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# *Turbulence Transport Equations for Variable-Density Turbulence and Their Relationship to Two-Field Models*

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# TURBULENCE TRANSPORT EQUATIONS FOR VARIABLE-DENSITY TURBULENCE AND THEIR RELATIONSHIP TO TWO-FIELD MODELS

by

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ABSTRACT

This study gives an updated account of our current ability to describe multimaterial compressible turbulent flows by means of a one-point transport model. Evolution equations are developed for a number of second-order correlations of turbulent data, and approximations of the gradient type are applied to additional correlations to close the system of equations. The principal fields of interest are the one-point Reynolds tensor for variable-density flow, the turbulent energy dissipation rate, and correlations for density-velocity and density-density fluctuations. This single-field description of turbulent flows is compared in some detail to two-field flow equations for nonturbulent, highly dispersed flow with separate variables for each field. This comparison suggests means for improved modeling of some correlations not subjected to evolution equations.

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## 1. INTRODUCTION

Turbulence in complex, high-speed, high-Reynolds number flows has been of wide Laboratory interest for many years. Predictive capabilities in the Inertial Confinement Fusion (ICF) and certain Strategic Defense Initiative (SDI) programs have relied crucially on modeling the effects of material mixing and enhanced momentum and thermal transport brought about by turbulence. The Laboratory's ability to model turbulence has improved significantly with the advent of high-speed computers and increased theoretical knowledge about the proper manner of modeling the ensemble-averaged Navier Stokes equations. Our recent goals have focused on understanding the theoretical foundations of variable-density turbulence and mixing and the implementations of simple models into existing computer

codes, like CAVEAT [1]. This manuscript will outline our current state of expertise in modeling variable-density turbulence and propose some simpler models for everyday use in laboratory codes.

We are primarily interested in describing multimaterial compressible turbulent flow; the different materials might not be initially mixed, which means that the mixing process itself must be modeled as well. The potential applications of such a description range from volcanic eruptions, where a plume of hot air containing ash and rocks mixes with surrounding cold air, to consideration of laser-driven ICF, where the mixing of the outer shell and the inner fuel may lead to decreased neutron yield. In the first case, the mixing is predominantly due to highly nonlinear stages of Kelvin-Helmholtz instability at the interface between hot and cold fluids; in the second instance, Richtmeyer-Meshkov and Rayleigh-Taylor instabilities can play a dominant role. Other temperature and pressure regimes can be studied through laboratory experiments, such as the shock-tube experiments of Sturtevant [2], Houas *et al.* [3], and Andronov *et al.* [4]; in these experiments, a thin (1 mm or less) membrane initially separating two test gases of different densities is shattered by an incident shock wave. The details of membrane destruction are poorly characterized, however, but subsequent shocks reflected from the end wall interact with the mixing zone established by initial shock passage to greatly increase the growth rate of the mixed region. In addition, the AWE in Great Britain has performed experiments by accelerating a tank containing two incompressible materials initially in a stable configuration downwards at about 40 times the acceleration due to gravity [5].

All of these applications are time-unsteady flows involving two or more materials. Turbulence models that attempt to analyze and characterize these flows need to pay attention to issues of initialization of turbulence field variables, which is a serious challenge for most usual turbulence theories. Ideally, the model should mimic the linear phase of instability as well as the fully turbulent late-stage mixing. Traditionally, two approaches have been taken. One scheme postulates the existence of multiphase flow equations

[6,7] while the other uses the more usual Reynolds decomposition of the Navier-Stokes equations for a single field with potentially large density variations [8-12]. The different approaches are compatible and, as we shall show here, an equivalence between schemes can be demonstrated in some interesting cases.

From our single-field modeling, we produced a report a few years ago that used standard turbulence closures [12], and the first part of this work will revisit those equations, modifying them at some points and looking more closely at the assumptions of closure. In that earlier effort, we realized that the Reynolds stress models must consistently include evolution equations for all relevant second-order correlations, in order to describe flows of this nature adequately. Since then, the formal parallels between two-field formulations and the unmodeled turbulence equations were exposed by us in an unpublished and unfinished working paper, and have more recently been completed by Lance Collins at Penn State. We will be reviewing these results near the end of this paper. First, however, in Section 3, we derive the turbulence equations in a standard fashion by dividing the flow variables into mean and fluctuating parts. The resulting equations are closed by postulating, with some (admittedly incomplete) physical justifications, appropriate models for unknown higher moments of the fluctuating variables. Because instability-driven mixing is of particular interest to laboratory programs, we then specialize the equations in Section 4 to the cases of Rayleigh-Taylor and Kelvin-Helmholtz instabilities and compare the behavior of our equations to other published work. Finally, in Section 5 we show an interesting correspondence between our unmodeled equations and the two-field flow equations describing nonturbulent highly-dispersed flow with separate field variables for two-field flow. We believe that new directions in variable-density turbulence modeling will arise from considering this correspondence.

## 2. DESCRIPTION OF TURBULENT FLOW OF COMPRESSIBLE FLUIDS

### 2.1. Formulation

Turbulent flows develop whenever incipient instabilities, driven by the advection terms in the flow dynamics, are not dissipated quickly enough by the action of fluid viscosity. As a result, fully developed turbulence is often characterized by the interactions of random, nonlinear modes of motion, typically swirling, overlapping eddies of fluid. Despite the appearance of complete disorder, turbulent flows often exhibit rather universal average behavior. Boundary layers, jets, and wakes all have been studied extensively in the past and, while the details of each experiment are not repeatable, even by a single researcher, the observables in each set of experiments have been well correlated and used to great advantage by engineers and scientists worldwide. The basic notion is that while turbulence cannot be analyzed in every detail, either by computer or by experiment, enough can be extracted from physical or numerical experiments to deduce the effects of turbulence on what we routinely observe in the typical design of aircraft, mixing vessels, heat exchangers, and piping systems.

The point of departure for nearly all engineering analysis of turbulent flows is the set of Navier-Stokes equations for compressible, variable-density flow of a single material. As convenience dictates, we denote vectors and tensors in Cartesian coordinate form or by bold letters. (The tensor symbols will be Latin capitals or Greek.) The equations for density, velocity, and internal energy are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \,, \tag{1}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} \,, \tag{2}$$

$$\frac{\partial \rho I}{\partial t} + \nabla \cdot (\rho \mathbf{u} I) = \boldsymbol{\sigma} : \nabla \mathbf{u} + \nabla \cdot (\kappa \nabla T) \,, \tag{3}$$

where $\sigma_{ij} = -P\delta_{ij} + \tau_{ij}$. Generally, the pressure $P$ is a function of species mass fractions $c_i$, as well as $\rho$ and $I$. The viscous stress $\tau$ is taken as

$$\tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot\mathbf{u}\right) . \tag{4}$$

The molecular viscosity $\mu$ and the thermal conductivity $\kappa$ are taken as constants for this analysis.

For the mass fraction, we apply Fick's law of diffusion with a constant diffusion coefficient $D$:

$$\frac{\partial \rho c_i}{\partial t} + \nabla\cdot(\rho \mathbf{u} c_i) = \nabla\cdot(\rho D \nabla c_i) . \tag{5}$$

Typically, we separate turbulent flow properties into mean parts, such as the turbulent velocity profile in a pipe, which for an incompressible fluid is a radial function only, and fluctuating parts that account for eddy motions that are not reproducible or describable in detail. The details of these fluctuations are determined in a strict sense by extremely fine-scale irregularities in the boundary and initial conditions of the experiment, but mean-flow properties are assumed to be deterministic and reproducible.

We denote average properties by overbars and fluctuations by primes. The appropriate average is taken over many members of an ensemble of experiments that are indistinguishable macroscopically, but may differ in microscopic detail in no controllable manner. Thus, $\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}'$, $P = \overline{P} + P'$, $\rho = \overline{\rho} + \rho'$, etc.

