

NOTES AND CORRESPONDENCE

The Relationship between the Transilient Matrix and the Green's Function for the Advection-Diffusion Equation

VINCENT E. LARSON

Program in Atmospheres, Oceans, and Climate, Massachusetts Institute of Technology, Cambridge, Massachusetts

19 March 1998 and 10 March 1999

ABSTRACT

The Green's function (or propagator) of the advection-diffusion equation is used to link the transilient matrix to the advection-diffusion equation. The Green's function framework allows one to construct more rigorous and general derivations of various mixing properties of the transilient matrix. Unlike the transilient matrix or one-dimensional convective parameterizations, the Green's function satisfies a composition property that allows a long-time propagator to be constructed from a series of short-time propagators.

1. Introduction

Many problems in meteorology involve fluid-mechanical mixing.¹ For example, the dynamics of a cumulus cloud is strongly influenced by (and strongly influences) the rapidity with which clear, dry air surrounding the cloud mixes into the cloud itself. Evaporative cooling occurs when, and only when, the mixing has proceeded to the molecular level. In this way, mixing at the finest cloud scales affects dynamics at the largest cloud scales. Another problem in which mixing is fundamental is the dispersal of pollutants emitted by a smokestack.

It is useful to place such mixing problems within a general theoretical framework, such as transilient matrix theory (Stull 1984, 1986, 1993; Stull and Hasegawa 1984). In this framework, the fluid domain is conceptually partitioned into disjoint, overlying horizontal slabs, or grid boxes. The transilient matrix is an array of numbers $G_{ij}(t; t')$ that represents tracer transport among the slabs between an initial time, t' , and a final time, t . To be more precise, we consider an ensemble, each member of which consists of a particular flow field and a particular initial dye distribution. Given the tran-

silient matrix and the ensemble-averaged tracer mixing ratio in the j th slab at the initial time, $\bar{c}_j(t')$, then the ensemble-averaged tracer mixing ratio in the i th slab at the final time, $\bar{c}_i(t)$, is computed from the matrix equation (Stull 1993):

$$\bar{c}_i(t) = \sum_{j=1}^N G_{ij}(t; t') \bar{c}_j(t'). \quad (1)$$

Here N denotes the number of slabs in the vertical, and an overbar denotes an ensemble average.

Stull (1984) and Ebert et al. (1989) offer a second definition of the transilient matrix in which the ensemble averages in (1) are replaced by slabwise spatial averages, and only a single realization of a flow is considered. According to the ergodic hypothesis, if the flow is statistically homogeneous in the horizontal, then as the slabs increase in horizontal extent and thereby encompass more eddies, the two definitions of the transilient matrix become equivalent. Operationally, the transilient matrix has been constructed as follows. A single realization of a flow is computed by a large eddy simulation model. At the initial time, tracers are spread *uniformly* throughout the slabs, using a different tracer for each slab. Then the transilient matrix is diagnosed from the amounts of the various tracers in each slab at the final time (Ebert et al. 1989). This operational definition of the transilient matrix can be thought of as a special case of the second definition, namely, the case in which the initial tracer distribution has no fluctuations within a slab. The operational definition thereby precludes the possibility of intraslab correlations between the initial tracer fluctuations and the flow. Because of this, the operational definition is not entirely equivalent

¹ In this paper, the term "mixing" shall subsume advection of material surfaces (i.e., transport) as well as tracer diffusion across material surfaces.

Corresponding author address: Vincent E. Larson, Cooperative Institute for Research in the Atmosphere, Colorado State University, Fort Collins, CO, 80523-1375.
E-mail: larson@cira.colostate.edu

to the first two definitions. The operational definition is, however, closely related to the statement in Stull (1993) that the transilient matrix is a matrix whose ij th element represents “the fraction of *air* mixed into a destination grid cell at vertical location index i from a source grid cell at location j ” (the italics are ours). This statement is in conformity with the operational definition of the transilient matrix, except that a tracer is not an exact marker of material fluid elements, since a tracer may diffuse from one element to another. This paper shall adhere to the first definition of the transilient matrix, given by (1).

Stull (1993) uses physical arguments to deduce various properties of $G_{ij}(t; t')$. For instance, Stull (1993) writes that each column of G_{ij} sums to unity,

$$\sum_{i=1}^N G_{ij}(t; t') = 1, \quad (2)$$

because “all of the air initially within each grid box must go somewhere.” Similarly, Stull (1993) writes that each row of G_{ij} also sums to unity,

$$\sum_{j=1}^N G_{ij}(t; t') = 1, \quad (3)$$

because “100% of the air at each destination must have come from somewhere.”

