A Unified Approach to the Various Formulations of the One-Dimensional-Turbulence Model

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Abstract

The One-Dimensional Turbulence (ODT) model has been successfully applied as a stand-alone model for predicting turbulence statistics in both nonreacting and reacting flows. There are several formulations of the model in the literature, and most of the variable-density formulations do not clearly distinguish the governing equations from the numerical algorithm used to solve them, resulting in confusion about exactly what form of the governing equations are being solved in the various existing ODT formulations. This paper presents a derivation of the governing equations for the various forms of the ODT model in the literature, and presents some suggestions for possible improvement to the present formulations. In addition, eddy selection and implementation are discussed in the context of the various forms of the governing equations to illustrate differences between various approaches.
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1 Introduction

The One-Dimensional Turbulence (ODT) model represents, conceptually, a line of sight through a turbulent flow field. First proposed by Kerstein [1], ODT is an outgrowth of the Linear Eddy Model [2–4], but includes the solution of the local velocity field to determine the rate and location of eddy occurrence. Although ODT (and its predecessor LEM) has been implemented as a sub-grid scale model in LES and RANS (see, e.g., [5–10]), much of its application has been as a stand-alone model.

In stand-alone applications, ODT is applicable in situations where there is a direction of predominant large-scale gradients such as shear-driven flow (channels, jets), buoyancy-driven flow (plumes), etc. The one-dimensional domain is aligned perpendicular to the direction of primary gradients (e.g., across the shear layer), thereby resolving the primary driving force for turbulence. Of primary importance in ODT modeling is resolution of the streamwise (x-direction) velocity component (perpendicular to the direction of the ODT domain), as this velocity component captures the shear that results in the turbulent cascade. Indeed, early ODT formulations considered only the streamwise component of velocity. Later, the model was extended to include multiple components of velocity [11]. We refer to the ODT-aligned coordinate as the y-direction, and the streamwise coordinate as x throughout this document. This inherently assumes a Cartesian coordinate system, which is consistent with most ODT applications to date. However, ODT has been formulated in cylindrical coordinates as well [12], where the ODT line is oriented in the radial direction, and the axial velocity component is the critical one that drives turbulence in the ODT model. ODT has been successfully applied as a stand-alone model for a variety of shear-dominated flows, both nonreacting [1,11,13,14] and reacting [12,15–19].

The ODT model consists of two primary ingredients:

- The governing equations written in terms of two independent variables: (t, y) for “temporal” ODT formulations and (x, y) for “spatial” ODT formulations.
- Discrete “eddy events” that occur at various points in (t, y) or (x, y). In ODT, these eddy events are influenced by the local shear rate. Therefore, the majority of ODT formulations solve an equation to evolve the streamwise component of velocity. A notable exception is application of ODT to Rayleigh convection [20].

Stand-alone ODT models (the focus of the remainder of this document) have been formulated as temporally evolving, with (t, y) as independent variables, and spatially evolving, with (x, y) as independent variables. With each of these approaches, both Lagrangian and Eulerian variants can be used. Particularly in the case of variable-density flows, virtually all of the literature regarding ODT combines the numerical solution algorithm with the discussion of the governing equations so that it is not immediately clear what the actual governing equations being solved are. In some cases, the equations presented are not the equations being solved. In this document, we formulate the various stand-alone ODT approaches under a single umbrella and illustrate the differences between them. This is done without discussion of specific numerical algorithms, except in cases to illustrate nuances of implementations presented in the literature. We hope to establish a mathematically sound basis for the various ODT formulations that will allow more clarity in comparing various approaches and will also allow a clear distinction between the equations being solved and the numerical method/algorithm used to solve the equations.

The remainder of this document is organized as follows: §2 presents the governing equations solved for
the ODT variants currently existing in the literature. The key modeling concepts in ODT, the triplet map and kernel transformation, are then addressed in §3. Both of these sections are supplemented with material presented in the appendices.

2 Governing Equations for ODT

In this section, we present several forms of the governing equations for use in ODT simulations.

As shown in Appendix A, the governing equations for a single phase reacting system can be written in Lagrangian form as

\[
\frac{d}{dt} \int_{V(t)} \rho \psi \, dV = - \int_{V(t)} \Phi_\psi \cdot a \, dS + \int_{V(t)} \sigma_\psi \, dV, \tag{1}
\]

\[
\rho \frac{d\psi}{dt} = -\nabla \cdot \Phi_\psi + \sigma_\psi, \tag{2}
\]

where \(\psi\) is an intensive quantity, \(\sigma_\psi\) is the net rate of production of \(\rho \psi\), and \(\Phi_\psi\) is the non-convective flux of \(\rho \psi\). Equations (1) and (2) are, respectively, the integral and differential forms of the Lagrangian evolution equations. In the Eulerian frame of reference, the corresponding equations are written in integral, strong differential, and weak differential forms as

\[
\int_{V(t)} \frac{\partial \rho \psi}{\partial t} \, dV + \int_{S(t)} \rho \psi \mathbf{v} \cdot a \, dS = - \int_{S(t)} \Phi_\psi \cdot a \, dS + \int_{V(t)} \sigma_\psi \, dV, \tag{3}
\]

\[
\frac{\partial \rho \psi}{\partial t} + \nabla \cdot \rho \rho \psi \mathbf{v} = -\nabla \cdot \Phi_\psi + \sigma_\psi, \tag{4}
\]

\[
\rho \frac{\partial \psi}{\partial t} + \rho \mathbf{v} \cdot \nabla \psi = -\nabla \cdot \Phi_\psi + \sigma_\psi, \tag{5}
\]

where \(\mathbf{v}\) is the mass-averaged velocity. Equation (2) is often most convenient for mathematical manipulation, while (1) and (3) are more readily applied in a finite-volume numerical solution approach. Table 1 shows the forms of \(\psi\), \(\Phi_\psi\), and \(\sigma_\psi\) for several common forms of the governing equations. Appendix A presents a derivation of the above equations and the terms in Table 1.

ODT formulations can be broadly classified into two categories:

- Temporal evolution, where \((t, y)\) are chosen as the independent variables, and (throughout this document) \(y\) refers to the direction associated with the one-dimensional ODT domain.

- Spatial evolution, where \((x, y)\) are chosen as the independent variables and \(x\) refers to the streamwise direction.

In each of these categories, there are both Eulerian and Lagrangian variants of ODT. Early ODT implementations were temporally evolving in a Lagrangian frame of reference. The spatially evolving ODT formulation was first introduced in the original description of ODT [1]. However, recent improvements to the model significantly broadened the range of flows and phenomena that the model can address [12,13,19,21,22]. Recently, Eulerian formulations for the temporal and spatial evolution have been demonstrated [14,18]. The following sections consider each of these variants in turn.

\[1\text{Note that the weak differential form is obtained by applying chain rule to (4) and substituting the continuity equation (} \psi = 1).]
Table 1: Forms of terms in the governing equations (1)-(5). Here \( p \) is the pressure, \( \tau = -\mu \left( \nabla v + (\nabla v)^T \right) + \frac{2}{3} \mu I \nabla \cdot v \) is the stress tensor, \( v \) is the mass-averaged velocity, \( g \) is the gravitational vector, \( Y_i \) is the mass fraction of species \( i \), \( j_i \) is the mass-diffusive flux of species \( i \) relative to a mass-averaged velocity, \( q = -\lambda \nabla T + \sum_{j=1}^{n} h_i j_i \) is the heat flux, \( \lambda \) is the thermal conductivity, \( T \) is the temperature, and \( h_i \) is the enthalpy of species \( i \).

<table>
<thead>
<tr>
<th>Equation</th>
<th>( \psi )</th>
<th>Non-convective Flux, ( \Phi_\psi )</th>
<th>Source Term, ( \sigma_\psi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Momentum</td>
<td>( v )</td>
<td>( pI + \tau )</td>
<td>( \rho g )</td>
</tr>
<tr>
<td>Species</td>
<td>( Y_i )</td>
<td>( j_i )</td>
<td>( \sigma_i )</td>
</tr>
<tr>
<td>Total Internal Energy</td>
<td>( e_0 )</td>
<td>( pv - \tau \cdot v + q )</td>
<td>( \rho g \cdot v )</td>
</tr>
<tr>
<td>Internal Energy</td>
<td>( e )</td>
<td>( q )</td>
<td>(-\tau : \nabla v - p \nabla \cdot v )</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>( h )</td>
<td>( q )</td>
<td>( \frac{\partial p}{\partial t} + v \cdot \nabla p - \tau : \nabla v )</td>
</tr>
</tbody>
</table>

2.1 Temporal ODT Evolution Equations

We first consider temporal evolution. In this context, the ODT equations will describe evolution of various quantities on a line oriented in the \( y \)-direction and evolving in time. We consider two general forms of the governing equations: the Eulerian and Lagrangian forms.

2.1.1 Eulerian Temporal Form

Retaining \((t, y)\) as independent variables, (4) becomes

\[
\frac{\partial \rho \psi}{\partial t} + \frac{\partial \rho \psi v}{\partial y} - \frac{\partial \Phi_\psi}{\partial y} + \sigma_\psi, \tag{6}
\]

where \( \Phi_{\psi,y} = \Phi_\psi \cdot y \) represents the component of \( \Phi_\psi \) in the \( y \)-direction, and \( v \) represents the local mass-averaged fluid velocity in the \( y \)-direction. Current approaches using the Eulerian form have solved the compressible form of these equations \([14,18]\). Specifically, (6) (or its integral form equivalent) is solved as follows:

- \( \psi = 1 \) is solved for \( \rho \).
- \( \psi = u \) is solved for the streamwise momentum \((\rho u)\) to provide the required information for the eddy selection (see §3). Note that the pressure gradient could be retained in this equation and imposed for pressure driven flow.
- \( \psi = v \) is solved for the lateral momentum \((\rho v)\), which is mainly required for the continuity equation \((\psi = 1)\). The pressure obtained from the equation of state is used to calculate the pressure gradient that appears in this equation.
- \( \psi = e_0 \) is solved for the total internal energy \((\rho e_0)\).
- \( \psi = Y_i \) is solved for the species masses \((\rho Y_i)\).

These equations are completed by an equation of state, \( p = p(\rho, T, Y_i) \). In a finite-volume context (as implemented in \([14,18]\)), the integral form of (6) is solved. While one could also solve the weak form of
these equations (corresponding to equation (5)), there have been no implementations to date using the weak form.