Two important measures of a turbulent regime are $K(\mathbf{x},t)$, the turbulent kinetic energy per unit mass, and $\epsilon(\mathbf{x},t)$, the rate of dissipation of turbulent kinetic energy per unit mass (i.e., irreversible conversion into internal energy). These are defined explicitly below by ensemble averages. One identifies a turbulent velocity scale $K^{1/2}$, a turbulent time scale $t_{\text{turb}} = K/\epsilon$, and a turbulent length scale $L_{\text{turb}} = K^{3/2}/\epsilon$. These may be thought to characterize the motion, period, and size of the dominant turbulent eddies. They may be compared to scales for the mean flow: $c_s$ = sound speed, $t_{\text{mean}} \approx |\partial\overline{u}_i/\partial x_j|^{-1}$, and $L_{\text{mean}}$ = scale for variation in physical space of mean-flow properties.

In conventional one-point analyses of constant-density flows, the assumption $L_{\text{turb}}/L_{\text{mean}} \lesssim 1$ is commonly made, explicitly or implicitly, and facilitates the modeling of the pressure-velocity correlation $\overline{p'\partial u_i'/\partial x_j}$. Realistically, $L_{\text{turb}}$ and $L_{\text{mean}}$ may have comparable size, though one expects $L_{\text{turb}}/L_{\text{mean}}$ not to exceed unity; otherwise, the logic of separation of variables into mean and fluctuating parts is sacrificed.

The assumption $t_{\text{turb}}/t_{\text{mean}} \ll 1$ is also frequently made. It suggests, as noted by Lumley [8], that the distribution of turbulence modes among different length scales has time to achieve approximate spectral equilibrium, and this underlies the logic of one-point modeling. It is an essential assumption in the argument for closures of otherwise undetermined correlations. In the case of constant-density fluids, the paradigm for such closures is (with account for symmetry if $X'$ has factors of $\mathbf{u}'$):

$$\overline{u_i'X'} = (\text{constant})\,\frac{K}{\epsilon}\,\overline{u_i'u_n'}\,\frac{\partial}{\partial x_n}\overline{X}\,. \tag{6}$$

Hereafter, we refer to this as a gradient closure or gradient approximation. Realistically, $t_{\text{turb}}$ need not be small compared with $t_{\text{mean}}$ in regimes of rapid time and space variation, such as shock-driven flows or interfacial instability flows. Therefore, it is preferable to construct evolution equations for what appear to be the more important second-order correlations. We cannot avoid gradient closures for some higher-order correlations entirely. By limiting their use to terms of presumed secondary importance, we hope to capture the main physical consequences of turbulence in evolution equations.

A third inequality assumed for the purposes of this paper is that the sound transit time $L_{\text{mean}}/c_s$ across typical mean-flow length scales be much less than the dominant-eddy turnover time, which translates into

$$\frac{\sqrt{K}}{c_s} \ll \frac{L_{\text{turb}}}{L_{\text{mean}}} \lesssim 1\,.$$

That is, the turbulent velocity scale is subsonic. Then the fluctuating velocity field may be taken as divergenceless; $\nabla \cdot \mathbf{u}' = 0$. We qualify this by allowing nonzero $\nabla \cdot \mathbf{u}'$ when heat conduction or mass diffusion between species is important; see Section 3.4.

Fourth, we assume that the turbulent Reynolds number of the system, defined by $(Re)_{\rm turb} = \rho K^2/(\mu\epsilon)$, be large compared to unity. This condition separates the dissipation scale from the dominant-eddy scales, allowing the neglect of viscous diffusion and viscous stresses relative to turbulent diffusion and pressure effects, respectively; and, as in the constant density case, is a requirement for the viability of a one-point model in which the dimensionless parameters of the model are hoped to have constant values valid for a general class of phenomena.

## 2.2. Mass-Weighted Averages and Mean Flow Equations

For any fluid variable $X$, the separation $X = \overline{X} + X'$ (Reynolds decomposition) is based on the uniformly-weighted ensemble average $\overline{X}$. The separation $X = \tilde{X} + X''$ (Favre decomposition) is based on the mass-weighted ensemble average $\tilde{X}$, defined as

$$\tilde{X} = \overline{\rho X}/\overline{\rho}\,.$$

Such averages, and especially the mass-averaged fluid velocity, appear naturally in conservation relations, as is the case in multispecies flow equations [13].

We shall use the following relations among these constructs repeatedly:

$$\begin{aligned}
\overline{X'} &= \overline{\rho X''} = 0\,,\\
\overline{XY} &= \overline{X}\,\overline{Y} + \overline{X'Y'}\,,\\
\overline{\rho XY} &= \overline{\rho}\tilde{X}\tilde{Y} + \overline{\rho X''Y''}\,,\\
\overline{X'Y} &= \overline{X'Y'} = \overline{X'Y''}\,,\\
\overline{X''} &= \overline{X} - \tilde{X} = -\overline{\rho' X'}/\overline{\rho}\,.
\end{aligned}$$

The list of important averages begins with $\overline{\rho}$ and the mass-weighted velocity $\tilde{\mathbf{u}} = \overline{\rho\mathbf{u}}/\overline{\rho}$. Then come the density-velocity correlation $\mathbf{A}$ and the associated velocity $\mathbf{a}$:

$$\mathbf{A} = \overline{\rho'\mathbf{u}'} = \overline{\rho'\mathbf{u}''} \quad ; \quad \mathbf{a} = \mathbf{A}/\overline{\rho} = -\overline{u''}\,. \tag{7}$$

Note that $\mathbf{A}$ is the net mass flux relative to $\overline{\mathbf{u}}$, the unweighted average velocity, and that

$$\tilde{\mathbf{u}} = \overline{\mathbf{u}} + \mathbf{A}/\overline{\rho} = \overline{\mathbf{u}} + \mathbf{a}\,, \tag{8}$$

$$\mathbf{u}'' = \mathbf{u}' - \mathbf{A}/\overline{\rho} = \mathbf{u}' - \mathbf{a}\,. \tag{9}$$

Next are the generalized Reynolds stress tensor $\mathbf{R}$ and the turbulent flux of internal energy $\mathbf{S}$:

$$R_{ij} = \overline{\rho u_i'' u_j''} = \overline{\rho}\,\overline{u_i' u_j'} - \overline{\rho} a_i a_j + \overline{\rho' u_i' u_j'}\,, \tag{10}$$

$$S_i = \overline{\rho I'' u_i''} = \overline{\rho}\,\overline{I' u_i'} - a_i \overline{\rho' I'} + \overline{\rho' I' u_i'}\,. \tag{11}$$

Ensemble averages of the flow equations (1), (2), (3), and (5) now yield the mean-flow equations:

$$\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial}{\partial x_n}(\overline{\rho}\tilde{u}_n) = 0\,, \tag{12}$$

$$\frac{\partial \overline{\rho}\tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_n}(\overline{\rho}\tilde{u}_n\tilde{u}_i) + \frac{\partial}{\partial x_n}R_{ni} = -\frac{\partial \overline{P}}{\partial x_i} + \frac{\partial \overline{\tau}_{ni}}{\partial x_n}\,, \tag{13}$$

$$\frac{\partial}{\partial t}\overline{\rho}\tilde{I} + \frac{\partial}{\partial x_n}\left(\overline{\rho}\tilde{u}_n\tilde{I}\right) + \frac{\partial}{\partial x_n}S_n = -\overline{P}\nabla\cdot\overline{\mathbf{u}} - \overline{P'\nabla\cdot\mathbf{u}'}$$

$$+ \overline{\tau}_{nm}\frac{\partial \overline{u}_n}{\partial x_m} + \overline{\tau'_{nm}\frac{\partial u'_n}{\partial x_m}} + \nabla\cdot(\kappa\nabla\overline{T})\,, \tag{14}$$

$$\frac{\partial}{\partial t}\overline{\rho}\tilde{c}_i + \frac{\partial}{\partial x_n}(\overline{\rho}\tilde{u}_n\tilde{c}_i) + \frac{\partial}{\partial x_n}\overline{\rho u_n'' c_i''} = \frac{\partial}{\partial x_n}\left(\overline{\rho}D\frac{\partial \tilde{c}_i}{\partial x_n}\right) + \frac{\partial}{\partial x_n}\overline{\rho D\frac{\partial}{\partial x_n}c_i''}\,. \tag{15}$$

With $\nabla\cdot\mathbf{u}' = 0$, as assumed above, the $P'\nabla\cdot\mathbf{u}'$ term drops, and

$$\overline{\tau'_{nm}\frac{\partial u'_n}{\partial x_m}} = \frac{1}{2}\mu\overline{\left(\frac{\partial u'_n}{\partial x_m} + \frac{\partial u'_m}{\partial x_n}\right)\left(\frac{\partial u'_n}{\partial x_m} + \frac{\partial u'_m}{\partial x_n}\right)}\,,$$

which is observed to be nonnegative. In the more general case, we can write

$$\overline{\tau'_{nm}\frac{\partial u'_n}{\partial x_m}} = \frac{1}{2}\mu\sum_{n,m}\overline{\left(\frac{\partial u'_n}{\partial x_m}+\frac{\partial u'_m}{\partial x_n}-\frac{2}{3}(\nabla\cdot\mathbf{u}')\delta_{nm}\right)^2},$$

which is still nonnegative.