The transilient matrix is more general than traditional eddy diffusivity formulations. An eddy diffusivity relates the tracer flux at a point in space to the *local* gradient in tracer concentration. In contrast, the transilient matrix relates the tracer profile at a final time, t , to the full, *nonlocal* tracer profile at an initial time, t' . Sometimes a local description of mixing fails. For instance, a planetary boundary layer whose interior lapse rate is adiabatic may be either convecting or not, depending on whether the lapse rate near the earth’s surface is superadiabatic or subadiabatic, respectively. Therefore, the interior lapse rate does not provide enough information to determine the interior vertical flux of potential temperature.

Stull (1993) has elucidated the physical content of the transilient matrix, but the following two questions may be raised. First, although the transilient matrix provides a fairly complete description of mixing, ultimately the mixing of a tracer is governed by the advection-diffusion equation; therefore, we may ask, can one find a rigorous connection between the transilient matrix and the advection-diffusion equation? Second, we may ask, how can the transilient matrix formalism be generalized to include sources of tracers and various tracer boundary conditions?

The bridge between the transilient matrix and the advection-diffusion equation is the Green’s function of the advection-diffusion equation. Stull (1993) notes that the transilient matrix “is essentially a Green’s function (Morse and Feshbach, 1953) matrix.” We shall demonstrate the more specific fact that, under several im-

portant restrictions, the transilient matrix is proportional to the ensemble-averaged advection-diffusion Green’s function. Use of Green’s functions permits us to rederive formulas (1), (2), and (3) with greater rigor and generality. Sobel (1997, 1999) has also related the transilient matrix to the advection-diffusion equation via a route in which he immediately discretizes the advection-diffusion equation. Unlike Sobel (1997, 1999), our derivation starts with a more general flow, does not discretize the advection-diffusion equation, and employs the Green’s function for the advection-diffusion equation.

Many prior authors have used Green’s functions to study mixing. For example, Holzer (1999) has used a coarse-grained Green’s function to study tropospheric transport of tracer in a general circulation model. Lin and Hildemann (1997) and references therein examine statistically steady-state turbulent dispersion in the atmospheric boundary layer. Phillips and Kaye (1996) study shear dispersion, and Fennel (1981) examines oceanic turbulent dispersion. Hamba (1995) uses the Green’s function of a horizontally averaged advection-diffusion equation to study nonlocal mixing in a large eddy simulation of an atmospheric boundary layer. The use of Green’s functions in the direct-interaction approximation (DIA) of Kraichnan (1959) is discussed in the text by Leslie (1973). Roberts (1961) applies DIA techniques to the turbulent dispersion problem with molecular diffusivity neglected. The review of Stull (1993) contains many references on transilient matrix theory and other approaches to mixing problems.

2. Development of the Green’s function framework

We consider an advection-diffusion equation of the form (see Gill 1982, 84)

$$\rho(\mathbf{x}, t) \frac{\partial c(\mathbf{x}, t)}{\partial t} + \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \nabla c(\mathbf{x}, t) - \nabla \cdot [\rho(\mathbf{x}, t) \kappa \nabla c(\mathbf{x}, t)] = \rho(\mathbf{x}, t) s(\mathbf{x}, t). \quad (4)$$

Here $c(\mathbf{x}, t)$ is the mixing ratio of tracer with units of mass of dye per mass of fluid. We shall use the term “tracer” and the more vivid term “dye” interchangeably. The function $s(\mathbf{x}, t)$ is a source of dye, such as a smokestack, specified as a function of space and time. The quantities \mathbf{u} , ρ , and κ denote a specified velocity field, fluid density, and (molecular) tracer diffusivity, respectively; then the advection-diffusion equation for $c(\mathbf{x}, t)$ is linear. The velocity field \mathbf{u} may be interpreted as the full velocity field down to the smallest fluid scale. Alternatively, it is easy to generalize the tracer diffusivity to include a space and time dependence; if we do so, we can interpret \mathbf{u} and κ as the large-scale velocity field and eddy diffusivity field output by a large eddy simulation. As a third alternative, one can even use a \mathbf{u} field that does not satisfy the Navier–Stokes equation.

The fluid is fully compressible and is enclosed within a volume V bounded by a surface S . We do not permit advection of dye through the boundary, although we do permit diffusion of dye through the boundary in some cases. The boundary may be removed to infinity. The time variables shall be ordered as follows, except when they are used as dummy variables of integration:

$$t'' < t' < t < t_j.$$

The variable τ shall denote an additional dummy variable of time integration.