2.1.2 Lagrangian Temporal Form

In the Lagrangian frame of reference, choosing \((t, y)\) as independent variables, (2) becomes

\[
\rho \frac{d\psi}{dt} = -\frac{\partial \Phi_{\psi,y}}{\partial y} + \sigma_{\psi}.
\]  

Equation (7) is written in integral form as

\[
\frac{d}{dt} \int \rho \psi \, dy = \int \left( -\frac{\partial \Phi_{\psi,y}}{\partial y} + \sigma_{\psi} \right) \, dy.
\]  

Equations (7) and (8) are the forms most often used for temporally evolving ODT simulations. In the Lagrangian reference frame, the volume of a finite material element \(V(t)\), and its associated surface \(S(t)\), change with time according to the local mass-averaged velocity, \(v\). To determine the locations of the cell centroids (and faces) ODEs may be solved for positions of cell centroids or faces by

\[
\frac{dy}{dt} = v,
\]

where \(v\) is the \(y\)-component of velocity. If we solve (7) for \(\psi = v\) then we have the lateral velocity component required for use in (9). Since \(v\) is the mass-averaged velocity, (9) describes the evolution of a surface defining a closed system for the mass, thereby enforcing continuity,

\[
\frac{d}{dt} \int \rho \, dy = \frac{dm}{dt} = 0.
\]  

Specifically, the limits of the integral in (8) are determined by (9), and (8) with \(\psi = 1\) implies (10). Thus, by solving (9), we evolve the size of the control volume that, by definition, enforces continuity. Note that (10) need not be solved because it simply states that mass is constant\(^3\).

A full solution approach would solve:

- Equation (9) for cell face positions to define the limits on the integral in (8).
- Equation (10) need not be solved since its solution is simply that mass is constant. Density is obtained using this constant mass and the volume determined by the evolution of (9).
- Equation (8) with \(\psi = u\) for the streamwise momentum to provide the required information for the eddy selection (see §3). Note that for pressure driven flow, the pressure gradient term can be specified accordingly. Otherwise, the streamwise pressure gradient is ignored.
- Equation (8) with \(\psi = v\) for the lateral momentum. This is required for use in (9).
- Equation (8) with \(\psi = e_0, e, \text{ or } h\) for energy conservation.
- Equation (8) with \(\psi = Y_i\) for species.

\(^2\)See §A.5 for details.

\(^3\)Note that in the case of a multiphase system, where the continuity equation for one phase may have source terms due to interphase mass transfer, (9) is still the appropriate equation for enforcing continuity. However, the mass of the system will no longer be constant, and (10) (with the appropriate interphase exchange terms) would need to be evolved.
• An equation of state \( p = p(p, T, Y_i) \). This is used in the lateral momentum equation (\( \psi = v \)).

Early ODT formulations did not solve the \( y \)-component of velocity (\( v \)), and even among the ones that do (e.g. [11]), it is typically not used to supply the velocity for (9). Indeed, most ODT formulations to date use the \( y \) and \( z \) velocity components as repositories of kinetic energy rather than advective velocities. Thus, even if \( v \) is solved, rather than solving (9) to determine the limits for the integral in (8), (10) is used to describe the change in cell size. Specifically, (10) is discretized using a first-order time approximation to find

\[
(\Delta y)^{n+1} = \frac{p^n (\Delta y)^n}{\rho^{n+1}},
\]

where the density is calculated from an equation of state (typically assuming constant pressure). This determines the new cell size, but does not specify position. In a time-split scheme, \( \rho^{n+1} \) is evaluated from the equation of state, \( Y_i^{n+1} \), and \( T^{n+1} \), where the pressure is typically assumed to be constant. Given the cell sizes at time \( n + 1 \), the new cell positions are determined by calculating \( e = \sum_i (\Delta y)_i^n - \sum_i (\Delta y)^{n+1}_i \), adding \( e/2 \) to the volume on each end of the domain, and then redistributing the control volumes with their new sizes over the domain length (which remains fixed). This approach has been employed in all variable-density temporal Lagrangian ODT simulations to date. Notably, it imposes a fixed domain size, whereas solution of (9) does not.

To summarize, most current ODT temporal Lagrangian formulations solve (8) with \( \psi = u, \psi = \varepsilon_0 \) (or an equivalent energy variable), \( \psi = Y_i \), and (10) to obtain cell volumes that maintain continuity. However, as was shown in this section, an alternative would be to solve (7) for \( \psi = v \) and use this in (9) to obtain the positions of the Lagrangian cell centroids and faces.

2.1.3 Space-Time Mapping

It is often useful to transform the time coordinate to an equivalent spatial coordinate. This can be done by solving an ODE for downstream position, and can be done in one of two ways:

\[
\frac{dx}{dt} = \bar{u}, \tag{12}
\]
\[
\frac{dx}{dt} = u, \tag{13}
\]

where \( u \) is the \( x \) (streamwise) component of the velocity. Equation (12) uses a suitably chosen average velocity (\( \bar{u} \)) to determine the downstream position for the ODT domain whereas (13) uses the local velocity at each point on the ODT line and solves a position equation for each point. Figure 1 illustrates the difference between these approaches for a hypothetical constant (in time) \( u \) profile and \( \bar{u} \) chosen in two different ways\(^4\):

\[
\bar{u} = u_x + \frac{\int \rho (u - u_x)^2 \, dy}{\int \rho (u - u_x) \, dy}, \tag{14}
\]
\[
\bar{u} = \left< u \right|_{u < u_c}, \quad u_c = \alpha (\max u - \min u) \tag{15}
\]

Figure 1 clearly shows that the space-time mapping can be highly approximate, and must be used cautiously.

\(^4\)Note that these are only two of many reasonable choices for \( \bar{u} \).
2.2 Spatially Evolving ODT Equations

Because of the ambiguity in determining a downstream location \( (x) \) in the temporally evolving approach, it may be advantageous in some situations to formulate the governing equations so that \( (x, y) \) rather than \( (t, y) \) are the independent variables. Below we consider Eulerian and Lagrangian equation sets that use \( (x, y) \) as independent variables.

2.2.1 Eulerian Spatial Form

The spatially evolving governing equations retain only \( (x, y) \) as independent variables in (4) to obtain

\[
\frac{\partial \rho \psi}{\partial x} = -\frac{\partial \rho \psi}{\partial y} - \frac{\partial \Phi_{\psi,x}}{\partial x} - \frac{\partial \Phi_{\psi,y}}{\partial y} + \sigma_{\psi},
\]

This is an elliptic equation, and is not readily amenable for use with the stochastic eddy events in ODT. If we neglect the term \( \frac{\partial \Phi_{\psi,x}}{\partial x} \), then we have

\[
\frac{\partial \rho \psi}{\partial x} = -\frac{\partial \rho \psi}{\partial y} - \frac{\partial \Phi_{\psi,y}}{\partial y} + \sigma_{\psi},
\]

which is an incompletely parabolic (convection-diffusion) equation set that may be solved using the method of lines for the streamwise fluxes, \( \rho \psi u \). Note that the continuity equation \( (\psi = 1) \),

\[
\frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} = 0,
\]

Figure 1: Downstream position \( (x) \) as a function of lateral position \( (y) \) for various times. The solid line uses (13) (solid line), the dashed line uses (12) with (14), and the dotted line uses (15) with \( \alpha = 0.05 \) (dotted line).
conserves mass flux rather than mass itself. The full set of equations to be solved is: (18), (17) with \( \psi = \{ u \ v \ Y_j \ e_0 \} \), and an equation of state. Note that we can obtain

\[
\begin{align*}
\rho &= \frac{\rho u u}{u} = \frac{(\rho u)^2}{\rho u}, \\
\psi &= \frac{\rho \psi u}{\rho u}, \quad \psi \neq \{ 1 \ u \}.
\end{align*}
\]

An alternative solution strategy is to solve the weak form of (17),

\[
\frac{\partial \psi}{\partial x} = -\frac{1}{\rho u} \left[ \rho u \frac{\partial \Phi}{\partial y} + \frac{\partial \Phi \psi, y}{\partial y} - \sigma \phi \right],
\]

(22)
together with an alternate form of (18)

\[
\frac{\partial p}{\partial x} = -\frac{1}{u} \left[ \frac{\partial \mu}{\partial x} + \frac{\partial \rho v}{\partial y} \right].
\]

(23)
The term \( \frac{\partial \psi}{\partial x} \) in (23) may obtained from (22) with \( \psi = u \). The full set of equations to be solved is: (23), (22) with \( \psi = \{ u \ v \ Y_j \ e_0 \} \), and an equation of state. As discussed in §2.1.1, the \( \frac{\partial \psi}{\partial x} \) term comes from the equation of state while \( \frac{\partial p}{\partial x} \) is only nonzero in the case where a pressure driven flow is considered, in which case a fixed value of \( \frac{\partial \psi}{\partial x} \) is assigned.

### 2.2.2 Lagrangian Spatial Form

Given that the independent variables for the spatial evolution equations are \((x, y)\), we can write

\[
\frac{d}{dx} = \frac{\partial}{\partial x} + \frac{dy}{dx} \frac{\partial}{\partial y} = \frac{\partial}{\partial x} + \frac{\partial}{\partial y}.
\]

(24)

Using (24), we can rewrite (22) in Lagrangian form as

\[
\frac{d \psi}{dx} = -\frac{1}{\rho u} \left[ \frac{\partial \Phi \psi, y}{\partial y} - \sigma \phi \right].
\]

(25)

This applies to all \( \psi \) except \( \psi = 1 \) (continuity), since (25) is in weak form. The Lagrangian form of the continuity equation can be obtained by substituting (24) into (18) to obtain

\[
\frac{d \rho u}{dx} = \frac{v \partial \rho u}{u \partial y} + \frac{\partial \rho v}{\partial y}.
\]

(26)

In (25), \( \frac{d \psi}{dx} \) is interpreted as the local rate of change in \( \psi \) as it moves with velocity \( v \). Equation (25) can also be written in integral form as

\[
\frac{d}{dx} \int \rho \psi u \, dy = \int \left( -\frac{\partial \Phi \psi, y}{\partial y} + \sigma \phi \right) \, dy.
\]

(27)
This is most easily shown by applying Leibniz’ rule to (27) to find

\[
\frac{d}{dx} \int_{y_1(x)}^{y_2(x)} \rho \psi u \, dy = \rho_2 \psi_2 u_2 \frac{dy_2}{dx} - \rho_1 \psi_1 u_1 \frac{dy_1}{dx} + \int_{y_1(x)}^{y_2(x)} \frac{\partial \psi u}{\partial x} \, dy
\]

\[
= \rho_2 \psi_2 u_2 - \rho_1 \psi_1 u_1 + \int_{y_1(x)}^{y_2(x)} \frac{\partial \psi u}{\partial x} \, dy
\]

\[
= \int_{y_1(x)}^{y_2(x)} \left( \frac{\partial \psi u}{\partial x} + \frac{\partial \psi v}{\partial y} \right) \, dy,
\]  

(28)

where subscripts 1 and 2 indicate that the quantities are evaluated at \(y_1\) and \(y_2\), respectively, and we have used (29). Equation (28) shows that (17) and (27) are equivalent. By virtue of the derivation of (25) from (17), we conclude that (25) and (27) are also equivalent.