## 2.3. Energy and Energy Dissipation

The inertial and advection terms of averaged evolution equations are best expressed by mass-weighted averages, because physical conservation applies to aggregates of mass, momentum, energy, etc. The stresses, lacking factors of $\rho$, are probably best described in terms of unweighted averages.

The Favre technique points to a conception that may usefully guide modeling. The Favre velocity $\tilde{u}$ is a mean variable that includes, in addition to $\overline{u}$, the part of the velocity fluctuation correlated with density fluctuation. Then $u''$ is not the whole of the velocity fluctuation, but only the part uncorrelated with density; $\overline{\rho u''} = 0$. How quadratic and higher functions of velocity fluctuation, whether in unweighted or in mass averages, contribute to density-correlated or uncorrelated effects is not, in general, easy to sort out.

For the ensemble average of total fluid kinetic energy density, we have

$$\overline{\tfrac{1}{2}\rho\mathbf{u}^2} = \tfrac{1}{2}\,\overline{\rho}(\tilde{\mathbf{u}})^2 + \tfrac{1}{2}\,\overline{\rho(\mathbf{u}'')^2}\,.$$

If we regard $\frac{1}{2}\,\overline{\rho}(\tilde{\mathbf{u}})^2$ as the energy density due to the combined mean and density-correlated turbulent motion, then $\frac{1}{2}\overline{\rho(\mathbf{u}'')^2} = \frac{1}{2}$ trace $R_{ij}$ measures the residual turbulent motion. The generalizations of $K$, the turbulent energy per unit mass, and $\epsilon$, the dissipation rate for $K$, as originally defined for constant-density one-phase flow, are now chosen to be

$$\overline{\rho}K = \tfrac{1}{2}\text{ trace } R_{ij}\,, \tag{16}$$

$$\overline{\rho}\epsilon = \overline{\tau'_{nm}\partial u'_n/\partial x_m}\,. \tag{17}$$

The first definition motivates the second, for $\overline{\rho}\epsilon$ as defined here represents the irreversible conversion of turbulent kinetic energy into internal energy in the $\overline{\rho}\tilde{I}$ evolution equation

and is also (one-half of) the decay term in the trace of the $R_{ij}$ evolution equation, to be given in Section 3.

Also suggestive are the equations

$$\overline{\rho u_i' u_j'} = \overline{\rho u_i'' u_j''} + \bar{\rho} a_i a_j \ ,$$

$$\overline{u_i'' u_j''} = \overline{u_i' u_j'} + a_i a_j \ .$$

These are relations between nonnegative definite tensors with nonnegative diagonal elements. They indicate that $\overline{\rho u_i' u_j'}$ and $\overline{u_i'' u_j''}$ carry more of the effect of the density-correlated turbulent motion than do $\overline{\rho u_i'' u_j''}$ and $\overline{u_i' u_j'}$, respectively.

### 2.4. Turbulence Variables of the Present Theory (Summary)

The flow equations for the mean variables $\bar{\rho}$, $\tilde{u}$, $\tilde{I}$, and $\tilde{c}_i$ introduce second-order averages, and equations for the latter introduce further correlations. A judgment must be made as to which turbulent variables are to be subjected to evolution equations and which are to be regarded as secondary and modeled by constraint equations, relating them to the more primary data at a common time.

In the present paper, we prescribe evolution equations for **R**, **S**, **a**, or equivalently $\mathbf{A} = \bar{\rho}\mathbf{a}$, and also for a density self-correlation $b$ defined by

$$b = -\overline{\rho' \left(\frac{1}{\rho}\right)'} \ . \tag{18}$$

Alternatively, because $-\overline{\rho'(1/\rho)'} = +\overline{(\bar{\rho} - \rho)/\rho}$,

$$b = \bar{\rho}\,\overline{\left(\frac{1}{\rho}\right)} - 1 \ . \tag{19}$$

A third alternative,

$$b = \overline{-\rho' \left(\frac{1}{\bar{\rho}+\rho'} - \frac{1}{\bar{\rho}}\right)} = \overline{(\rho')^2/(\rho\bar{\rho})} \ ,$$

makes clear that $b$ is nonnegative and that the approximation $b \approx \overline{(\rho')^2}/(\bar{\rho})^2$ would apply if $\rho' \ll \bar{\rho}$. We also encounter $w = \overline{\rho' I'}/\bar{\rho}$ in the evolution equation for **S** and write an evolution equation for $w$ but without modeling it in detail.

As a simplified alternative to the $\mathbf{R}$ equations, we can set forth $K$ and $\epsilon$ equations as generalizations of the $K$–$\epsilon$ model for incompressible flow. In these, the anisotropic part of $\mathbf{R}$ is replaced by its gradient approximation:

$$R_{ij} - \frac{2}{3}\bar{\rho}K\delta_{ij} = -\mu_t\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\nabla\cdot\tilde{\mathbf{u}}\right) , \tag{20}$$

with $\mu_t$ the turbulent viscosity, given by

$$\mu_t = C_\mu \bar{\rho} K^2/\epsilon \quad ; \quad c_\mu = \text{ constant} .$$

The a equation requires consideration of $\overline{u_i'u_j'}$. We shall finesse this by expressing $\overline{u_i'u_j'}$ in terms of primary data and a triple correlation, then applying a gradient approximation to the latter:

$$\overline{u_i'u_j'} = a_i a_j + R_{ij}/\bar{\rho} \; - \overline{\rho' u_i' u_j'}/\bar{\rho} , \tag{21}$$

$$\overline{\rho' u_i' u_j'} = -C_{Da}\frac{K}{\epsilon}\left(R_{in}\frac{\partial a_j}{\partial x_n} + R_{jn}\frac{\partial a_i}{\partial x_n}\right) \; ; \; C_{Da} = \text{ constant} . \tag{22}$$

Some of the gradient closures involved in the next section have a rationale based on consideration of terms likely to be dominated in evolution equations for the next higher-order equations as noted in Section 3.2.

## 2.5. Realizability

Realizability, the notion applied by Schumann to constant-density flows, also applies to variable-density flows. If $v_i$ , $1 \le i \le N$, is any sequence of fluid variables, and $e_i$ , $1 \le i \le N$, is any constant vector, then $\rho(e_i v_i)^2 \ge 0$ and hence

$$e_i e_j \, \overline{\rho v_i v_j} \ge 0 .$$

Then $\overline{\rho v_i v_j}$ is a nonnegative definite tensor, and all of its principal minors have nonnegative determinants. From this, we can infer that

$$R_{11} \ge 0 , \quad R_{11}R_{22} - (R_{12})^2 \ge 0 , \quad \det R_{ij} \ge 0 ,$$

and

$$\overline{\rho} a_1 = \overline{\rho' u_1''} = \overline{(\rho'/\rho^{1/2})\,\rho^{1/2} u_1''} \leq \left(\overline{(\rho')^2/\rho}\right)^{1/2} \left(\overline{\rho u_1'' u_1''}\right)^{1/2} ,$$

whence, applying the third definition of $b$ in the previous section,

$$a_1^2 \leq b R_{11}/\overline{\rho} .$$

Gradient approximations are not always consistent with realizability and should be checked in practical applications.