The Green's function $G(\mathbf{x}, t; \mathbf{x}', t')$ is defined by the equation

$$\begin{aligned} \rho(\mathbf{x}, t) \frac{\partial G(\mathbf{x}, t; \mathbf{x}', t')}{\partial t} + \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \nabla G(\mathbf{x}, t; \mathbf{x}', t') \\ - \nabla \cdot [\rho(\mathbf{x}, t) \kappa \nabla G(\mathbf{x}, t; \mathbf{x}', t')] = \delta^3(\mathbf{x} - \mathbf{x}') \delta(t - t'), \end{aligned} \tag{5}$$

where δ denotes the Dirac delta function. The $G(\mathbf{x}, t; \mathbf{x}', t')$ field may be taken to represent a "dye," which we shall call "G-dye." Comparison of (5) and (4) shows that G-dye is like the dye $c(\mathbf{x}, t)$, except that G-dye has a delta function source at \mathbf{x}' and t' . Also, as shown later, G-dye must obey a homogeneous boundary condition. To interpret Eq. (5), we imagine that at location \mathbf{x}' and time t' we inject into the fluid an infinitesimally small, instantaneous puff of G-dye of unit mass, which subsequently evolves according to the given flow field. Then $G(\mathbf{x}, t; \mathbf{x}', t')$ is proportional to the mixing ratio of G-dye at a later time t and position \mathbf{x} . It is important to note that the Green's function governs the propagation of dye in a particular flow field, whereas the transilient matrix, as defined by this paper, concerns the propagation of dye in an ensemble of flows and initial dye distributions.

Before deriving the equation governing the propagation of tracer, it is necessary to note the *reciprocity condition*:

$$G(\mathbf{x}, t; \mathbf{x}', t') = \tilde{G}(\mathbf{x}', t'; \mathbf{x}, t), \tag{6}$$

where \tilde{G} is the adjoint function, which satisfies the equation

$$\begin{aligned} \rho(\mathbf{x}, t) \frac{\partial \tilde{G}(\mathbf{x}, t; \mathbf{x}'', t'')}{\partial t} + \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \nabla \tilde{G}(\mathbf{x}, t; \mathbf{x}'', t'') \\ + \nabla \cdot [\rho(\mathbf{x}, t) \kappa \nabla \tilde{G}(\mathbf{x}, t; \mathbf{x}'', t'')] = -\delta^3(\mathbf{x} - \mathbf{x}'') \delta(t - t''). \end{aligned} \tag{7}$$

Here G propagates an initial dye distribution forward in time to its final distribution, whereas \tilde{G} propagates a final distribution of dye backward in time to its initial distribution. We omit the derivation of the reciprocity condition here. A similar derivation for the diffusion equation may be found in Morse and Feshbach (1953, 857–859). We simply note various conditions that must be imposed in the course of the derivation. To avoid violating causality, we must require that

$$G(\mathbf{x}', t'; \mathbf{x}, t) = 0 \quad t' < t, \tag{8}$$

that is, that a puff injected at t has no effect at earlier times t' . Likewise, we require that

$$\tilde{G}(\mathbf{x}, t; \mathbf{x}', t') = 0 \quad t' < t.$$

Furthermore, we insist either that (a) there is no flow through the boundary $\mathbf{u} \cdot \mathbf{n}|_S = 0$ and G satisfies the homogeneous Neumann boundary condition $\mathbf{n} \cdot \nabla G(\mathbf{x}, t; \mathbf{x}', t')|_S = 0$ where \mathbf{n} is the unit outward normal to the boundary; or that (b) G obeys the homogeneous Dirichlet boundary condition $G(\mathbf{x}, t; \mathbf{x}', t')|_S = 0$. We let G and \tilde{G} satisfy the same boundary conditions.

With the reciprocity condition in hand, we proceed to derive the equation governing the propagation of tracer, again following Morse and Feshbach (1953, 859–860). From the defining equation for the adjoint function (7) and the reciprocity condition (6), we find

$$\begin{aligned} \rho(\mathbf{x}', \tau) \frac{\partial G(\mathbf{x}, t; \mathbf{x}', \tau)}{\partial \tau} + \rho(\mathbf{x}', \tau) \mathbf{u}(\mathbf{x}', \tau) \cdot \nabla' G(\mathbf{x}, t; \mathbf{x}', \tau) \\ + \nabla' \cdot [\rho(\mathbf{x}', \tau) \kappa \nabla' G(\mathbf{x}, t; \mathbf{x}', \tau)] = -\delta^3(\mathbf{x} - \mathbf{x}') \delta(t - \tau). \end{aligned} \tag{9}$$