When (25) is solved, an equation for \(y\) is also required to determine the position of the Lagrangian system

\[
\frac{dy}{dx} = \frac{v}{u},
\]

(29)

where \(u\) and \(v\) are the local fluid velocities in the \(x\) and \(y\) directions, respectively. If solving the integral form of the Lagrangian evolution equations, the position is required to determine the limits on the integral in (27) for each discrete volume element. If solving the differential form of the equations (via, e.g. a finite difference method) then the position is required to evaluate the fluxes and their divergences. In both cases, the role of the velocity is to maintain the proper definition of the Lagrangian control volume as discussed in §2.1.2.

Together with an equation of state, (25) and (29) form a complete set of equations. When solving these equations, primitive variables are obtained using (19)-(21).

To date, ODT implementations using the spatial form of the governing equations have solved (25) - see, e.g., [19, 21, 22]. All of these formulations present equations (17) (Eulerian forms) as the governing equations to be solved, but the form of the governing equations actually solved in these formulations is (25) (Lagrangian forms)\(^5\). As discussed in §2.1.2, the \(v\) component of velocity was not solved in the early ODT formulations. Rather than solving (29), these formulations (and the ones cited above) obtain Lagrangian position \((y)\) via (27) with \(\psi = 1\),

\[
\frac{d}{dx} \int \rho u \, dy = 0,
\]

(30)

so that a first-order time discretization results in

\[
(\Delta y)^{n+1} = \left( \frac{\rho u \Delta y}{\rho u} \right)^n, \quad (31)
\]

where \(n\) refers to the solution at streamwise position \(x_n\) while \(n + 1\) refers to the solution at position \(x_{n+1}\). From the updated volume sizes, the local positions are obtained as described in §2.1.2.

Alternatively (and equivalently), an equation for \(v\) could be solved (including the pressure term as shown in Table 1) and (29) could be solved for cell and face positions. However, as with the analogous approach in §2.1.2, this has not yet been demonstrated in ODT.

\(^5\)References [19, 21, 22] only present the discrete form of the equations they are actually solving, but they are the discrete form of (25).
Independent of which approach is taken to obtain the position evolution, the evolution streamwise mass flux, $\rho u$, need not be solved since it remains constant (as is evident from (27) with $\psi = 1$). The exception is for multiphase flow where there may be a source term in the flux continuity equation, as discussed in §2.1.2 for the mass conservation analogue.

### 2.2.3 Time-Space Mapping

Occasionally in a spatially evolving formulation we are interested in determining a “residence time,” e.g., in order to advance a chemical-kinetic mechanism [15,16]. In analogy to the discussion in §2.1.3 this can be obtained by solving one of

$$\frac{dt}{dx} = u^{-1}, \quad (32)$$

$$\frac{dt}{dx} = \bar{u}^{-1}. \quad (33)$$

Equation (32) accounts for the variation of residence time due to variation in $u$ while (33) obtains a characteristic residence time for the domain assuming that it moves with some characteristic velocity $\bar{u}$. As discussed in §2.1.3, the choice for $\bar{u}$ in (33) is somewhat arbitrary.

### 2.3 Summary

This section has presented four general approaches for ODT formulations. These can be categorized as temporally developing and spatially developing equations, with Lagrangian and Eulerian variants of each. When solving the Eulerian equations (see §2.1.1 and §2.2.1), the $y$-component of velocity advects fluid and serves to enforce continuity. On the other hand, when solving the Lagrangian equations (see §2.1.2 and §2.2.2) continuity reduces to a statement that mass (temporal form) or mass flux (spatial form) remains constant. However, in the Lagrangian form, the position must be evolved. This can be done one of two ways:

1. Use the $y$-component of velocity to determine the system position by solving (9) (temporal) or (29) (spatial). No boundary conditions are imposed on this ODE for position, but the boundary conditions on $v$ velocity directly influence the evolution of this equation.

2. Use an operator-splitting approach along with a discrete form of the continuity equation (11) (temporal) or (31) (spatial). This also requires imposition of boundary conditions directly, as discussed in §2.1.2 and §2.2.2.

The boundary conditions mentioned in these two options are important as they directly affect entrainment, large-scale flapping, etc., but details of their implementation are beyond the scope of this work. In addition, initial conditions may be particularly important in the case of spatially developing flows because of the approximation discussed in §2.2 that eliminated the elliptical nature of the problem [12].
3 Eddy Events in One Dimensional Turbulence

As discussed in §1, stand-alone modeling of turbulent flows using ODT requires a dominant direction of the flow (which we refer to as the x-direction) to be identified a priori. To mimic the three dimensional nature of turbulence in one spatial dimension, a stochastic process is adopted whereby motions that accelerate mixing are modeled through a series of stochastic rearrangement events. These events may be interpreted as the model analogue of individual turbulent eddies which are referred to as “eddy events” or simply “eddies”. Each eddy event modifies fields by applying an instantaneous transformation over some spatial interval \((y_0, y_0 + \ell)\), where \(y_0\) represents the eddy starting location and \(\ell\) is the eddy length.

A complete definition of the model for an eddy event requires specification of:

1. A procedure for selecting the candidate eddy starting location \((y_0)\), length \((\ell)\), and the eddy rate distribution (which is a function of \(y_0\) and \(\ell\)).

2. The transformation (mapping), which is the effect of an eddy on the solution variables.

The following sections address these elements of the eddy model.

3.1 Transformations

In ODT, each eddy is an instantaneous event and has no opportunity to interact directly with other eddies. Rather, the interaction is indirect, mediated by the flow evolution. An eddy event is represented by an instantaneous rearrangement in the form of a “triplet map.” For a selected eddy event the triplet map of a function \(\phi(y)\) is \(\phi(f(y; y_0, \ell))\), with \(f(y; y_0, \ell)\) given as

\[
f(y; y_0, \ell) = \begin{cases} 
3(y - y_0) & y_0 \leq y \leq y_0 + \frac{1}{3}\ell \\
2\ell - 3(y - y_0) & y_0 + \frac{1}{3}\ell \leq y \leq y_0 + \frac{2}{3}\ell \\
3(y - y_0) - 2\ell & y_0 + \frac{2}{3}\ell \leq y \leq y_0 + \ell \\
y - y_0 & \text{otherwise}
\end{cases}
\]  

(34)

The triplet map defined by (34) forms the heart of any ODT modeling approach, representing the effects of a three-dimensional eddy with a one-dimensional rearrangement. Triplet maps are qualitatively similar to turbulence in that they have the effect of increasing gradients by redistributing the fluid elements along the 1-D domain. The functional form chosen for the triplet mapping function is the simplest of a class of mappings that satisfy the physical requirements of measure preservation, continuity and scale locality over the eddy interval and also strengthen the local stretch rate just as turbulent fluctuations do [1].

While the triplet map itself is measure preserving, occasionally we wish to augment the transformation imposed by the eddy event to ensure conservation of other properties. For example, application of the triplet map to \(\rho \phi\) results in conservation of momentum, energy, and mass. However, kinetic energy is not necessarily conserved. If an eddy occurs in the presence of a gravitational field, then there is an exchange of potential and kinetic energy that must be accounted for when the transformation is applied to the \(\rho \phi\). To ensure conservation of kinetic energy when applied to the momentum fields, the triplet map can be augmented by a “kernel transformation,” \(cJ(y)\), which ensures conservation of kinetic energy. Applying such a kernel transformation to velocity components rather than momentum components can lead to a violation of momentum conservation, so that a second kernel, \(bJ(y)\), must be added to repair momentum...
conservation in the situation where transformations are applied to $\psi$ rather than $\rho \psi$. In this context, we can write the effect of an eddy on a velocity/momentum field as

$$\phi_i(y) = \phi_i(f(y; y_0, \ell)) + c_i K(y) + b_i J(y), \quad (35)$$

where

$$K(y) = y - f(y; y_0, \ell), \quad (36)$$
$$J(y) = |K(y)|. \quad (37)$$

The $K(y)$ kernel enforces conservation of kinetic energy while the $J(y)$ kernel enforces conservation of momentum [13]. If $\rho \psi$ rather than $\psi$, is transformed, then $J$ is not required (or $b_i = 0$) since momentum will be conserved by construction when (35) is applied to $\rho u, \rho v, \rho w$.

Generally speaking, selection of a kernel transformation is influenced by two primary considerations:

1. What variables are being transformed? Typically this will be one of $\psi, \rho \psi$, since it it typically most convenient to transform the solution variables. However, one could impose a transformation on any set of variables in general.

2. What constraints are placed on the transformation? Most frequently we seek to impose constraints on the momentum and kinetic energy when solving a temporal form of the equations and on the fluxes of momentum and kinetic energy when solving the spatial form of the equations. However, these are modeling considerations, not fundamental requirements. Additional constraints could be added as necessary.

The derivation of the transformations for various choices of transformed variables and constraints is presented in Appendix B. The coefficients $c_i$ and $b_i$ can be represented generally as

$$c_i = \frac{1}{2S} \left( -P_i + \text{sgn}(P_i) \sqrt{P_i^2 + \alpha \sum_j T_{ij} P_j^2} \right), \quad (38)$$
$$b_i = HC_i, \quad (39)$$

with specific forms for $S, P_i$ and $H$ presented in Appendix B and summarized in Table 2. Table 2 summarizes the transformations for designed for $\psi$ and $\rho \psi$ with constraints on conservation of kinetic energy and momentum and the fluxes of kinetic energy and momentum.