## 3. TURBULENCE EQUATIONS

A summary of the evolution equations to be developed for the primary turbulence variables is given in Section 3.9.

### 3.1. Preliminaries

We note that, in view of (1), (12),

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_n}(\rho u_n u_i) = \rho \frac{\partial u_i}{\partial t} + \rho u_n \frac{\partial u_i}{\partial x_n} ,$$

and

$$\frac{\partial}{\partial t}(\overline{\rho} \tilde{u}_i) + \frac{\partial}{\partial x_n}(\overline{\rho} \tilde{u}_n \tilde{u}_i) = \overline{\rho} \frac{\partial \tilde{u}_i}{\partial t} + \overline{\rho} \tilde{u}_n \frac{\partial \tilde{u}_i}{\partial x_n} .$$

Subtracting $(\rho/\overline{\rho})$ times Eq. 13 from Eq. 2, and utilizing the above, we get a useful form for the $\mathbf{u}''$ equation:

$$\begin{aligned} \frac{\partial}{\partial t}(\rho u_i'') + \frac{\partial}{\partial x_n}(\rho u_n u_i'') + \rho u_n'' \frac{\partial \tilde{u}_i}{\partial x_n} - \frac{\rho}{\overline{\rho}} \frac{\partial}{\partial x_n} R_{ni} \\ = -(\rho/\overline{\rho}) \frac{\partial \overline{\sigma}_{ni}}{\partial x_n} + \frac{\partial \sigma_{ni}}{\partial x_n} . \end{aligned} \tag{23}$$

A second useful form (set $\tilde{u}_i = u_i - u_i''$ in the third term of (23)) is

$$\frac{\partial u_i''}{\partial t} + \tilde{u}_n \frac{\partial u_i''}{\partial x_n} + u_n'' \frac{\partial u_i}{\partial x_n} - \frac{1}{\overline{\rho}} \frac{\partial R_{ni}}{\partial x_n} = -\frac{1}{\overline{\rho}} \frac{\partial \overline{\sigma}_{ni}}{\partial x_n} + \frac{1}{\rho} \frac{\partial \sigma_{ni}}{\partial x_n} . \tag{24}$$

As a notational device aimed at conciseness without loss of clarity, we write

$$\sum{}^{\bullet} \text{(product of tensors)}$$

to denote a symmetrizing procedure with respect to the free indices in [illegible] ed product of tensors. Specifically, $\sum^s$ is the instruction, first, to replace each [illegible] tensors by its symmetric part with respect to its free indices, and second, to supplement the result by adding to it the minimal number of like terms, with free indices permuted, to make the final result symmetric. One could also make the notation more complete by writing $\sum^{N\,s}$ to show that there are $N$ permutations in the final result. For example,

$$\sum{}^s \frac{\partial}{\partial x_n}(B_i C_{njk}) = \sum{}^s \frac{\partial}{\partial x_n}\left[B_i\left(C_{njk} + C_{nkj}\right)/2\right]$$
$$= \frac{1}{2}\frac{\partial}{\partial x_n}\left(B_i C_{njk} + B_i C_{nkj} + B_j C_{nki} + B_j C_{nik} + B_k C_{nij} + B_k C_{nji}\right),$$

and, if $a_i = b_i + c_i$,

$$a_i a_j a_k = b_i b_j b_k + \sum{}^{3\,s} b_i b_j c_k + \sum{}^{3\,s} b_i c_j c_k + c_i c_j c_k\,.$$

Note that $\sum^s \frac{\partial}{\partial x_n}(B_i C_{njk})$ differs from $\frac{\partial}{\partial x_n}\sum^s(B_i C_{njk})$ because the latter is to be symmetrized over four free indices.

Now let the definition of the $R$ tensor be generalized to

$$R_{ijk\ldots m} = \overline{\rho u_i'' u_j'' u_k'' \ldots u_m''}\,.$$

We observe that

$$\sum{}^s \overline{u_j'' \ldots u_m''\left[\frac{\partial}{\partial t}(\rho u_i'') + \frac{\partial}{\partial x_n}(\rho u_n u_i'')\right]} = \frac{\partial}{\partial t}R_{ij\ldots m} + \frac{\partial}{\partial x_n}(\bar{u}_n R_{ij\ldots m}) + \frac{\partial}{\partial x_n}R_{nij\ldots m}\,.$$

More generally, if $X_1, X_2, \ldots X_m$ are any fluid variables, then

$$\sum{}^{m\,s} \overline{X_2 X_3 \ldots X_m\left[\frac{\partial}{\partial t}(\rho X_1) + \frac{\partial}{\partial x_n}(\rho u_n X_1)\right]} = \frac{\partial}{\partial t}\overline{\rho X_1 X_2 \ldots X_m}$$
$$+ \frac{\partial}{\partial x_n}\overline{\rho u_n X_1 X_2 \ldots X_m}\,.$$

### 3.2. Equation for the Generalized Reynolds Stress

To obtain an evolution equation for **R**, multiply (23) by $u_j''$, apply $\sum^s$, and take the ensemble average. Apply $\overline{\rho \mathbf{u}''} = 0$ and

$$\overline{u_j''\frac{\partial \sigma_{ni}}{\partial x_n}} = \overline{u_j''\left(\frac{\partial \bar{\sigma}_{ni}}{\partial x_n} + \frac{\partial \sigma'_{ni}}{\partial x_n}\right)} = -a_j\frac{\partial \bar{\sigma}_{ni}}{\partial x_n} + \overline{u_j'\frac{\partial \sigma'_{ni}}{\partial x_n}}\,,$$

and integrate the last term by parts. Then

$$\frac{\partial}{\partial t}R_{ij} + \frac{\partial}{\partial x_n}(\tilde{u}_n R_{ij}) + \frac{\partial}{\partial x_n}R_{nij} + R_{in}\frac{\partial \tilde{u}_j}{\partial x_n} + R_{jn}\frac{\partial \tilde{u}_i}{\partial x_n}$$
$$= \sum{}^{s}\left\{a_i\left(\frac{\partial \overline{P}}{\partial x_j} - \frac{\partial}{\partial x_n}\overline{\tau}_{nj}\right) - \frac{\partial}{\partial x_n}\overline{u_i'(\delta_{nj}P' - \tau_{nj}')}\right.$$
$$\left. + \overline{P'\frac{\partial u_i'}{\partial x_j}} - \overline{\frac{\partial u_i'}{\partial x_n}\tau_{nj}'}\right\}.$$

The terms requiring modeling are, in order of occurrence in this equation, (1) the triple correlations $R_{nij}$, (2) stress-velocity correlations occurring in a transport term, (3) a correlation of pressure and velocity gradient that is traceless for the assumed case $\nabla\cdot\mathbf{u}' = 0$, and (4) the average of $(\partial u_i'/\partial x_n)\tau_{nj}'$, whose trace represents the dissipation of turbulent energy, and whose residual, traceless part may be grouped with the term (3). Insight provided by a spectral approach to constant-density flow suggests, by analogy to the present case, that the term (4) will be diagonal for large turbulent Reynolds number, that is, for large $\rho K^2/(\mu\epsilon)$; see Section VA of [14].