Here ∇' denotes the gradient operator with respect to the \mathbf{x}' coordinate. A change of variables in the advection-diffusion equation [(4)] leads to

$$\begin{aligned} \rho(\mathbf{x}', \tau) \frac{\partial c(\mathbf{x}', \tau)}{\partial \tau} + \rho(\mathbf{x}', \tau) \mathbf{u}(\mathbf{x}', \tau) \cdot \nabla' c(\mathbf{x}', \tau) \\ - \nabla' \cdot [\rho(\mathbf{x}', \tau) \kappa \nabla' c(\mathbf{x}', \tau)] = \rho(\mathbf{x}', \tau) s(\mathbf{x}', \tau). \end{aligned} \tag{10}$$

We now multiply Eq. (9) by $c(\mathbf{x}', \tau)$, Eq. (10) by $G(\mathbf{x}, t; \mathbf{x}', \tau)$, and add. Let ϵ denote a positive, infinitesimal time interval. Then applying the operator $\int_V d^3x' \int_{t'}^{t'+\epsilon} d\tau$ to the resulting equation and using continuity yields the propagation equation:

$$\begin{aligned} c(\mathbf{x}, t) = & \underbrace{\int_V d^3x' \rho(\mathbf{x}', t') G(\mathbf{x}, t; \mathbf{x}', t') c(\mathbf{x}', t')}_{\text{I}} \\ & + \underbrace{\int_{t'}^{t'+\epsilon} d\tau \int_V d^3x' \rho(\mathbf{x}', \tau) G(\mathbf{x}, t; \mathbf{x}', \tau) s(\mathbf{x}', \tau)}_{\text{II}} \\ & + \int_{t'}^{t'+\epsilon} d\tau \int_S dA' \mathbf{n} \cdot \rho(\mathbf{x}', \tau) \kappa \\ & \times \left[\underbrace{G(\mathbf{x}, t; \mathbf{x}', \tau) \nabla' c(\mathbf{x}', \tau)}_{\text{III}} \right. \\ & \left. - \underbrace{c(\mathbf{x}', \tau) \nabla' G(\mathbf{x}, t; \mathbf{x}', \tau)}_{\text{IV}} \right]. \end{aligned} \tag{11}$$

The advection term has vanished. To ensure its disappearance, we have had to demand either that no fluid flows through the boundary, or that G satisfies a homogeneous Dirichlet boundary condition. Furthermore, the causality condition on the Green's function [(8)] has caused the time-integrated term to vanish at $\tau = t + \epsilon$.

We require that G obey the homogeneous form of the boundary condition on c . For instance, if c satisfies a homogeneous or inhomogeneous Dirichlet condition, then we choose a homogeneous Dirichlet condition on G , so that term III vanishes and Eq. (11) becomes an explicit solution for $c(\mathbf{x}, t)$. By way of example, we list two possible sets of boundary conditions. If the dye mixing ratio on the boundary $c|_S$ is a specified function, then

$$G|_S = 0.$$

If the diffusive flux of dye through the boundary $\mathbf{n} \cdot \nabla c|_S$ is a specified function, then

$$\mathbf{n} \cdot \nabla G|_S = 0 \quad \mathbf{n} \cdot \mathbf{u}|_S = 0.$$

In term I of Eq. (11), the operator $\int d^3x' \rho(\mathbf{x}', t')$ $G(\mathbf{x}, t; \mathbf{x}', t')$ propagates the dye from its distribution $c(\mathbf{x}', t')$ at the initial time to its distribution $c(\mathbf{x}, t)$ at any later time. Hence the Green's function may be called a "propagator." It is similar to the propagator of quantum mechanics, which, when applied to an initial wave function, yields the wave function at a later time (Sakurai 1985, 110). Term II of Eq. (11) propagates each infinitesimal puff of dye emitted by the source to its destination at time t . Terms III and IV add the contribution of dye diffused through the boundary. The propagation equation [(11)] provides a simple interpretation of G : if c satisfies a homogeneous boundary condition and $s = 0$, then $\rho(\mathbf{x}', t')G(\mathbf{x}, t; \mathbf{x}', t')$ is proportional to the dye distribution that arises from a delta function initial dye distribution. The fact that integral operators and not differential operators appear in the propagation equation [(11)] reflects the fact that mixing may depend on the flow field and dye concentration at remote points, that is, that mixing may be nonlocal.