In the original ODT model formulation, a single velocity component was considered along with a set of scalars [1]. The application of the model to buoyant stratified flows, where conversion between kinetic energy and potential energy was the key concern, motivated the development of a kernel transformation to enforce the kinetic energy conservation [23]. Subsequently, a “vector” ODT formulation was considered, where an eddy event incorporated energy transfer between velocity components [11].

The rules governing the partitioning of kinetic energy among velocity components, which have been referred to as the “pressure-scrambling model,” also incorporate an element of three-dimensionality into the 1D model. This model is derived in Appendix B for various ODT formulations, and the key results are summarized in Table 2.

---

6Note that in cases where there are momentum sources from, e.g., a dispersed phase, a kernel ensuring momentum conservation must be applied even if $\rho \psi$ is transformed.
Table 2: Transformations for various quantities given the constraint of conservation of (a) momentum and kinetic energy, and (b) fluxes of momentum and kinetic energy. Derivations of the results shown here are presented in Appendix B. See equations (38) and (39) for how $S$, $T_{ij}$, $P_i$, and $H$ (whose defining equations are enumerated in the table) are used in obtaining the kernel coefficients $b_i$ and $c_i$ for use in (35).

<table>
<thead>
<tr>
<th>Transformed Quantity</th>
<th>Transformations</th>
<th>Kernel Coefficients for Conserving Quantities</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Momentum and KE</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$T_{ij}$</td>
</tr>
<tr>
<td>$\psi$</td>
<td>$u_i(y) \rightarrow u_i[f(y; y_0, \ell)] + c_iK(y) + b_iJ(y)$, $\psi(y) \rightarrow \psi[f(y; y_0, \ell)]$, $\psi \neq u_i$</td>
<td>(B.46)</td>
</tr>
<tr>
<td>$\rho \psi$</td>
<td>$(\rho u_i)[y] \rightarrow (\rho u_i)[f(y; y_0, \ell)] + c_iK(y)$, $(\rho \psi)_i[y] \rightarrow (\rho \psi)_i[f(y; y_0, \ell)]$, $\psi \neq u_i$</td>
<td>(B.46)</td>
</tr>
</tbody>
</table>
3.2 Eddy selection

The procedure to select an eddy event is described here in the context of temporally evolving flows. A similar analysis with appropriate scaling can be used for spatial flows. Unlike LEM, where frequency and eddy-size distribution of the events are based on a predefined kinetic energy spectrum [2], the eddy events are influenced by the local flow field in ODT. Similar to the dimensional relationship applied to turbulent eddies, for events defined in ODT, a relationship can be formulated between an eddy’s size, time scale, and kinetic energy. Since ODT resolves one or more components of the velocity/momentum vector, the “turnover” time ($\tau_e$) for an eddy can be calculated from the local kinetic energy and the length of a candidate eddy$^7$. From $\tau_e$, the eddy rate distribution ($\lambda$) that governs the eddy events is calculated from

$$\lambda = \frac{C}{\ell^2 \tau_e},$$

where $C$ is a model constant often referred to as the “eddy rate constant.” The models used to identify the turnover time ($\tau_e$) are summarized in Table 3 for different ODT model variants. The quantity $\ell/\tau_e$ is interpreted as an eddy velocity and $\rho\ell^3/\tau_e^2$ is interpreted as a measure of the kinetic energy of eddy motion. Based on the streamwise velocity ($x$-component), the kinetic energy will be computed and equated to eddy energy to formulate an expression for eddy velocity ($\ell/\tau_e$)$^8$.

The model constant $Z$ that appears Table 3 is a “viscous cutoff” parameter that provides a lower limit on the eddy size roughly analogous to the Kolmogorov scale. In principle, this is not necessary (and could be set to zero) since eddies smaller than the Kolmogorov and Batchelor scales will have a negligible effect on the physical evolution of the system$^9$.

Because $\rho\psi$ and $\psi$ evolve continuously in time between eddy events, $\lambda$ also evolves continuously in time. The unsteadiness of the eddy rate distribution is both a fundamental property of the model and a key consideration in its numerical implementation. $\lambda$ is used to compute the probability of the eddy occurring,

$$p_e = \frac{\lambda \Delta t}{f(y_0) g(\ell)},$$

where $f(y_0)$ and $g(\ell)$ are the probability density functions for $y_0$ and $\ell$ for respectively. The functional forms for $f(y_0)$ and $g(\ell)$ can influence the computational cost of the simulation, but do not affect the results [1]. The probability ($p_e$) is compared with a randomly selected number on the interval [0,1]. If the random number is less than $p_e$ then the eddy will be implemented.

For spatially evolving flows (see §2.2) $\Delta t$ is replaced by $\Delta x/\bar{u}$, where

$$\bar{u} = \frac{1}{\ell} \int_{y_0}^{y_0+\ell} u \, dy$$

is the average velocity defined over the eddy interval. This results in a definition of the probability of an

$^7$Note that $\tau_e$ can be interpreted as an eddy turnover time or the time between eddies (inverse of the eddy frequency). These two quantities are closely related, but there are situations where a clear distinction is important, such as in particle-laden flows where particle-eddy interaction is important. In these cases, $\tau_e^{-1}$ is interpreted as an eddy frequency governing eddy sampling and the eddy turnover time is calculated using an adjustable constant of proportionality [24].

$^8$More recent formulations that employ the “vector” formulation and solve several components of velocity use the kinetic energy from all velocity components in determining the eddy velocity and time scale [25].

$^9$See [1] for exceptions.
Table 3: Models for the eddy time scale, $\tau_e$, in terms of the eddy velocity, $\ell/\tau_e$. More details are found in Appendix B.

<table>
<thead>
<tr>
<th>ODT variant</th>
<th>Eddy time scale, $\tau_e$</th>
<th>Model Parameters</th>
<th>Relevant Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\psi$, conserving KE and momentum</td>
<td>$\left(\frac{\ell}{\tau_e}\right)^2 \approx \frac{4\ell^2}{27\rho_{kk}} \left[ \frac{8}{27} \left( Q_y + \alpha \sum_j T_{y,j} Q_j \right) - Z \frac{\nu^2}{\rho \ell} \right]$</td>
<td>$\alpha, C, Z$</td>
<td>See §B.1.1 and equations (B.46), (B.50), (B.55), (B.90), (B.91).</td>
</tr>
<tr>
<td>$\rho \psi$, conserving KE and momentum</td>
<td>$\left(\frac{\ell}{\tau_e}\right)^2 \approx \left[ \frac{Q_2 + \alpha \sum_j T_{y,j} Q_j - Z \frac{\nu^2}{\rho \ell}}{\rho \ell} \right]$</td>
<td>$\alpha, C, Z$</td>
<td>See §B.1.2 and equations (B.46), (B.64), (B.91), (B.92).</td>
</tr>
<tr>
<td>$\psi$, conserving KE and momentum fluxes</td>
<td>$\left(\frac{\ell}{\tau_e}\right)^2 \approx \frac{2}{\nu_0} \frac{2}{\rho_{u,kk}} \left[ Q_2 + \alpha \sum_j T_{y,j} Q_j - Z \frac{\nu^2}{\rho \ell} \right]$</td>
<td>$\alpha, C, Z$</td>
<td>See §B.2.1 and equations (B.46), (B.69), (B.74), (B.92).</td>
</tr>
<tr>
<td>$\rho \psi$, conserving KE and momentum fluxes</td>
<td>$\left(\frac{\ell}{\tau_e}\right)^2 \approx \frac{1}{\nu_0} \frac{2}{\rho_{u,yy}} \left[ Q_2 + \alpha \sum_j T_{y,j} Q_j - Z \frac{\nu^2}{\rho \ell} \right]$</td>
<td>$\alpha, C, Z$</td>
<td>See §B.2.2 and equations (B.46), (B.88), (B.92).</td>
</tr>
</tbody>
</table>
3.3 Large Eddy Suppression

While the viscous cutoff parameter $Z$ suppresses the least energetic eddies, we require a mechanism to prevent the occurrence of unphysically large eddies that result in unrealistic behaviour. We briefly outline the common methods for large eddy suppression in the following subsections.

3.3.1 Eddy Time Scale Method

Even though eddies are implemented as instantaneous events, the turnover time associated with each eddy event can be calculated from the scaling analysis as summarized in Table 3. The eddy turnover time can be compared with the simulation elapsed time ($t$), and eddy events are allowed only when $t \geq \beta \tau$, where $\beta$ is a model parameter. This large eddy suppression mechanism is used in most of the temporal formulations [15–18]. However, this approach can also be used in a spatially evolving simulation by using $x \geq \beta \ell$ as the criteria for eliminating large eddies.

3.3.2 Median Method

In this method, the eddy event rate ($\lambda$) for a given eddy event is evaluated two different ways and the smaller of the two results is used in evaluating the probability. One evaluation is by the expressions formulated in §3.2. The other evaluation replaces each velocity profile $u_i(y)$ by a profile that is linear in $y$, and evaluates of $\lambda$ based on these linear profiles. The slope of each profile is taken to be the median value $|\frac{du_i}{dy}|$ within the eddy range $[y_0, y_0 + \ell]$. The procedure assigns a zero rate to any event for which each velocity profile is flat (zero slope) in more than half of the eddy range, thereby suppressing large eddies [11].

3.3.3 Scale reduction method

The scale reduction method is the most common method for suppressing large eddies in spatially developing flows [12, 13, 21], although it could be applied to temporally evolving flows as well. It involves auxiliary eddy-rate computations for each of three equal sub-intervals of the eddy interval $[y_0, y_0 + \ell]$. For the selected eddy event, $\lambda$ is evaluated as if the eddy interval were $[y_0 + (j - 1) \frac{\ell}{3}, y_0 + j\frac{\ell}{3}]$, for $j = 1, 2,$ and $3$, respectively. If any of these three candidate eddies are disallowed due to dominance of the viscous penalty, as described in §3.2, then the eddy is discarded. Otherwise it is unchanged from its value computed for the complete eddy interval $[y_0, y_0 + \ell]$.

4 Conclusions

We intend that this document will serve as a reference for those interested in ODT as a modeling approach by providing a survey of the various ODT formulations along with a sound mathematical basis for
the equations being solved.