We now exhibit a rationale for a gradient approximation of the $R_{nij}$ term. Multiply (23) by $u_j''u_k''$, apply $\sum^s$, and take the ensemble average. The left side of the resulting equation is

$$\frac{\partial}{\partial t}R_{ijk} + \frac{\partial}{\partial x_n}(\tilde{u}_n R_{ijk}) + \frac{\partial}{\partial x_n}R_{nijk} + \sum{}^{s}\left\{R_{ijn}\frac{\partial \tilde{u}_k}{\partial x_n} - (R_{jk}/\overline{\rho})\frac{\partial}{\partial x_n}R_{ni}\right\}.$$

Set

$$R_{nijk} = R^c_{nijk} + \sum{}^{s}{}^{3} R_{ij}R_{nk}/\overline{\rho}\,.$$

This is, in the first instance, simply a definition of the fourth-order cumulant $\mathbf{R}^c$. But if $\rho$ were constant and the velocity fluctuations followed a gaussian random distribution law, then $\mathbf{R}^c$ would vanish. Let us disregard $\mathbf{R}^c$ in the present case. Then the left side simplifies to

$$\frac{\partial}{\partial t}R_{ijk} + \frac{\partial}{\partial x_n}(\tilde{u}_n R_{ijk}) + \sum{}^{s}\left\{R_{in}\frac{\partial}{\partial x_n}(R_{jk}/\overline{\rho}) + R_{ijn}\frac{\partial \tilde{u}_k}{\partial x_n}\right\}.$$

Next, we suppose that in the absence of the source term $\sum^s R_{in}\frac{\partial}{\partial x_n}\left(R_{jk}/\overline{\rho}\right)$, the turbulent stresses on the right-hand side of the $R_{ijk}$ equation would drive $R_{ijk}$ to zero on the turbulent time scale $t_{\text{turb}}$, and let this effect be modeled by a decay term proportional to $(\epsilon/K)R_{ijk}$. If the inertial terms and any transport terms implicit in the stresses change on a time scale of $t_{\text{mean}}$, and $t_{\text{mean}} \gg t_{\text{turb}}$, then we may have an approximate equilibrium set up, expressed by

$$R_{ijk} = -C_{DR}\frac{K}{\epsilon}\sum^s R_{in}\frac{\partial}{\partial x_n}\left(R_{jk}/\overline{\rho}\right) .$$

This takes care of the modeling of $\frac{\partial}{\partial x_n}R_{nij}$. If there were residual effects correlated with density, they might be simulated by terms proportional to $\sum^s \frac{\partial}{\partial x_n}\left(a_i R_{nj}\right)$ and requiring an additional dimensionless phenomenological constant; we do not include such terms in the present theory.

Next, we discard the transport terms of the form

$$\frac{\partial}{\partial x_n}\left[\overline{u'_j\left(\delta_{nj}P' - \tau'_{nj}\right)} + \overline{u'_j\left(\delta_{ni}P' - \tau'_{ni}\right)}\right] .$$

This follows the precedent established for treatment of constant-density one-phase flow, though the justification remains obscure.

Next, we consider the pressure-velocity gradient correlations. Again, we make extensive use of ideas of other researchers. For constant-density flows, one usually solves a Poisson equation for $P'$, forms the correlations of interest, and notices that there are two types of terms involved: those specified by a product of turbulence variables and those with explicit factors of mean velocity gradient. For variable-density flows, even if $\nabla\cdot\mathbf{u}' = 0$ is assumed, the analog of the Poisson equation is more complex:

$$-\frac{\partial}{\partial x_n}\left(\frac{1}{\rho}\frac{\partial}{\partial x_n}P\right)' = \frac{\partial}{\partial x_m}\frac{\partial}{\partial x_n}\left(2\overline{u_n}u'_m + u'_n u'_m - \overline{u'_n u'_m}\right) - u'_m\frac{\partial}{\partial x_m}\frac{\partial}{\partial x_n}\overline{u_n} ,$$

and more difficult to solve for $P'$. We adopt a simpler approach and model the pressure-velocity gradient correlations in complete analogy to the constant-density case. For the "slow" part, we set

$$(\pi^s_R)_{ij} = -C_{1R}\frac{\epsilon}{K}\left(R_{ij} - \frac{1}{3}\delta_{ij}R_{nn}\right) , \tag{25}$$

and for the "rapid" part, we use the straightforward extension of Launder, Reece, and Rodi's [15] simpler model to the variable-density case:

$$(\pi_R^r)_{ij} = C_{2R}\left(R_{in}\frac{\partial \tilde{u}_j}{\partial x_n} + R_{jn}\frac{\partial \tilde{u}_i}{\partial x_n} - \frac{2}{3}\delta_{ij}R_{mn}\frac{\partial \tilde{u}_m}{\partial x_n}\right) . \tag{26}$$

In principle, we should also consider a third contribution arising from the interactions of **a** and the mean pressure gradient. This model would presumably look like

$$(\pi_R^P)_{ij} = -C_{3R}\left(a_i\frac{\partial \overline{P}}{\partial x_j} + a_j\frac{\partial \overline{P}}{\partial x_i} - \frac{2}{3}\delta_{ij}\,\mathbf{a}\cdot\nabla\overline{P}\right) , \tag{27}$$

though we have not explored this possibility in detail in our simulations.

The fourth and last group of terms to be modeled make up the dissipation tensor. Again proceeding from experience with constant-density models, we assume it to be adequately modeled by

$$-\sum{}^{*}\overline{\frac{\partial u_i'}{\partial x_n}\tau_{nj}'} = -\frac{2}{3}\overline{\rho}\epsilon\delta_{ij} + \text{ traceless part} .$$

In the limit of high Reynolds number, $\epsilon$ is expected to be independent of visco[illegible] traceless part is either zero or is lumped with the pressure-velocity gradient correlations [8].

### 3.3. Equation for the Density-Velocity Correlation

We work with $\mathbf{a} = \mathbf{A}/\overline{\rho}$ as our primary variable, instead of $\mathbf{A}$. Because $\mathbf{a} = -\overline{\mathbf{u}''}$, we average (24), and then multiply by $\overline{\rho}$. Observe that with $\nabla\cdot\mathbf{u}' = 0$,

$$\overline{u_n''\frac{\partial}{\partial x_n}u_i} = \overline{u_n''\frac{\partial}{\partial x_n}\overline{u}_i} + \overline{u_n''\frac{\partial}{\partial x_n}u_i'} = -a_n\frac{\partial}{\partial x_n}\overline{u_i} + \frac{\partial}{\partial x_n}\overline{u_n'u_i'} ,$$

and with $b = \overline{\rho}\,\overline{(1/\rho)} - 1$,

$$-\frac{\partial}{\partial x_n}\overline{\sigma}_{ni} + \overline{\frac{\overline{\rho}}{\rho}\frac{\partial}{\partial x_n}\sigma_{ni}} = b\frac{\partial}{\partial x_n}\overline{\sigma}_{ni} + \overline{\rho}\overline{\left(\frac{1}{\rho}\right)'\frac{\partial}{\partial x_n}\sigma_{ni}'} .$$

Hence

$$\frac{\partial}{\partial t}(\overline{\rho}a_i) + \frac{\partial}{\partial x_n}(\overline{\rho}\tilde{u}_n a_i) + \overline{\rho}a_n\frac{\partial}{\partial x_n}\overline{u_i} = \overline{\rho}\frac{\partial}{\partial x_n}\overline{u_n'u_i'} - \frac{\partial}{\partial x_n}R_{ni}$$

$$-b\frac{\partial}{\partial x_n}\overline{\sigma_{ni}} + \overline{\rho}\overline{\left(\frac{1}{\rho}\right)'\left(\frac{\partial P'}{\partial x_i} - \frac{\partial}{\partial x_n}\tau_{ni}'\right)} . \tag{28}$$

Again, we are prepared to ignore the viscous stress terms when compared to pressure effects at high Reynolds number. The contributions from $\overline{\mathbf{u}'\mathbf{u}'}$ and $\mathbf{R}$ from (28) can be written as

$$\overline{\rho}\frac{\partial}{\partial x_n}\overline{u_n'u_i'} - \frac{\partial}{\partial x_n}R_{ni} = \frac{\left(\overline{\rho' u_i' u_n'} - R_{in}\right)}{\overline{\rho}}\frac{\partial\overline{\rho}}{\partial x_n} + \overline{\rho}\frac{\partial}{\partial x_n}(a_n a_i) - \frac{\partial}{\partial x_n}\overline{\rho' u_n' u_i'}\,. \tag{29}$$

The modeled form of $\overline{\rho' u_n' u_i'}$ was given in (22). Finally, the density-pressure correlation in the $\mathbf{a}$ equation is split into two parts: that which responds to mean flow gradients and that which involves only turbulence. The latter ("slow" part) becomes a decay term

$$\pi_a^s = \quad C_{1a}\overline{\rho}\frac{\epsilon}{K}\mathbf{a}\,, \tag{30}$$

while the rapid part introduces a mean velocity gradient term that is modeled as

$$\pi_a^r = C_{2a}\overline{\rho}(\mathbf{a}\cdot\nabla)\tilde{\mathbf{u}}\,. \tag{31}$$

Also, as in the $\mathbf{R}$ equation, terms containing the mean pressure gradient could emerge from the pressure-density correlation in a manner something like

$$\pi_a^p = -C_{3a}b\nabla\overline{P}\,, \tag{32}$$

but this has not been utilized in the current implementations of the model. This completes our specification of the $\mathbf{a}$ equation.