Mixing often depends strongly on both the flow field and the initial distribution of dye. We may wish, however, to gain information about a flow's mixing properties abstracted from any particular initial dye distribution. The Green's function provides such information. The governing equation for the Green's function [(5)] reveals that the Green's function can be constructed solely from the flow field (i.e., \mathbf{u} , ρ , and κ), and the boundary condition on G (which depends on the form of the boundary condition for c). On the other hand, if one desires to know the mixing properties associated with any particular initial condition, one may find this information by performing the integrations in (11), once G , ρ , κ , and s are given. In this sense, the Green's function "knows" about the mixing processes associated with all initial dye distributions that are compatible with G 's boundary condition.

Regardless of whether or not a source is present or the boundary condition on c is inhomogeneous, the *composition property* may be proven:

$$G(\mathbf{x}, t; \mathbf{x}'', t'') = \int_V d^3x' \rho(\mathbf{x}', t') G(\mathbf{x}, t; \mathbf{x}', t') G(\mathbf{x}', t'; \mathbf{x}'', t''). \quad (12)$$

An analogous identity arises in quantum mechanics (Sakurai 1985, 115). To derive the composition property, we multiply the equation

$$\begin{aligned} & \rho(\mathbf{x}', \tau) \frac{\partial G(\mathbf{x}', \tau; \mathbf{x}'', t'')}{\partial \tau} \\ & + \rho(\mathbf{x}', \tau) \mathbf{u}(\mathbf{x}', \tau) \cdot \nabla' G(\mathbf{x}', \tau; \mathbf{x}'', t'') \\ & - \nabla' \cdot \rho(\mathbf{x}', \tau) \kappa \nabla' G(\mathbf{x}', \tau; \mathbf{x}'', t'') \\ & = \delta^3(\mathbf{x}' - \mathbf{x}'') \delta(\tau - t'') \end{aligned} \quad (13)$$

by $G(\mathbf{x}, t; \mathbf{x}', \tau)$, Eq. (9) by $G(\mathbf{x}', \tau; \mathbf{x}'', t'')$, add the two resulting equations, and operate with $\int_V d^3x' \int_{t'}^{t'+\epsilon} d\tau$. Using the continuity equation, the causality condition [(8)], and homogeneous Dirichlet or Neumann boundary conditions, we may eliminate various time-integrated and boundary terms, as in the derivation of (11), and obtain the composition property [(12)]. The composition property states that propagating an infinitesimal puff of G-dye from (\mathbf{x}'', t'') to (\mathbf{x}, t) is equivalent to propagating it from (\mathbf{x}'', t'') to an intermediate point (\mathbf{x}', t') and then from (\mathbf{x}', t') to (\mathbf{x}, t) , integrating over all possible intermediate positions \mathbf{x}' . When the diffusivity κ is non-zero, a particle of G-dye may take many paths from (\mathbf{x}'', t'') to (\mathbf{x}, t) ; we must sum the contributions from all such paths to calculate the concentration of G-dye at (\mathbf{x}, t) . A long-time-interval propagator may be constructed from a series of short-time-interval propagators by generalizing the composition property [(12)].

Under certain assumptions, ensemble averaging the propagation equation [(11)] yields the transilient matrix equation [(1)], and ensemble averaging the Green's function yields essentially the transilient matrix. We partition the Green's function and dye distribution into an ensemble-averaged part, denoted by an overbar, and a deviation part, denoted by a hat:

$$\begin{aligned} G(\mathbf{x}, t; \mathbf{x}', t') &= \overline{G}(\mathbf{x}, t; \mathbf{x}', t') + \hat{G}(\mathbf{x}, t; \mathbf{x}', t') \\ c(\mathbf{x}', t') &= \overline{c}(\mathbf{x}', t') + \hat{c}(\mathbf{x}', t'). \end{aligned}$$

We assume that the domain is a rectangular parallelepiped, partitioned into a stack of overlying horizontal slabs. Furthermore, we assume that c obeys a homogeneous boundary condition, that there is no source of dye, and that ρ is constant. Then, upon ensemble averaging the propagation equation [(11)], we find

$$\begin{aligned} \overline{c}(\mathbf{x}, t) &= \int_V d^3x' \rho \overline{G}(\mathbf{x}, t; \mathbf{x}', t') \overline{c}(\mathbf{x}', t') \\ &+ \int_V d^3x' \rho \overline{\hat{G}(\mathbf{x}, t; \mathbf{x}', t') \hat{c}(\mathbf{x}', t')}. \end{aligned} \quad (14)$$