Most ODT formulations (particularly for variable density flows) have not clearly distinguished the governing equations being solved from the numerical method employed to solve them. The equations are often written in fully discrete form. This paper attempts to clarify the equations being solved by the various ODT formulations and, in so doing, raise alternative solution techniques. Specifically, this paper has formulated the governing equations for use in ODT simulations in several forms:

- Temporally evolving Eulerian,
- Temporally evolving Lagrangian,
- Spatially evolving Eulerian,
- Spatially evolving Lagrangian.

In addition, the models for “eddy events” in ODT, including the transformations applied to the solution variables (with appropriate kernel transformations) and the eddy selection criteria, were discussed and compared for the various ODT formulations.

Both the governing equations and the variable transformations associated with the eddy events are presented in a general manner assuming variable density and a multicomponent reacting system. Simplifications can be made in the event where density or composition is constant. In such cases, the discussion here simplifies to many of the early forms for ODT presented in the literature.

5 Acknowledgements

Several people have provided valuable insight into the development of the ideas presented herein. We are grateful to David Lignell, Philip Smith, Jeremy Thornock, and Yuxin Wu for their insightful comments.

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Work at Sandia was supported by the US Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Energy Biosciences. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the US Department of Energy under contract DE-AC04-94AL85000.
A Reynolds’ Transport Theorem and the Governing Equations

Consider an extensive property $\Psi$ with a corresponding intensive property $\psi = \frac{\partial \Psi}{\partial m}$. We can define the following relationships involving $\psi$ and $\Psi$

$$\frac{\partial \psi}{\partial V} = 0, \quad \frac{\partial \Psi}{\partial V} = \frac{\partial \Psi}{\partial m} \frac{dm}{\partial V} = \frac{1}{\rho} \frac{\partial \Psi}{\partial m'}$$

$$\Psi = \int \rho \psi \, dV = m \psi. \quad (A.1)$$

Consider a control volume (CV) of volume $V$ enclosed by an arbitrary surface $S$ which may change in time, i.e. $V(t)$, $S(t)$, as depicted in Figure A.1. Furthermore, consider a control volume $V_\psi(t)$ with a corresponding surface $S_\psi(t)$ that is defined such that it moves with the local velocity of the property $\psi$, $v_\psi$. The Reynolds’ transport theorem may be written for an intensive property $\psi$ moving with velocity $v_\psi$ as

$$\frac{d}{dt} \int_{V_\psi(t)} \rho \psi \, dV = \int_{V(t)} \frac{\partial \rho \psi}{\partial t} \, dV + \int_{S(t)} \rho \psi v_\psi \cdot \mathbf{a} \, dS. \quad (A.2)$$

The terms in (A.2) are interpreted as:

1. The change in $\Psi$ in a closed system defined by $V_\psi(t)$. A closed system implies that the boundary surface $S_\psi(t)$ moves locally at $v_\psi$. Also note that $\frac{d}{dt} \int_{V_\psi(t)} \rho \psi \, dV = \frac{d\Psi}{dt}$.

2. The instantaneous change in $\rho \psi$ at a point in space.

3. The flux of $\Psi$ across a differential element $dS$ due to advection. Note that Gauss’ theorem states $
\int_{S(t)} \rho \psi v_\psi \cdot \mathbf{a} \, dS = \int_{V(t)} \nabla \cdot (\rho \psi v_\psi) \, dV$.

The LHS of (A.2) represents the change of $\Psi$ in a Lagrangian frame of reference traveling through space at velocity $v_\psi$, while the RHS of (A.2) represents the change of $\Psi$ in an Eulerian reference frame (at a point in space).
space and time). The utility of (A.2) is that it relates the Eulerian reference frame to the Lagrangian reference frame.

Note that, in principle, each different quantity \( \psi \) could have a unique \( \mathbf{v}_\psi \) and thus a unique \( \mathcal{V}_\psi(t) \) associated with it. Rather than have a different velocity for each property \( \psi \), it is convenient to define a mass-averaged velocity,

\[
\mathbf{v} = \sum_{i=1}^{n_s} \rho_i Y_i \mathbf{v}_i \tag{A.3}
\]

where \( Y_i \) is the mass fraction of species \( i \) and \( \mathbf{v}_i \) is the velocity of species \( i \) in the mixture. Using this definition of the mass-averaged velocity, (A.2) can be written as

\[
\frac{d}{dt} \int_{\mathcal{V}(t)} \rho \psi \, dV = \int_{\mathcal{V}(t)} \frac{\partial \rho \psi}{\partial t} \, dV + \int_{\mathcal{S}(t)} \left( \rho \psi \mathbf{v} + j_\psi \right) \cdot \mathbf{a} \, dS, \tag{A.4}
\]

where

\[
j_\psi = \rho \psi (\mathbf{v}_\psi - \mathbf{v}) \tag{A.5}
\]

represents the flux of \( \psi \) relative to the mass-averaged velocity. Indeed, the quantity \( \mathbf{v}_\psi^0 = \mathbf{v}_\psi - \mathbf{v} \) can be interpreted as a "diffusion velocity."

If we want to use the same volume \( \mathcal{V}(t) \) for all \( \psi \) then we must account for the fact that \( \mathcal{V}(t) \) may not define a closed system for \( \Psi \). For convenience, we define \( \mathcal{V}(t) \) as a Lagrangian control volume that moves with the local mass-averaged velocity, \( \mathbf{v} \). Making this choice, we can relate the Lagrangian volume associated with \( \mathcal{V}_\psi(t) \) to the one associated with the mass averaged velocity, \( \mathcal{V}(t) \), by

\[
\frac{d}{dt} \int_{\mathcal{V}_\psi(t)} \rho \psi \, dV = \frac{d}{dt} \int_{\mathcal{V}(t)} \rho \psi \, dV + \int_{\mathcal{S}(t)} j_\psi \cdot \mathbf{a} \, dS. \tag{A.6}
\]

Note that in this case, we can define the evolution of any point in our Lagrangian system by \( \frac{dt}{dt} = \mathbf{v} \). In deriving various forms of the governing equations, we seek:

1. The diffusive flux, \( j_\psi \). Of course, this is only nonzero if \( \mathbf{v}_\psi \neq \mathbf{v} \).
2. An expression for \( \frac{d}{dt} \int_{\mathcal{V}_\psi(t)} \rho \psi \, dV \), the change of \( \Psi \) in a closed system whose boundaries move at \( \mathbf{v}_\psi \).

With this information, equations (A.4) and (A.6) allow us to describe evolution of \( \psi \) or \( \Psi \) in an Eulerian or Lagrangian frame of reference. As we will see, it is possible to cast the governing equations in the form

\[
\frac{d}{dt} \int_{\mathcal{V}(t)} \rho \psi \, dV = - \int_{\mathcal{S}(t)} \Phi_\psi \cdot \mathbf{a} \, dS + \int_{\mathcal{V}(t)} \sigma_\psi \, dV, \tag{A.7}
\]

\[
\int_{\mathcal{V}(t)} \frac{\partial \rho \psi}{\partial t} \, dV + \int_{\mathcal{S}(t)} \rho \psi \mathbf{v} \cdot \mathbf{a} \, dS = - \int_{\mathcal{S}(t)} \Phi_\psi \cdot \mathbf{a} \, dS + \int_{\mathcal{V}(t)} \sigma_\psi \, dV, \tag{A.8}
\]

where \( \Phi_\psi \) is the flux of \( \psi \) apart from the flux associated with the mass-averaged velocity, \( \rho \psi \mathbf{v} \). Equation (A.7) is the Lagrangian conservation equation for \( \psi \) using a Lagrangian control volume moving at \( \mathbf{v} \), and (A.8) is the Eulerian conservation equation for \( \psi \). The following subsections will detail the definitions of \( \Phi_\psi \) and \( \sigma_\psi \) for various governing equations.
A.1 Continuity

For the continuity equation, we have $\psi = m$ and $\psi = \frac{\partial \psi}{\partial t} = 1$. Also, $v_{\psi-1} = v$, i.e., the velocity advecting the density is the mass averaged velocity. Because of this, $j_{\psi-1} = 0$ and, from (A.6), $V_{\psi-1}(t) = \mathcal{V}(t)$. Now since mass is conserved for a closed system, we have

$$\frac{d}{dt} \int_{\mathcal{V}(t)} \rho \, dV = 0,$$

which, together with (A.4), implies

$$\frac{d}{dt} \int_{\mathcal{V}(t)} \rho \, dV = 0,$$

$$\int_{\mathcal{V}(t)} \frac{\partial \rho}{\partial t} \, dV + \int_{S(t)} \rho v \cdot a \, dS = 0.$$

Comparing these with (A.7) and (A.8), we can identify

$$\Phi_{\psi-1} = 0,$$

$$\sigma_{\psi-1} = 0.$$

A.2 Momentum

For the momentum equation, we have $\psi = m_{\nu}$ and $\psi = v$. It is commonly assumed that $v_{\nu} = v$, i.e., that the mass averaged velocity is the one that advects momentum in a closed system. Therefore, $j_{v} = 0$ and $V_{v}(t) = \mathcal{V}(t)$ so (A.2) becomes

$$\frac{d}{dt} \int_{\mathcal{V}(t)} \rho v \, dV = \int_{\mathcal{V}(t)} \frac{\partial \rho v}{\partial t} \, dV + \int_{S(t)} \rho v \otimes v \cdot a \, dS.$$

Furthermore, Newton’s second law of motion states that

$$\frac{d}{dt} \int_{\mathcal{V}(t)} \rho v \, dV = \int_{S(t)} (pI + \tau) \cdot a \, dS + \int_{\mathcal{V}(t)} \rho g \, dV,$$

where $\tau$ is the deviatoric stress tensor, $p$ is the pressure, $I$ is the unit tensor, and $g$ is the gravitational acceleration vector. From (A.7) we conclude

$$\Phi_{v} = pI + \tau,$$

$$\sigma_{v} = \rho g.$$

A.3 Species

For the species equations, we have $\psi = mY_{i}$ and $\psi = Y_{i}$. Clearly, individual species velocities ($v_{i}$) can differ, which implies that $v \neq v_{i}$. We define $j_{i} = \rho \gamma_{i} (v_{i} - v)$ as the species mass diffusive flux. For an ideal system, the Maxwell-Stefan equations relate the species mass diffusion fluxes to their mole fraction
gradients as\(^{10}\)

\[
\nabla x_i = \frac{M}{\rho} \sum_{j=1}^{n} \frac{1}{D_{ij}} \left( \frac{x_i j - x_j j_i}{M_j - M_i} \right),
\]

(A.18)

where \(D_{ij}\) are the binary diffusion coefficients, \(x_i\) are species mole fractions, \(M_i\) are the species molecular weights, and \(M\) is the mixture molecular weight. The Maxwell-Stefan equations can be cast in Fick’s law form as

\[
j_i = -\rho \sum_{j=1}^{n-1} D_{ij} \nabla x_j,
\]

(A.19)

where \(D_{ij}\) are the multicomponent diffusion coefficients, and are functions of the local thermodynamic state of the system as well as the binary diffusion coefficients, \(D_{ij}\).