### 3.4. Equation for the Modified Density Self-Correlation

From the mass equation, one may deduce an equation for the specific volume, $v = 1/\rho$, and hence for $\overline{v}$:

$$\frac{\partial\overline{v}}{\partial t} + \overline{\mathbf{u}}\cdot\nabla\overline{v} = \overline{v}\nabla\cdot\overline{\mathbf{u}} - \overline{\mathbf{u}'\cdot\nabla v'} + \overline{v'\nabla\cdot\mathbf{u}'}\,. \tag{33}$$

From this, the equation for $b = \overline{\rho}\,\overline{v} - 1$ follows:

$$\frac{\partial b}{\partial t} + (\overline{\mathbf{u}}\cdot\nabla)b + \frac{b+1}{\overline{\rho}}\nabla\cdot\overline{\rho}\mathbf{a} + \overline{\rho}\nabla\cdot\left(\overline{\left(\frac{1}{\rho}\right)'\mathbf{u}'}\right) - 2\overline{\rho}\overline{\left(\frac{1}{\rho}\right)'\nabla\cdot\mathbf{u}'} = 0 \tag{34}$$

There are two expressions to be modeled. We apply a gradient closure to the first and apply (19):

$$\overline{\left(\frac{1}{\rho}\right)' u_i'} = -C_{Db}\frac{k}{\epsilon}\frac{R_{in}}{\bar{\rho}}\frac{\partial}{\partial x_n}\left(\frac{1+b}{\bar{\rho}}\right) . \tag{35}$$

The last term provides for decay of $b$ and requires some care. As previously stated in this report, we are considering only subsonic turbulence. Therefore, $\nabla \cdot \mathbf{u}'$ is nonzero only in the presence of heat conduction and/or mass diffusion. For example, when two species with different microscopic densities are interdiffusing with a constant diffusion coefficient $D$ at an equilibrium pressure and temperature, then $\rho$ is a function of concentration only and

$$\nabla \cdot \mathbf{u} = -\nabla \cdot \left(\frac{D}{\rho}\nabla\rho\right) . \tag{36}$$

Then

$$\overline{\left(\frac{1}{\rho}\right)' \nabla \cdot \mathbf{u}'} = -\overline{\left(\frac{1}{\rho}\right)' \nabla \cdot \left(\frac{D}{\rho}\nabla\rho\right)'}$$

In the limit of high Peclet number for mass transfer, which is also the limit of small $D$, we model this decay term for $b$ to be independent of $D$, in the same way that energy dissipation $\epsilon$ is independent of viscosity in the limit of high Reynolds number. Thus

$$\bar{\rho}\overline{\left(\frac{1}{\rho}\right)' \nabla \cdot \mathbf{u}'} = -C_{1b}\frac{\epsilon b}{K} . \tag{37}$$

We note two circumstances in which this form is not appropriate. First, if $D$ is large (small Peclet number), the rate of $b$-decay will depend directly on $D$, and not merely on turbulence variables. Second, if $D$ is strictly zero, e.g., for a system of two immiscible incompressible fluids, then $\nabla \cdot u' = 0$ and $b$ would not decay. Questions related to $b$ decay need further study and are not resolved here.

### 3.5. Equation for the Turbulent Heat Flux

From the internal energy equation, the fluctuating momentum equation for $\mathbf{u}''$, and the mass equation, it is straightforward to derive an equation, in the limit of incompressible turbulence, for the turbulent flux of internal energy $\overline{\rho \mathbf{u}'' I''} = \mathbf{S}$:

$$\frac{\partial S_i}{\partial t} + \frac{\partial}{\partial x_n}(\tilde{u}_n S_i) + R_{in}\frac{\partial \tilde{I}}{\partial x_n} + S_n\frac{\partial \tilde{u}_i}{\partial x_n} + \frac{\partial}{\partial x_n}\overline{\rho u_n'' u_i'' I''} = w\frac{\partial \bar{\sigma}_{ni}}{\partial x_n} + \left(a_i\bar{\sigma}_{nm} - \overline{u_i'\sigma_{nm}'}\right)\frac{\partial \tilde{u}_m}{\partial x_n}$$

$$+ \overline{\frac{\partial \sigma'_{ni}}{\partial x_n} I'} - a_i \bar{\rho} \epsilon + \overline{u'_i \frac{\partial u'_n}{\partial x_m} \tau_{nm}} - a_i \frac{\partial}{\partial x_n} \left( \kappa \frac{\partial \bar{T}}{\partial x_n} \right) - \overline{u'_i \frac{\partial}{\partial x_n} \left( \kappa \frac{\partial T'}{\partial x_n} \right)} , \tag{38}$$

where $w = \overline{\rho' I'}/\bar{\rho} = -\overline{I''}$. We will not attempt to propose closures here for all these unknown terms, because we have not had much experience with this equation. We merely point out that pressure-internal energy correlations and pressure-density correlations, such as those found in the **a** equation, should behave in analogous fashions, thereby introducing a decay term and some modified production terms. Furthermore, the triple correlation $\overline{\rho \mathbf{u}'' \mathbf{u}'' I''}$ could also be modeled by the approach used for $\overline{\rho \mathbf{u}'' \mathbf{u}'' \mathbf{u}''}$.

As a simpler alternative for **S**, one could use the standard analogy to the gradient approximation, appealing to the concept of an effective turbulent thermal conductivity:

$$\overline{\rho \mathbf{u}'' I''} = \overline{\rho \mathbf{u}' I''} = -C_{DI} \frac{K}{\epsilon} (\mathbf{R} \cdot \nabla) \tilde{I} . \tag{39}$$

For completeness, an equation for $w$ can be derived to give

$$\frac{\partial \bar{\rho} w}{\partial t} + \frac{\partial}{\partial x_n} (\bar{\rho} \bar{u}_n w) + \bar{\rho} a_n \frac{\partial \bar{I}}{\partial x_n} + (S_n - \overline{\rho' u'_n I'}) \frac{\partial \bar{\rho}}{\partial x_n} \Big/ \bar{\rho} - \bar{\rho} \frac{\partial}{\partial x_n} (a_n w) + \frac{\partial}{\partial x_n} \overline{\rho' u'_n I'}$$

$$= -b \overline{\sigma_{mn}} \frac{\partial \bar{u}_n}{\partial x_n} - \bar{\rho} \overline{\left(\frac{1}{\rho}\right)' \sigma'_{mn}} \frac{\partial \bar{u}_m}{\partial x_n} - b \bar{\rho} \epsilon - \bar{\rho} \overline{\left(\frac{1}{\rho}\right)' (\bar{\tau}_{nm} + \tau'_{nm})} \frac{\partial u'_m}{\partial x_n} \tag{40}$$

$$- b \nabla \cdot (\kappa \nabla \bar{T}) - \bar{\rho} \overline{\left(\frac{1}{\rho}\right)' \nabla \cdot (\kappa \nabla T')} .$$

The last two terms on the right-hand side could be modeled as decay of $w$. Once again, we would model the triple correlation by a gradient approximation leading to a diffusion term.