The second term is an “error term,” similar to that derived by Sobel (1997, 1999). The error term is nonzero if, for instance, the ensemble of flows contains rising plumes surrounded by subsiding regions, and the initial dye is placed preferentially in the plumes. In order to derive the transilient matrix equation, however, we must assume that the dye is initially distributed such that the error term vanishes. Then, to discretize (14), we spatially average over individual slabs. Denote a spatial average over the \mathbf{x} coordinate of the i th slab by $\langle \rangle_i$, and a spatial average over the \mathbf{x}' coordinate of the j th slab by $\langle \rangle_j$. Assume that either $\langle \overline{G}(\mathbf{x}, t; \mathbf{x}', t') \rangle_i$, or $\overline{c}(\mathbf{x}', t')$ is approximately slabwise uniform in \mathbf{x}' . Upon averaging (14) over slabs, we find

$$\langle \overline{c}(\mathbf{x}, t) \rangle_i = \sum_{j=1}^N m_j \langle \overline{G}(\mathbf{x}, t; \mathbf{x}', t') \rangle_i \langle \overline{c}(\mathbf{x}', t') \rangle_j. \quad (15)$$

Here m_j denotes the mass of fluid contained within slab j . If we identify the transilient matrix $G_{ij}(t; t')$ with $m_j \langle \overline{G}(\mathbf{x}, t; \mathbf{x}', t') \rangle_i$, then we recover the transilient matrix equation [(1)]. The *integral* operator of Green’s function theory has become the *matrix* operator of transilient theory. When the volumes of the slab are equal, m_j is a constant number, and the transilient matrix is simply proportional to $\langle \overline{G}(\mathbf{x}, t; \mathbf{x}', t') \rangle_i$. Stull (1993) also shows how the transilient matrix may account for slabs of different mass m_j , but he absorbs m_j into the transilient matrix using a different convention than ours.

Neither the transilient matrix nor the ensemble-averaged Green’s function satisfies a composition property analogous to (12). Ensemble averaging the composition property [(12)] yields, if ρ is constant,

$$\begin{aligned} \overline{G}(\mathbf{x}, t; \mathbf{x}'', t'') &= \int_V d^3x' \rho \overline{G}(\mathbf{x}, t; \mathbf{x}', t') \overline{G}(\mathbf{x}', t'; \mathbf{x}'', t'') \\ &+ \int_V d^3x' \overline{\rho \hat{G}(\mathbf{x}, t; \mathbf{x}', t') \hat{G}(\mathbf{x}', t'; \mathbf{x}'', t'')}. \end{aligned} \quad (16)$$

The second term on the right-hand side represents the correlation between the perturbation transport from (\mathbf{x}'', t'') to (\mathbf{x}', t') and the perturbation transport from (\mathbf{x}', t') to (\mathbf{x}, t) . The correlation term does not vanish in general. A nonnegligible correlation term can arise when the flow is not random, but instead contains persistent, large-scale, organized structures. For instance, consider an ensemble of flows, each of which contains rising plumes surrounded by subsiding regions. Suppose a puff of dye starts in the base of a plume at (\mathbf{x}'', t'') , then rises within the plume to a moderate altitude (\mathbf{x}', t') , and continues to rise until it reaches (\mathbf{x}, t) . The transport within the plume during the two time intervals $[t'', t']$ and $[t', t]$ is strongly correlated. Consideration of the fate of many such puffs indicates that the correlation term is likely to be nonnegligible. The transilient matrix, however, destroys information about the

correlations by averaging at the intermediate time step. Loosely speaking, after an application of the transilient matrix, we do not know whether dye that was originally in a plume still resides within the plume or resides elsewhere in the slab. The lack of a composition property may also be explained as follows. Even if the error term $\int_V d^3x'' \rho \overline{\hat{G}(\mathbf{x}', t'; \mathbf{x}'', t'') \hat{c}(\mathbf{x}'', t'')}$ for the first time interval vanishes, the error term $\int_V d^3x' \rho \overline{\hat{G}(\mathbf{x}, t; \mathbf{x}', t') \hat{c}(\mathbf{x}', t')}$ for the second time interval is unlikely to vanish, because of dye transport by the plumes during the first time interval. Therefore, errors arise when the transilient matrix is applied the second time. An analysis of such “convective structure memory” effects is contained in Ebert et al. (1989), Stull (1993), and Sobel (1997, 1999).