In a closed system defined by \(V(t)\) which moves at the species velocity \(v_i\), the \(i^{th}\) species mass may be changed via chemical reaction,

\[
\frac{d}{dt} \int_{V(t)} \rho Y_i \, dV = \int_{V(t)} \omega_i \, dV,
\]

(A.20)

\[
\frac{d}{dt} \int_{V(t)} \rho Y_i \, dV = \int_{V(t)} \omega_i \, dV - \int_{S(t)} j_i \cdot a \, dS
\]

(A.21)

where the second equation comes from applying (A.6) to the first equation. Comparing with (A.7), we can define

\[
\Phi_{Y_i} = j_i,
\]

(A.22)

\[
\sigma_{Y_i} = \omega_i.
\]

(A.23)

**A.4 Total Internal Energy**

For total internal energy we have \(\Psi = m e_0 = E_0, \psi = e_0\). As with momentum, it is customary to define \(v_{e_0} = v\) so that \(f_{e_0} = 0\) and \(V_{e_0}(t) = V(t)\). From the first law of thermodynamics, we have

\[
\frac{dE_0}{dt} = \frac{dQ}{dt} + \frac{dW}{dt}
\]

\[
= -\int_{S(t)} q \cdot a \, dS - \int_{S(t)} (\tau \cdot v + pv) \cdot a \, dS + \int_{V(t)} \rho g \cdot v \, dV,
\]

(A.24)

where \(q = -\lambda \nabla T + \sum_{i=1}^{nSi} h_i j_i\) is the diffusive flux of heat\(^{11}\). We can thus define

\[
\Phi_{e_0} = pv + \tau \cdot v + q,
\]

(A.25)

\[
\sigma_{e_0} = \rho g \cdot v.
\]

(A.26)

(A.27)

\(^{10}\)For thermodynamically nonideal systems and systems with pressure diffusion, electrical fields, or thermal diffusion, additional terms are required. See, e.g. [26] for more details.

\(^{11}\)Here we have neglected the Dufour effect. Inclusion of this effect should be accompanied by modification of the species diffusive fluxes to include the Soret effect.
A.5 Differential Forms

Using (A.1) and (A.5), (A.2) can be written in differential form by taking the derivative with respect to the system volume,

$$\frac{\partial}{\partial V} \frac{d\Psi}{dt} = \frac{\partial \rho \psi}{\partial t} + \nabla \cdot \rho \psi \mathbf{v}. \quad (A.28)$$

Since $\Psi = m \psi$ then $\frac{d\Psi}{dt} = m \frac{d\psi}{dt} + \psi \frac{dm}{dt}$. By virtue of the continuity equation ($\frac{dm}{dt} = 0$), we have $\frac{d\Psi}{dt} = m \frac{d\psi}{dt}$. Therefore,

$$\frac{\partial}{\partial V} \frac{d\Psi}{dt} = \frac{\partial m}{\partial V} \frac{d\psi}{dt} + m \frac{d}{dt} \frac{\partial \psi}{\partial V}. \quad (A.29)$$

Since $\psi$ is an intensive quantity, $\frac{\partial \psi}{\partial V} = 0$ so that we have

$$\frac{\partial}{\partial V} \frac{d\Psi}{dt} = \rho \frac{d\psi}{dt}. \quad (A.29)$$

Substituting (A.29) into (A.28), we obtain the differential form of the Reynolds Transport Theorem,

$$\rho \frac{d\psi}{dt} = \frac{\partial \rho \psi}{\partial t} + \nabla \cdot \rho \psi \mathbf{v}. \quad (A.30)$$

We can thus write differential forms of (A.7) and (A.8) (the governing equations in the Lagrangian and Eulerian frames, respectively) as

$$\rho \frac{d\phi}{dt} = -\nabla \cdot \Phi_\psi + \sigma_\phi, \quad (A.31)$$

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot \rho \mathbf{v} + \rho \mathbf{v} \cdot \nabla \phi = -\nabla \cdot \Phi_\phi + \sigma_\phi. \quad (A.32)$$

Note that (A.32) also follows directly from applying Gauss' theorem and differentiating (A.8) with respect to $V$. The Eulerian form can be written in weak form by rewriting (A.32)

$$\rho \frac{\partial \phi}{\partial t} + \psi \frac{\partial \rho}{\partial t} + \rho \mathbf{v} \cdot \nabla \phi + \psi \nabla \cdot \rho \mathbf{v} = -\nabla \cdot \Phi_\phi + \sigma_\phi \quad (A.33)$$

and then using the continuity equation ($\psi = 1$) to obtain

$$\rho \frac{\partial \phi}{\partial t} + \rho \mathbf{v} \cdot \nabla \phi = -\nabla \cdot \Phi_\phi + \sigma_\phi. \quad (A.34)$$

The terms $\Phi_\phi$ and $\sigma_\phi$ are summarized in Table A.1 for various governing equations.

A.6 Other Forms of the Energy Equation

Table A.1 shows definitions of $\Phi_\psi$ and $\sigma_\phi$ for internal energy ($\psi = c$) and enthalpy ($\psi = h$). The following subsections show a derivation of these equations.
Table A.1: Definitions of $\Phi_\psi$ and $\sigma_\psi$, for use in equations (A.7), (A.8), (A.31), (A.32) and (A.34).

<table>
<thead>
<tr>
<th>Equation</th>
<th>$\psi$</th>
<th>$\Phi_\psi$</th>
<th>$\sigma_\psi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Continuity</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Momentum</td>
<td>$v$</td>
<td>$pI + \tau$</td>
<td>$\rho g$</td>
</tr>
<tr>
<td>Species</td>
<td>$Y_i$</td>
<td>$j_i$</td>
<td>$\omega_i$</td>
</tr>
<tr>
<td>Total Internal Energy</td>
<td>$e_0$</td>
<td>$q + \tau \cdot v + pv$</td>
<td>$\rho g \cdot v$</td>
</tr>
<tr>
<td>Internal Energy</td>
<td>$e$</td>
<td>$q$</td>
<td>$-p \nabla \cdot v - \tau : \nabla v$</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>$h$</td>
<td>$q$</td>
<td>$\frac{dp}{dt} - p \nabla \cdot v - \tau : \nabla v$</td>
</tr>
</tbody>
</table>

A.6.1 The Internal Energy Equation

Beginning with the momentum equation in Lagrangian form (equation (A.31) with $\psi = v$)

$$\rho \frac{dv}{dt} = -\nabla \cdot \tau - \nabla p + \rho g,$$  \hspace{1cm} (A.35)

we take the dot product with the velocity to obtain (after applying the chain rule)

$$\rho \frac{dk}{dt} = -v \cdot \nabla \cdot \tau - v \cdot \nabla p + v \cdot \rho g,$$ \hspace{1cm} (A.36)

where $k = vv/2$. Now since $e_0 = e + k$, we have $\frac{de_0}{dt} = \frac{de}{dt} - \frac{dk}{dt}$. From §A.4 and (A.31) we have

$$\rho \frac{de_0}{dt} = -\nabla \cdot (pv + \tau \cdot v + q) + \rho g \cdot v.$$ \hspace{1cm} (A.37)

Subtracting (A.36), we find

$$\rho \frac{de}{dt} = -p \nabla \cdot v - \tau : \nabla v - \nabla \cdot q.$$ \hspace{1cm} (A.38)

Comparing (A.31) and (A.38), we identify

$$\Phi_e = q,$$ \hspace{1cm} (A.39)

$$\sigma_\psi = -p \nabla \cdot v - \tau : \nabla v.$$ \hspace{1cm} (A.40)

A.6.2 The Enthalpy Equation

The relationship between enthalpy and internal energy is $e = h - \frac{p}{\rho}$ so that $\rho \frac{dh}{dt} = \rho \frac{de}{dt} + \frac{dp}{dt}$. Substituting (A.38), we find

$$\rho \frac{dh}{dt} = \frac{dp}{dt} - p \nabla \cdot v - \tau : \nabla v - \nabla \cdot q.$$ \hspace{1cm} (A.41)

Comparing with (A.31), we conclude

$$\Phi_h = q,$$ \hspace{1cm} (A.42)

$$\sigma_h = \frac{dp}{dt} - p \nabla \cdot v - \tau : \nabla v.$$ \hspace{1cm} (A.43)
B Kernels for Kinetic Energy Conservation

As described in §3.1, when energy is transferred between velocity/momentum components, conservation laws are enforced through kernel transformations. As shown in §3.1, the effect of an eddy on a velocity/momentum field is given by (35),

\[ \phi_i(y) = \phi_i(f(y; y_0, \ell)) + c_i K(y) + b_i J(y), \]  

(35)

where \( K(y) \) is given by (36), and \( J(y) \) is given by (37). The coefficients, \( c_i \) and \( b_i \), for the kernel transformation that augments the triplet map closely depends on the fields transformed in the model and conservation laws applied on them.

In the following sections, we derive kernel coefficients for the situations summarized in Table 2. Specifically, §B.1 discusses kernel transformations designed to conserve momentum and kinetic energy while §B.2 discusses kernel transformations designed to conserve the flux of momentum and kinetic energy. This appendix is not meant to be exhaustive. Rather, it summarizes some of the key kernel transformations in the literature, provides a few new transformations not present in the literature, and illustrates the strategy for deriving such transformations.

The coefficients for kernels are derived based on the following constraints,

1. Enforce kinetic energy conservation:

\[ \sum \Delta E_i = 0, \]  

(35)

where \( \Delta E_i \) is the change in kinetic energy associated with the \( i \)th velocity component due to the transformation.