### 3.6. Equation for the Rate of Turbulent Energy Dissipation

An exact $\epsilon$ equation could, in principle, be derived from the Navier-Stokes equations, much as an equation for $\overline{(\partial u'_i/\partial x_n)(\partial u'_i/\partial x_n)}$ was originally derived by Daly and Harlow

[16]. More concisely, however, most researchers have merely formed the equation for $K$ by taking the trace of the $R_{ij}$ equation:

$$\frac{\partial}{\partial t}(\bar{\rho}K) + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n K) + R_{nm}\frac{\partial \tilde{u}_m}{\partial x_n} = a_n \frac{\partial \overline{P}}{\partial x_n} + \frac{\partial}{\partial x_n}\left(\mu_t \frac{\partial K}{\partial x_n}\right) - \bar{\rho}\epsilon \tag{41}$$

where the anisotropic part of $\mathbf{R}$ is given by the gradient approximation stated earlier (Eq. 20). Then, we form a dimensionally correct equation for $\epsilon$ from the $K$ equation. Supplying constants to all production terms, we get

$$\frac{\partial \bar{\rho}\epsilon}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n \epsilon) + C_{1\epsilon}\frac{\epsilon}{K}R_{nm}\frac{\partial \tilde{u}_m}{\partial x_n} = C_{3\epsilon}\frac{\epsilon}{K}a_n\frac{\partial \overline{P}}{\partial x_n} + C_{D\epsilon}\frac{\partial}{\partial x_n}\left(\frac{\bar{\rho}K^2}{\epsilon}\frac{\partial \epsilon}{\partial x_n}\right) - C_{2\epsilon}\frac{\epsilon^2\bar{\rho}}{K}. \tag{42}$$

This is the natural generalization of the most frequently used form of the constant-density $\epsilon$ equation. We shall, however, modify it slightly, adding another production term on the right hand side ($-C_{4\epsilon}\bar{\rho}\epsilon\nabla\cdot\tilde{\mathbf{u}}$) to give the correct length scale behavior during compression and expansion [17].

### 3.7. The Concentration Equation

The ensemble-averaged mass conservation equation for a species $i$ interdiffusing in a mixture was given in (15). Once again, we identify the last term on the left side as a turbulent diffusion of species mass fraction, and model it as

$$\overline{\rho c_i'' \mathbf{u}''} = \overline{\rho c_i' \mathbf{u}'} = -C_{Dc}\frac{K}{\epsilon}(\mathbf{R}\cdot\nabla)\tilde{c}_i. \tag{43}$$

To complete this set of equations, the equation of state needs to be specified.

### 3.8. Mixture Equation of State Considerations

Generally, the pressure can be expressed as a function of all but one of the mass concentrations, the system density and internal energy:

$$P = f(\rho, I, c_1, c_2, \ldots, c_{n-1}). \tag{44}$$

Hence

$$\overline{P} = \overline{f(\rho, I, c_1, c_2, \ldots, c_{n-1})} \tag{45}$$

which is not necessarily the same as $f(\bar{\rho}, \tilde{I}, \tilde{c}_1, \ldots)$, but this last approximation is accurate up to inclusion of second order correlations. What we can say is that, because of the assumptions of nearly incompressible turbulence outlined in the introduction, the pressure is constant among a group of eddies encompassing a region small compared to the mean flow gradient length. This constancy implies relationships among the fluctuations in density, internal energy and concentrations, such that

$$\overline{P} = f(\bar{\rho} + \rho', \tilde{I} + I'', \tilde{c}_1 + c_1'', \ldots) = P \tag{46}$$

everywhere. For a single material gamma-law gas with constant specific heat, $P = \overline{P}$ implies $\rho I = \overline{\rho I}$; hence $\rho(\tilde{I} + I'') = \bar{\rho}\tilde{I} = (\rho - \rho')\tilde{I}$. Then

$$\frac{\rho'}{\rho} = -\frac{I''}{\tilde{I}}, \tag{47}$$

but no specific relationship can be inferred about $\rho'/\bar{\rho}$. The assumption of eddy pressure equilibrium breaks down in a shock but holds after a shock has left the mixing zone between two materials. A self-consistent description of the interactions of the shock and the fluctuations is not possible with this postulate. Nonetheless, we expect that the jumps of mean and turbulent quantities can be sufficiently well described by this model.

### 3.9. Summary of Turbulence Model Equations

We now summarize our model equations, which should be most relevant in the limit of fully developed turbulence:

$$\frac{\partial R_{ij}}{\partial t} + \frac{\partial}{\partial x_n}(\tilde{u}_n R_{ij}) + R_{in}\frac{\partial \tilde{u}_j}{\partial x_n} + R_{jn}\frac{\partial \tilde{u}_i}{\partial x_n}$$

$$= \sum{}' \left\{ a_i \left( \frac{\partial \overline{P}}{\partial x_j} - \frac{\partial \overline{\tau}_{nj}}{\partial x_n} \right) + C_{DR}\frac{\partial}{\partial x_m}\left[ \frac{K}{\epsilon} R_{in} \frac{\partial}{\partial x_n}\left( \frac{R_{mj}}{\bar{\rho}} \right) \right] \right\} \tag{48}$$

$$- C_{1R}\frac{\epsilon}{K}\left( R_{ij} - \frac{1}{3}\delta_{ij}R_{nn} \right) - C_{2R}\left( R_{in}\frac{\partial \tilde{u}_j}{\partial x_n} + R_{jn}\frac{\partial \tilde{u}_i}{\partial x_n} - \frac{2}{3}\delta_{ij}R_{mn}\frac{\partial \tilde{u}_m}{\partial x_n} \right) - \frac{2}{3}\delta_{ij}\bar{\rho}\epsilon ,$$

$$\frac{\partial \bar{\rho} a_i}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n a_i) + \bar{\rho} a_n \frac{\partial \bar{u}_i}{\partial x_n} = b\left(\frac{\partial \bar{P}}{\partial x_i} - \frac{\partial \bar{\tau}_{ni}}{\partial x_n}\right) - \frac{R_{in}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial x_n}$$

$$+ C_{Da}\bar{\rho}\frac{\partial}{\partial x_m}\left[\frac{K}{\epsilon\bar{\rho}}\left(R_{in}\frac{\partial a_m}{\partial x_n} + R_{mn}\frac{\partial a_i}{\partial x_n}\right)\right]$$

$$+ \bar{\rho}\frac{\partial}{\partial x_n}(a_n a_i) - C_{1a}\bar{\rho}\frac{\epsilon}{K}a_i + C_{2a}\bar{\rho}a_n\frac{\partial \tilde{u}}{\partial x_n}, \qquad (49)$$

$$\frac{\partial b}{\partial t} + \bar{u}_n\frac{\partial b}{\partial x_n} + \frac{b+1}{\bar{\rho}}\frac{\partial}{\partial x_n}(\bar{\rho}a_n) = \bar{\rho}C_{Db}\frac{\partial}{\partial x_n}\left(\frac{K}{\epsilon\bar{\rho}}R_{nm}\frac{\partial}{\partial x_m}\left(\frac{1+b}{\bar{\rho}}\right)\right) - C_{1b}\frac{\epsilon}{K}b \qquad (50)$$

$$\frac{\partial \bar{\rho}\epsilon}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n\epsilon) + C_{1\epsilon}\frac{\epsilon}{K}R_{mn}\frac{\partial \tilde{u}_m}{\partial x_n} = C_{3\epsilon}\frac{\epsilon}{K}a_n\frac{\partial \bar{P}}{\partial x_n}$$

$$+ C_{D\epsilon}\frac{\partial}{\partial x_n}\left(\frac{\bar{\rho}K^2}{\epsilon}\frac{\partial \epsilon}{\partial x_n}\right) - C_{2\epsilon}\frac{\epsilon^2\bar{\rho}}{K} - C_{4\epsilon}\bar{\rho}\epsilon\frac{\partial \tilde{u}_n}{\partial x_n}, \qquad (51)$$

$$\frac{\partial S_i}{\partial t} + \frac{\partial}{\partial x_n}(\tilde{u}_n S_i) + R_{in}\frac{\partial \tilde{I}}{\partial x_n} + S_n\frac{\partial \tilde{u}_i}{\partial x_n} = w\left(-\frac{\partial \bar{P}}{\partial x_i} + \frac{\partial \bar{\tau}_{ni}}{\partial x_n}\right) + a_i\left(\bar{P}\frac{\partial \bar{u}_n}{\partial x_n} - \bar{\tau}_{mn}\frac{\partial \bar{u}_m}{\partial x_n}\right)$$