In some cases we may be interested in fluid transport to and from irregularly shaped or overlapping regions. For instance, we might want to know how much environmental air at time t' has been entrained into a cloud by time t . If we ignore tracer diffusion from one material element to another, we might compute this by performing a numerical simulation in which we spread dye of unit mixing ratio uniformly throughout the volume $V_{o'}$ that excludes the cloud at time t' . Then we would observe how much dye is contained within the volume V_c occupied by the cloud at time t . If we let c satisfy homogeneous boundary conditions and $s = 0$, then the quantity we desire can be written in terms of the Green’s function:

$$\begin{aligned} &\int_{V_c} d^3x \rho(\mathbf{x}, t) c(\mathbf{x}, t) \\ &= \int_{V_c} d^3x \rho(\mathbf{x}, t) \int_{V_{o'}} d^3x' \rho(\mathbf{x}', t') G(\mathbf{x}, t; \mathbf{x}', t'). \end{aligned} \quad (17)$$

This connection between tracer numerical experiments and the Green’s function may be conceptually helpful. On the one hand, one may use the Green’s function point of view to help interpret tracer calculations. On the other hand, tracer calculations may be used to compute integrals over the Green’s function when direct computation of the Green’s function is impossible. Ebert et al. (1989) have demonstrated the usefulness of this procedure.

We now derive generalized versions of Eqs. (2) and (3). An analog to the transilient matrix condition (2) may be derived directly from the defining equation for the Green’s function [(5)] by applying the operator $\int_V d^3x \int_{t'-\epsilon}^{t'} dt$ to it. Using appropriate boundary conditions and the causality condition [(8)], we obtain

$$\begin{aligned} &\int_V d^3x \rho(\mathbf{x}, t_f) G(\mathbf{x}, t_f; \mathbf{x}', t') \\ &= 1 + \int_{t'-\epsilon}^{t'} dt \int_S dA \mathbf{n} \cdot \rho(\mathbf{x}, t) \kappa \nabla G(\mathbf{x}, t; \mathbf{x}', t'). \end{aligned} \quad (18)$$

To interpret this equation, imagine that a point-source

puff of G-dye is injected into the flow at \mathbf{x}' and t' . Then the left-hand side represents the amount of G-dye within the volume V at a later time t_f . With our normalization, this is equal to unity minus the portion of the original puff that has diffused out the boundary between times $t' - \epsilon$ and t_f . With Neumann boundary conditions on c , the final term in Eq. (18) vanishes, and the equation becomes analogous to the transilient matrix equation [(2)]. Thuburn and McIntyre (1997) note that when c obeys homogeneous Neumann boundary conditions and $s = 0$, Eq. (18) is equivalent to conservation of tracer mass, as can be seen by applying $\int_V d^3x \rho(\mathbf{x}, t)$ to the propagation equation [(11)].

Similarly, an analog to the transilient matrix condition (3) is derived by applying $\int_V d^3x' \int_{t'}^{t'+\epsilon} d\tau$ to (9):

$$\begin{aligned} & \int_V d^3x' \rho(\mathbf{x}', t') G(\mathbf{x}, t; \mathbf{x}', t') \\ &= 1 + \int_{t'}^{t'+\epsilon} d\tau \int_S dA' \mathbf{n} \cdot \rho(\mathbf{x}', \tau) \kappa \nabla' G(\mathbf{x}, t; \mathbf{x}', \tau). \end{aligned} \quad (19)$$

This equation sums the contributions of all those particles of G-dye at an initial time t' that contribute to the concentration of G-dye present at (\mathbf{x}, t) . All such contributions integrate to unity, minus the loss due to diffusion out the boundary. With Neumann boundary conditions on c , Eq. (19) reduces to an analog of the transilient formula [(3)]. Thuburn and McIntyre (1997) note that when c obeys homogeneous Neumann boundary conditions and $s = 0$, Eq. (19) is equivalent to requiring that a spatially uniform initial dye distribution remain uniform, as can be seen by inspection of the propagation equation [(11)].

3. Conclusions

This note has argued that the Green's function for the advection-diffusion equation provides a useful way to attach mathematical rigor to ideas about nonlocal mixing that have been developed over the past several decades. The Green's function is well suited to this purpose for several reasons. It is a rigorously defined mathematical entity that contains within it all relevant information about a flow's capacity for mixing. Yet the Green's function is independent of the initial distribution of dye. Although local mixing may be adequately represented by a differential operator, nonlocal mixing is probably best represented by an integral operator. The Green's function appears as part of an *integral* operator in the propagation equation [(6)], but in addition the Green's function has a direct mathematical connection to the *differential* equation that governs the advection and diffusion of dye. Finally, the composition property [(12)] allows us to construct a single long-time Green's function by stringing together many short-time Green's

functions. The transilient matrix lacks such a composition property.