2. When more than one velocity component is transformed during eddy event applying (35) imposes only one constraint. Two additional constraints are needed to define all the kernel coefficients. One such constraint is based on the following observation. \( c_i \) for given \( i \) can be chosen so as to add an arbitrarily large amount of kinetic energy to component \( i \), but the maximum amount that can be removed is a finite value, which is evaluated by maximizing the kinetic energy change with respect to \( c_i \). To identify the maximum energy \((Q_i)\), \( \Delta E_i \) is differentiated with respect to \( c_i \), equated to zero and the corresponding expression for \( c_i \) will be substituted back in to \( \Delta E_i \).

3. An additional constraint is based on the motivated phenomenological interpretation of pressure scrambling as a tendency to restore isotropy. This dictates the kernel coefficients to be invariant under the exchange of indices. So the kinetic energy changes imposed on the velocity components must be of the form

\[ \Delta E_i = a \sum_j T_{ij} Q_j \]  

(35)

where \( T_{ij} \) is defined by

\[ T_{ij} = \frac{1}{2} \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}. \]  

(35)
The change in kinetic energy for component \( i \) can be written as

\[
\Delta E_i = \alpha \left[ -Q_i + \frac{1}{2} (Q_j + Q_k) \right],
\]

where \( \alpha \) is a model parameter and \( \{i, j, k\} \) is any permutation of the component indices \( \{1, 2, 3\} \). The value \( \alpha = 1 \) maximizes the inter-component transfer.

### B.1 Transformations Conserving Momentum and Kinetic Energy

#### B.1.1 Transformations Involving \( \psi \)

When applying the transformation to \( \psi \), the change in the \( i \)th component of velocity, \( u''_i \), due to an eddy event is represented as

\[
u''_i = u'_i + c_i K(y) + b_i J(y),
\]

where \( u'_i \) represents the velocity field after application of the triplet map as defined by (34).

Following step 1, the change in kinetic energy associated with the \( i \)th velocity component during an eddy event is

\[
\Delta E_i = \frac{1}{2} \int_{y_0}^{y_0+t} \rho' \left[ (u''_i)^2 - (u'_i)^2 \right] \, dy.
\]

\[
= \frac{1}{2} \int_{y_0}^{y_0+t} \rho' \left[ (u'_i + b_i J + c_i K)^2 - (u'_i)^2 \right] \, dy.
\]

(B.49)
Expanding (B.49), we can define the following [13]:

\[
\begin{align*}
\rho_I & = \int_{y_0}^{y_0 + \ell} \rho' J \, dy = \frac{4}{9} \int_{y_0}^{y_0 + \ell} \left( \ell + y_0 - y \right) \rho(y) \, dy \left. + \int_{y_0 + \ell/2}^{y_0 + \ell} \left( y - y_0 \right) \rho(y) \, dy \right], \\
\rho_K & = \int_{y_0}^{y_0 + \ell} \rho' K \, dy = \frac{4}{9} \int_{y_0}^{y_0 + \ell} \left( \ell - 2 \left| y - y_0 \right| \right) \rho(y) \, dy, \\
\rho_{JK} & = \int_{y_0}^{y_0 + \ell} \rho' J K \, dy = \frac{8}{27} \int_{y_0}^{y_0 + \ell} \left[ \left( \ell^2 - 3 \ell \left| y - y_0 \right| + 2 \left| y - y_0 \right|^2 \right) \rho(y) \, dy \right. \\
& \quad + \left. \int_{y_0 + \ell/2}^{y_0 + \ell} \left( y - y_0 \right) \left[ \ell - 2 \left( y - y_0 \right) \right) \rho(y) \, dy \right], \\
\rho_{KK} & = \int_{y_0}^{y_0 + \ell} \rho' \rho'' \, dy = \frac{8}{27} \int_{y_0}^{y_0 + \ell} \left[ \ell^2 - 3 \ell \left( y - y_0 \right) + 3 \left( y - y_0 \right)^2 \right] \rho(y) \, dy, \\
\rho_i & = \int_{y_0}^{y_0 + \ell} \rho' u_i' J \, dy = \frac{4}{9} \int_{y_0}^{y_0 + \ell} \left( \ell + y_0 - y \right) \rho(y) u_i(y) \, dy \left. + \int_{y_0 + \ell/2}^{y_0 + \ell} \left( y - y_0 \right) \rho(y) u_i(y) \, dy \right], \\
\rho_{ij} & = \int_{y_0}^{y_0 + \ell} \rho' u_i' J \, dy = \frac{4}{9} \int_{y_0}^{y_0 + \ell} \left( \ell - 2 \left| y - y_0 \right| \right) \rho(y) u_i(y) \, dy, \\
H & = \frac{\rho_K}{\rho_I}, \\
P_i & = \rho_{ij} - H \rho_{ij}, \\
S & = \frac{1}{2} \left( H^2 + 1 \right) \rho_{KK} - H \rho_{JK}. 
\end{align*}
\]

From these definitions, (B.49) can be rewritten as

\[
\Delta E_i = P_i c_i + S c_i^2, 
\]

and following step 2, the maximum energy available with velocity component \(i\) is

\[
Q_i = \frac{p_i^2}{4S}. 
\]

From (B.44), (B.47), (B.49) and (B.55), expressions for the kernel amplitudes \(c_i\) are obtained as

\[
c_i = \frac{1}{2S} \left( -P_i \pm \sqrt{P_i^2 \left( 1 - \alpha \right) + \frac{\alpha}{2} \left( P_i^2 + P_k^2 \right)} \right), 
\]

\[
= \frac{1}{2S} \left( -P_i + \text{sgn}(P_i) \sqrt{P_i^2 + \alpha \sum_j T_{ij} P_j^2} \right). 
\]

An additional kernel must be applied on the velocity components to enforce momentum conservation during an eddy event. Momentum conservation over the eddy interval is given by

\[
\int_{y_0}^{y_0 + \ell} \rho' u_i'' \, dy = \int_{y_0}^{y_0 + \ell} \rho' u_i' \, dy. 
\]
From the identities defined above, it may be shown that (B.57) implies

\[ b_i = -Hc_i. \]  

(B.58)

Note that here and below, significant simplifications are afforded when the density is constant.

**B.1.2 Transformations Involving \( \rho \psi \)**

When applying the transformation to \( \rho \psi \), the change in the \( i^{th} \) component of momentum, \( (\rho u)^i'' \), due to an eddy event is represented as

\[ (\rho u)^i'' = (\rho u)^i' + c_iK(y), \]  

(B.59)

where \( (\rho u)^i' \) represents the momentum field after application of the triplet map as defined by (34).

Following step 1, the change in kinetic energy associated with the \( i^{th} \) velocity component during an eddy event is

\[
\Delta E_i = \frac{1}{2} \int_{y_0}^{y_0+\ell} \left[ (\rho u)^i''(u'')_i - (\rho u)^i'_i u'_i \right] \, dy,
\]

(B.60)

Combining (B.59) and (B.60), \( \Delta E_i \) is represented as

\[
\Delta E_i = \frac{1}{2} \int_{y_0}^{y_0+\ell} \left[ \frac{(\rho u)^i' + c_iK}{\rho'} - \frac{(\rho u)^i'}{\rho'} \right]^2 \, dy,
\]

(B.61)

where

\[
S = \int_{y_0}^{y_0+\ell} 2\frac{K^2}{\rho'} \, dy, \]

(B.62)

\[
P_i = \int_{y_0}^{y_0+\ell} 2\frac{(\rho u)^i'K}{\rho'} \, dy. \]

(B.63)

Following step 2, the maximum energy that is available with velocity component \( i \) is

\[ Q_i = \frac{P_i^2}{4S}. \]  

(B.64)

From (B.44), (B.47), (B.61), and (B.64), expressions for the kernel amplitudes \( (c_i) \) are obtained as

\[
c_i = \frac{P_i}{2S} \pm \sqrt{\left( \frac{P_i}{2S} \right)^2 (1 - \alpha) + \frac{\alpha}{2} \left( \left( \frac{P_j}{2S} \right)^2 + \left( \frac{P_k}{2S} \right)^2 \right)},
\]

(B.65)

\[
= \frac{1}{2S} \left( -P_i + \text{sgn}(P_i) \sqrt{P_i^2 + \alpha \sum_j T_j P_j^2} \right).
\]
B.2 Transformations Conserving Fluxes of Momentum and Kinetic Energy

In the following subsections, we consider transformations on $\psi$ and $\rho \psi$ that conserve the flux of momentum and kinetic energy.

B.2.1 Transformations Involving $\psi$

The ODT model was first proposed with only the streamwise component of velocity [1], and was later extended to a velocity vector formulation with kernel transformations to allow for inter-component energy transfer [13, 24]. When energy transfer is enabled between the velocity components, mass is necessarily conserved but mass flux may not be. When an eddy event is implemented, mass flux conservation over the eddy interval in the continuous form is given by

$$\int_{y_0}^{y_0+\ell} \rho' u' \, dy = \int_{y_0}^{y_0+\ell} \rho' u'' \, dy', \quad (B.66)$$

where $u'_i$ represents the velocity field after application of the triplet map as defined by (34) and $u''_i$ is given by

$$u''_i = u'_i + c_i K(y) + b_i f(y). \quad (B.67)$$

To ensure mass flux conservation, each cell volume will be modified to account for acceleration and expansion. The cumulative effect of these control volume adjustments requires adjustment of the overall eddy length [24].

