggest that penetrative convection in general may be more efficient in transporting tracer particles into the overshoot region than suggested by estimates involving diffusion (reviewed by Michaud & Charbonneau 1991) or by naively extending the “effective” (in terms of chemical homogenization) convection zone as in the *extra mixing* models of D’Antona & Mazzitelli (1984).

4. Conclusions

The transilient matrix method is a Green function approach (with the initial condition playing the role of the source term) to describing the non-diffusive, non-local transport of passive tracer particles in fluid flows. It is more general and more accurate than the more common and simpler parameterizations of turbulent transport in terms of *eddy* or *turbulent* diffusivities and similar expansion coefficients and it (or another non-local approach) may be required in some astrophysical and geophysical scenarios where long-range correlations or broad velocity distribution functions exist and such local parameterizations

break down. The method was originally developed by Stull and collaborators (Stull 1984; Ebert et al. 1989; Stull 1993) and applied by them to large-eddy simulations of atmospheric convection.

In this paper, we have developed further some of the diagnostic capabilities of the matrix, have presented a more efficient (but less rigorous) method of calculating it based on following the trajectories of tracer particles, and have applied the approach for the first time to astrophysical flows; to several numerical simulations of compressible, stratified, MHD, rotating, convective turbulence with overshoot in a three-dimensional rectangular geometry. Our primary purpose is not to provide an alternative turbulence model, but rather to use the matrix as a quantitative descriptor of flow properties and a useful tool in addressing specific transport questions such as the means of light element depletion in stars and the dispersal of chemical tracers having some arbitrary initial distribution. The method is therefore quite general and can be applied to a wide range of flow systems and processes. However, as with any such tool, it must be remembered that its utility with regard to real physical systems is limited by the applicability of the numerical simulations themselves.

In computing the matrices, we have used both snapshots of the velocity field and velocity fields incorporating the full time dependence of the governing MHD equations and find little difference in the results between otherwise identical runs.

To describe vertical transport, we in general chose to bin the matrix in layers of constant mass to take into account the anisotropic effects of the density stratification. Vertical transport in the lower resolution run, case 1 (see Table 1), is found to be dominated by large-scale, overturning motions, (see Fig 4 and the associated discussion), with downward transport typically occurring on scales comparable to the size of the convection zone, and upward transport typically associated with relatively smaller eddies (see Fig. 12). Case 2, on the other hand, which had a higher resolution and higher stratification, is dominated by transport on smaller scales, although downward transport is still associated with relatively larger scales than upward transport.

In all cases considered, the turbulent transport is found to be more advective than diffusive, as indicated by the temporal scaling of the variance in particle displacements following their injection on a particular source level (see Figures 6 and 7). This is also true for the temporal scaling associated with horizontal transport, which is less sensitive to the source depth. The non-diffusive, asymmetric, and advective nature of the transport is also suggested by examining qualitatively the matrices themselves in Figures 1, 2, and 14. Nonlocal transport coefficients were computed (Fig. 10) which relate the temporal derivatives of the concentration (and thereby particle fluxes) to spatial derivatives of the Green function and are found to converge exponentially with increasing order of the derivatives (Fig. 11). This convergence again suggests that advective transport is relatively more pronounced than diffusive. The advective nature of transport in the convection zone is likely due to the presence of vertical plumes and coherent, converging and diverging horizontal flows. Advective transport in the penetrative layer could be due to particle trapping in gravity waves (see section 3.4). Interestingly, the usual reason advanced for success of the local approximation, namely that the velocity correlation length is small, is not borne out by our calculations of the nonlocal fluxes, which show that vertical transport is dominated by large eddies (see Figure 11).

The normalized fourth moment, or kurtosis, with respect to either destination or source indices, often remains approximately invariant as the transilient matrix evolves in time and therefore provides a good quantitative descriptor of that evolution. For horizontal transport, the kurtosis tends to lie close to the value 3 for all source depths, which is the result predicted by classical diffusion, in contrast to vertical transport, where it is strongly

depth dependent. In both cases 1 and 2, the kurtosis describing downward transport has a strong peak near the base of the convection zone (of order 20), indicating the importance, relative to diffusion, of long-range displacements deep into the stable region. If the tracer particles are identified with light elements in stars, then this suggests that the depletion of those elements by transporting them deep into the radiative interior where they are burned is more efficient than would be expected for diffusive processes. Indeed, when the depletion is calculated using the transilient matrix (section 3.4), it is found to increase in time more rapidly than predicted by either diffusion or simple advection. Thus, penetrative convection may play a significant role in light element depletion even when the layer at which the elements are burned lies several pressure scale heights below the convection zone. However, the limitations of computer simulations in general make direct application of these results to actual stars somewhat uncertain, although more work in this area seems justified.

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