Unfortunately, for many flows of interest, direct computation of the truly point-source Green's function is not feasible. Here the transilient matrix, which averages over extended volumes, has a great advantage. Users of the transilient matrix may find it helpful, however, to interpret each element of the transilient matrix as an average of the Green's function over source and destination slabs. The shapes of the volumes may be generalized, if desired. Also, the Green's function formalism makes it clear how to incorporate sources of dye and inhomogeneous boundary conditions into the transilient matrix framework.

Finally, we speculate that convective structure memory effects may significantly degrade the accuracy of vertical transport of scalars, such as chemical species, in large-scale models. In such models, vertical fluxes are accomplished partly by convective parameterizations. These are one-dimensional schemes that compute average properties over the large horizontal area spanned by a grid box. As with the transilient matrix, therefore, convective parameterizations lose information each time they are applied. It may be worthwhile to seek ways to minimize convective structure memory effects in such parameterizations. For instance, one might attempt to optimize the time interval between successive applications of the convective parameterization, as in Ebert et al. (1989).

Acknowledgments. The author greatly appreciates the helpful suggestions of Roland Stull, Glenn Flierl, R. Alan Plumb, Kerry Emanuel, Pablo Zurita, Adam Sobel, Bjorn Stevens, and Alejo Sison. Glenn Flierl suggested the use of the adjoint function to formulate and derive the reciprocity condition. The author is also grateful to the Department of Energy for financial support of this research via Grant DE-FG02-91ER61220.

REFERENCES

- Ebert, E. E., U. Schumann, and R. B. Stull, 1989: Nonlocal turbulent mixing in the convective boundary layer evaluated from large-eddy simulation. *J. Atmos. Sci.*, **46**, 2178–2207.
- Fennel, W., 1981: Turbulent diffusion in wind-driven currents. *Deep-Sea Res.*, **A28**, 695–703.
- Gill, A. E., 1982: *Atmosphere–Ocean Dynamics*. Academic Press, 662 pp.
- Hamba, F., 1995: An analysis of nonlocal scalar transport in the convective boundary layer using the Green's function. *J. Atmos. Sci.*, **52**, 1084–1095.
- Holzer, M., 1999: Analysis of passive tracer transport as modeled by an atmospheric general circulation model. *J. Climate*, **12**, 1659–1684.
- Kraichnan, R. H., 1959: The structure of isotropic turbulence at very high Reynolds numbers. *J. Fluid Mech.*, **5**, 497–543.
- Leslie, D. C., 1973: *Developments in the Theory of Turbulence*. Clarendon Press, 368 pp.
- Lin, J.-S., and L. M. Hildemann, 1997: A generalized mathematical scheme to analytically solve the atmospheric diffusion equation with dry deposition. *Atmos. Environ.*, **31**, 59–71.

- Morse, P. M., and H. Feshbach, 1953: *Methods of Theoretical Physics, Part I*. McGraw-Hill, 997 pp.
- Phillips, C. G., and S. R. Kaye, 1996: A uniformly asymptotic approximation for the development of shear dispersion. *J. Fluid Mech.*, **329**, 413–443.
- Roberts, P. H., 1961: Analytical theory of turbulent diffusion. *J. Fluid Mech.*, **11**, 257–283.
- Sakurai, J. J., 1985: *Modern Quantum Mechanics*. Addison-Wesley, 474 pp.
- Sobel, A. H., 1997: Quantitative diagnostics of stratospheric mixing. Ph.D. dissertation, Massachusetts Institute of Technology, 134 pp. [Available from Program in Atmospheres, Oceans, and Climate, Room 54-1712, Massachusetts Institute of Technology, Cambridge, MA 02139.]
- , 1999: Diffusion versus nonlocal models of stratospheric mixing, in theory and practice. *J. Atmos. Sci.*, **56**, 2571–2584.
- Stull, R. B., 1984: Transient turbulence theory. Part I: The concept of eddy-mixing across finite distances. *J. Atmos. Sci.*, **41**, 3351–3367.
- , 1986: Transient turbulence theory. Part III: Bulk dispersion rate and numerical stability. *J. Atmos. Sci.*, **43**, 50–57.
- , 1993: Review of non-local mixing in turbulent atmospheres: Transient turbulence theory. *Bound.-Layer Meteor.*, **62**, 21–96.
- , and T. Hasegawa, 1984: Transient turbulence theory. Part II: Turbulent adjustment. *J. Atmos. Sci.*, **41**, 3368–3379.
- Thuburn, J., and M. E. McIntyre, 1997: Numerical advection schemes, cross-isentropic random walks, and correlations between chemical species. *J. Geophys. Res.*, **102**, 6775–6797.