The kernel coefficients are derived in the same manner as in §B.1.1, except that conservation of momentum and kinetic energy fluxes are enforced here. Following step 1, the kinetic energy flux change for velocity component $i$ over the modified eddy interval ($\ell'$) is given by

$$\Delta E_i = \frac{1}{2} \int_{y_0}^{y_0+\ell'} \rho' u' (u''_i)^2 \, dy' - \int_{y_0}^{y_0+\ell} \rho' u' (u'_i)^2 \, dy \quad (B.68)$$
In (B.68), we define the following by neglecting the eddy interval change (i.e. \( \ell = \ell' \) and \( y_0 = y_0' \)),

\[
\begin{align*}
\rho_{u,i} &= \int_{y_0}^{y_0+\ell} \rho' u_1' \, dy, \\
\rho_{u,K} &= \int_{y_0}^{y_0+\ell} \rho' u_i K \, dy, \\
\rho_{u,KK} &= \int_{y_0}^{y_0+\ell} \rho' u_i^2 K^2 \, dy, \\
\rho_{u,JK} &= \int_{y_0}^{y_0+\ell} \rho' u_i' K \, dy, \\
\rho_{u,ui} &= \int_{y_0}^{y_0+\ell} \rho' u_i'u_i' \, dy, \\
\rho_{u,ui} &= \int_{y_0}^{y_0+\ell} \rho' u_i'u_i' \, dy, \\
\rho_{u,ui} &= \int_{y_0}^{y_0+\ell} \rho' u_i'u_i' \, dy, \\
P_i &= \rho_{u,ui} - H \rho_{u,K} - H \rho_{u,JK} \\
H &= \frac{\rho_{u,K}}{\rho_{u,ui}}, \\
S &= \frac{1}{2} \left( H^2 + 1 \right) \rho_{u,KK} - H \rho_{u,JK}.
\end{align*}
\]  

(B.69)

From these definitions, (B.68) becomes

\[\Delta E_i = P_i c_i + S c_i^2.\]  

(B.73)

Following step 2, the maximum energy that is available with velocity component \( i \) is

\[Q_i = \frac{p_i^2}{4S}.\]  

(B.74)

From (B.44), (B.47), (B.73) and (B.74), expressions for the kernel amplitudes \( c_i \) are obtained as

\[c_i = \frac{1}{2S} \left( -P_i \pm \sqrt{P_i^2 \left( 1 - \alpha \right) + \frac{\alpha}{2} \left( P_i^2 + P_k^2 \right)} \right),\]

\[c_i = \frac{1}{2S} \left( -P_i + \text{sgn}(P_i) \sqrt{P_i^2 + \alpha \sum_i T_{ij} P_j^2} \right).\]  

(B.75)

The momentum flux conservation over the eddy interval is given by

\[\int_{y_0}^{y_0+\ell} \rho' u_i' u_i' \, dy = \int_{y_0}^{y_0+\ell} \rho' u_i'' u_i'' \, dy'.\]  

(B.76)

Using the identities above, it can be shown that (B.76) implies

\[b_i = -Hc_i.\]  

(B.77)

Equations (B.75) and (B.77) complete the specification of the triplet map and kernel transformation for the case where \( \psi \) is transformed and flux conservation for momentum and kinetic energy is desired.
B.2.2 Transformations Involving $\rho \psi$

When applying the transformation to $\rho \psi$, the change in the $i$th component of momentum, $(\rho u)'$, due to an eddy event is represented as

$$
(\rho u)' = (\rho u)' + c_i K + b_i J.
$$

where $(\rho u)'$ represents the momentum field after application of the triplet map as defined by (34).

Following step 1, the change in kinetic energy flux associated with the $i$th velocity component during an eddy event is

$$
\Delta E_i = \frac{1}{2} \int_{y_0}^{y_0 + \ell} \left[ (\rho u)' (u_i' u_i') - (\rho u)' (u_i')^2 \right] \, dy.
$$

Combining (B.78) and (B.79), $\Delta E_i$ is represented as

$$
\Delta E_i = \frac{1}{2} \int_{y_0}^{y_0 + \ell} \left[ \frac{(\rho u)'}{(\rho')^2} \left( \left[ (\rho u)' + c_i K + b_i J \right]^2 - [(\rho u)']^2 \right) \right] \, dy.
$$

Momentum flux conservation through the kernel transformation requires

$$
\int_{y_0}^{y_0 + \ell} (\rho u)' u_i' \, dy = \int_{y_0}^{y_0 + \ell} (\rho u)' u_i'' \, dy,
$$

$$
\int_{y_0}^{y_0 + \ell} \frac{(\rho u)'}{\rho'} \left[ c_i K + b_i J \right] \, dy = 0.
$$

Defining

$$
A_1 = \int_{y_0}^{y_0 + \ell} (\rho u)' K \, dy, \quad A_2 = \int_{y_0}^{y_0 + \ell} (\rho u)' J \, dy,
$$

equation (B.81) can be rewritten to identify the relationship between $b_i$ and $c_i$,

$$
b_i = -\frac{A_1}{A_2} c_i.
$$
Defining

\[ A_3 \equiv \int_{y_0}^{y_0 + \ell} \frac{(\rho u)' K^2}{2 (\rho')^2} \, dy = \int_{y_0}^{y_0 + \ell} \frac{2 (\rho u)'}{2 (\rho')^2} \, dy, \]
\[ A_4 \equiv \int_{y_0}^{y_0 + \ell} \rho u' K (\rho u)'_i \, dy, \]
\[ A_5 \equiv \int_{y_0}^{y_0 + \ell} (\rho u)'_i (\rho u)_i' \, dy, \]
\[ A_6 \equiv \int_{y_0}^{y_0 + \ell} \frac{(\rho u)' K}{(\rho')^2} \, dy, \]

\[ P_i \equiv A_4 - A_5 \frac{A_1}{A_2}, \quad (B.84) \]
\[ S \equiv A_5 \left( 1 + \frac{(A_1}{A_2} \right)^2 - A_6 A_1, \quad (B.85) \]

equation (B.80) can be written as

\[ \Delta E_i = P_i c_i + Sc_i^2. \quad (B.87) \]

Following step 2, the maximum energy that is available with velocity component \( i \) is

\[ Q_i = \frac{P_i^2}{4S^2}. \quad (B.88) \]

From (B.44), (B.47), (B.87) and (B.88), expressions for the kernel amplitudes \( c_i \) are obtained as

\[ c_i = \frac{1}{2S} \left( -P_i \pm \sqrt{P_i^2 (1 - \alpha) + \frac{\alpha}{2} \left( P_i^2 + P_k^2 \right)} \right), \quad (B.89) \]

\[ = \frac{1}{2S} \left( -P_i + \text{sgn}(P_i) \sqrt{P_i^2 + \alpha \sum_i T_{ij} P_j^2} \right). \]

### B.3 Eddy time scale

As described in §3.2, the eddy time scale \( \tau_e \) is defined based on scaling analysis. Dimensions of various quantities defined as part of the pressure scrambling model are given in Table B.2.

Expressions for the eddy energy are constructed from the quantities described in Table B.2 and the following average quantities defined over the eddy interval:

\[ \mu_e = \left[ \frac{1}{\ell} \int_{y_0}^{y_0 + \ell} \frac{dy}{\mu} \right]^{-1}, \quad (B.90) \]
\[ \rho_e = \frac{1}{\ell} \int_{y_0}^{y_0 + \ell} \rho \, dy, \quad (B.91) \]
\[ \gamma_e = \left[ \frac{1}{\ell} \int_{y_0}^{y_0 + \ell} \frac{\rho}{\mu} \right]^{-1}. \quad (B.92) \]
Table B.2: Units for variables used in the kernel transformations. The equation numbers for the corresponding quantities are also indicated for reference.

<table>
<thead>
<tr>
<th>Transformed Quantity</th>
<th>Conserved Quantity</th>
<th>See section</th>
<th>( P_i )</th>
<th>( S )</th>
<th>( Q_i )</th>
<th>( C_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \psi )</td>
<td>KE and Momentum</td>
<td>B.2.1</td>
<td>( \text{kg/s} )</td>
<td>( \text{kg} )</td>
<td>( \text{kg/s}^2 )</td>
<td>( \text{s}^{-1} )</td>
</tr>
<tr>
<td>( \rho \psi )</td>
<td>KE and Momentum</td>
<td>B.1.2</td>
<td>( \text{m}^3/\text{s} )</td>
<td>( \text{m}^6/\text{kg} )</td>
<td>( \text{kg/s}^2 )</td>
<td>( \text{kg/m}^3 \text{s} )</td>
</tr>
<tr>
<td>( \psi )</td>
<td>Fluxes of KE and Momentum</td>
<td>B.2.1</td>
<td>( \text{kg/m/s}^2 )</td>
<td>( \text{kg/m/s} )</td>
<td>( \text{kg/m/s}^3 )</td>
<td>( \text{s}^{-1} )</td>
</tr>
<tr>
<td>( \rho \psi )</td>
<td>Fluxes of KE and Momentum</td>
<td>B.2.2</td>
<td>( \text{m}^4/\text{s}^2 )</td>
<td>( \text{m}^7/\text{kg} \text{s} )</td>
<td>( \text{kg/m/s}^3 )</td>
<td>( \text{kg/m}^3 \text{s} )</td>
</tr>
</tbody>
</table>

In the following section we derive eddy time scale for cases which involve transformation of \( \rho \psi \). For situations where \( \psi \) is transformed, the expressions are given based on what is available in the literature [13, 24].

B.3.1 Transformations Involving \( \rho \psi \)

When \( \rho \psi \) is transformed, the eddy energy (\( Q_e \)) can be denoted as

\[
Q_e = Q_y + \sum_j T_{yj} Q_j. \tag{B.93}
\]

The dimensions for \( Q_e \) depends on the conservation laws enforced during kernel transformation. When momentum and kinetic energy are conserved, \( Q_e \) scaled with density (\( \rho_e \)) and eddy length (\( \ell \)) has the dimensions of \( \text{m}^2/\text{s}^2 \). Now the following relationship can be developed based on scaling analysis,

\[
\left( \frac{\ell}{\tau_e} \right)^2 \sim \frac{Q_e}{\rho_e \ell^2}. \tag{B.94}
\]

Some of the energy available with the eddy is dissipated by the viscous effects. To account for these effects a model constant \( Z \) is introduced, as discussed in §3.2. However, following the same arguments of scaling analysis the term representing these effects should have the dimensions of \( \text{m}^2/\text{s}^2 \), and the time scale expression can be denoted as

\[
\left( \frac{\ell}{\tau_e} \right)^2 \sim \left[ \frac{Q_e}{\rho_e \ell^2} - Z \left( \frac{\nu_e}{\ell} \right)^2 \right], \tag{B.95}
\]

where \( \nu_e^2/\ell^2 \) has units of \( \text{m}^2/\text{s}^2 \).

Following the same procedure, when momentum and kinetic energy fluxes are conserved, \( Q_e \) is scaled with \( \int_{y_0}^{y_0 + \ell} \rho u \, dy \), to obtain dimensions of \( \text{m}^2/\text{s}^2 \). In this case, the time-scale expression can be denoted as

\[
\left( \frac{\ell}{\tau_e} \right)^2 \sim \left[ \frac{Q_e}{\int_{y_0}^{y_0 + \ell} \rho u \, dy} - Z \left( \frac{\nu_e}{\ell} \right)^2 \right]. \tag{B.96}
\]
References