$$+ C_{DS}\frac{\partial}{\partial x_n}\left[\frac{K}{\epsilon}\left(R_{nm}\frac{\partial}{\partial x_m}\left(\frac{S_i}{\bar{\rho}}\right) + R_{im}\frac{\partial}{\partial x_m}\left(\frac{S_n}{\bar{\rho}}\right)\right)\right]$$

$$- \bar{\rho}a_i\epsilon - a_i\frac{\partial}{\partial x_n}\left(\kappa\frac{\partial \bar{T}}{\partial x_n}\right) - C_{1s}\frac{\bar{\rho}\epsilon}{K}S_i + C_{2s}S_n\frac{\partial \tilde{u}_i}{\partial x_n}, \qquad (52)$$

$$\frac{\partial \bar{\rho}w}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n w) + \bar{\rho}a_n\frac{\partial \tilde{I}}{\partial x_n} + \frac{S_n}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial x_n} - \bar{\rho}\frac{\partial}{\partial x_n}(a_n w) = b\left(\bar{P}\frac{\partial \bar{u}_n}{\partial x_n} - \bar{\tau}_{mn}\frac{\partial \bar{u}_n}{\partial x_m}\right)$$

$$+ C_{Dw}\bar{\rho}\frac{\partial}{\partial x_n}\left[\frac{K}{\epsilon\bar{\rho}}R_{nm}\frac{\partial w}{\partial x_m}\right] - \bar{\rho}\epsilon b$$

$$- b\frac{\partial}{\partial x_n}\left(\kappa\frac{\partial \bar{T}}{\partial x_n}\right) - C_{1w}\frac{\bar{\rho}\epsilon}{K}w - C_{2w}\bar{\rho}a_n\frac{\partial \bar{I}}{\partial x_n}, \tag{53}$$

$$\frac{\partial \bar{\rho}\tilde{c}_i}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n\tilde{c}_i) = \frac{\partial}{\partial x_n}\left(\bar{\rho}D\frac{\partial \tilde{c}_i}{\partial x_n}\right) + C_{Dc}\frac{\partial}{\partial x_n}\left(\frac{K}{\epsilon}R_{nm}\frac{\partial \tilde{c}_i}{\partial x_m}\right). \tag{54}$$

The equations for S and $w$ could be omitted if (39) is adopted as a simpler model for the turbulence heat flux.

## 4. SPECIALIZATION OF EQUATIONS TO INSTABILITY-DRIVEN TURBULENCE

One of the major goals of our work is to utilize these model equations to describe instability-driven turbulence accurately. The different types of instabilities encompassed by the equations are pressure-gradient driven, as in Rayleigh-Taylor instability or its shock-driven counterpart, Richtmeyer-Meshkov instability, and shear instability, commonly known as Kelvin-Helmholtz instability. To show that our model can reproduce the statistical effects of these instabilities, we first specify that the flow is nearly incompressible, but variable-density, and we define a coordinate system for the general case of variable-density turbulence in a combined pressure gradient and shear flow. Let us dictate that the initial flow velocity ($u$) is aligned with the x-axis, while the pressure gradient acts in the y-direction, which is the same direction in which the x-velocity varies. Furthermore, we are interested in the ability of the model to predict how mean flow variations affect these instabilities, and so we ignore the secondary effects of turbulence on itself. Triple correlations, decay terms, and the "slow" parts of the pressure-containing correlations will be dropped. This amounts to rapid distortion theory applied to instability-driven turbulence. Further, in source terms, gradients of turbulence variables are dropped and $\tilde{u}$

is replaced by $\overline{u}$. The turbulence equations for the Reynolds stresses and the turbulence mass flux vector components are, in this special case (with $D/Dt = \partial/\partial t + \tilde{\mathbf{u}} \cdot \nabla$),

$$\frac{DR_{yy}}{Dt} = 2a_y \frac{\partial \overline{P}}{\partial y} - \frac{2}{3} C_{2R} R_{xy} \frac{\partial \overline{u}}{\partial y} , \tag{55}$$

$$\frac{DR_{xy}}{Dt} = -(1 - C_{2R}) R_{yy} \frac{\partial \overline{u}}{\partial y} + a_x \frac{\partial \overline{P}}{\partial y} , \tag{56}$$

$$\frac{DR_{xx}}{Dt} = \left( -2 + \frac{1}{3} C_{2R} \right) R_{xy} \frac{\partial \overline{u}}{\partial y} , \tag{57}$$

$$\frac{Da_y}{Dt} = \frac{b}{\overline{\rho}} \frac{\partial \overline{P}}{\partial y} - \frac{R_{yy}}{\overline{\rho}^2} \frac{\partial \overline{\rho}}{\partial y} , \tag{58}$$

$$\frac{Da_x}{Dt} = -\frac{R_{xy}}{\overline{\rho}^2} \frac{\partial \overline{\rho}}{\partial y} . \tag{59}$$

The rapid parts of the pressure-velocity are included here because they affect the qualitative conclusions about forms of instability growth rates. We are now in a position to examine the description of instabilities by these simplified equations.

For pure shear flow in a constant density medium, the pressure and density gradient terms disappear. If the mean flow gradient is taken to be approximately constant over the time scale of interest, then differentiation of Eq. 55 gives

$$\begin{aligned} \frac{D^2 R_{yy}}{Dt^2} &= -\frac{2}{3} C_{2R} \frac{DR_{xy}}{Dt} \frac{\partial \overline{u}}{\partial y} \\ &= \frac{2}{3} C_{2R} (1 - C_{2R}) R_{yy} \left( \frac{\partial \overline{u}}{\partial y} \right)^2 \approx \frac{1}{6} R_{yy} \left( \frac{\Delta u}{L_u} \right)^2 \end{aligned} \tag{60}$$

if $C_{2R}$ is near 0.5. The resulting expression for the growth rate of the instability is

$$\omega = \frac{1}{\sqrt{6}} k_u \Delta u , \tag{61}$$

where $k_u = (L_u)^{-1}$, which nearly corresponds to the growth rate of Kelvin-Helmholtz instability [18] at a wavenumber characteristic of the mixing layer width.

On the other hand [illegible] pressure gradient driven circumstances, with no initial flow in the x-direction, all equations with time-derivatives of x-direction variables disappear. By differentiating Eq. 55 in [illegible] manner as above for Kelvin-Helmholtz instability, we get

$$\frac{D^2 R_{yy}}{Dt^2} = 2\frac{Da_y}{Dt}\frac{\partial \overline{P}}{\partial y} = 2\left(\frac{b}{\overline{\rho}}\frac{\partial \overline{P}}{\partial y} - \frac{R_{yy}}{\overline{\rho}^2}\frac{\partial \overline{\rho}}{\partial y}\right)\frac{\partial \overline{P}}{\partial y} . \tag{62}$$

The first term on the right side of this equation describes the effect of a pressure gradient (acceleration or shock) interacting with the turbulent density fluctuations, as measured by $b$. This always leads to increase of turbulent energy but is not present in purely Rayleigh-Taylor instability.

The second term on the right, proportional to mean-density gradient, gives the effect of Rayleigh-Taylor unstable conditions on turbulence, as these are characterized by the interaction of density gradient and acceleration. This term gives exponential growth to $R_{yy}$ at a rate determined by

$$\pm\sqrt{2\left(\frac{1}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial y}\right)g} = \pm\sqrt{2}\omega_{RT} , \tag{63}$$

where $g = -\frac{1}{\overline{\rho}}\frac{\partial \overline{P}}{\partial y}$ wherever $g\frac{\partial \overline{\rho}}{\partial y} > 0$. If we interpret $\frac{1}{\overline{\rho}}\frac{\partial \overline{\rho}}{\partial y}$ to be a density difference between two superposed fluids divided by their sum times the reciprocal of a gradient scale length ($\beta_\rho$), we recover the form of the expression for the growth rate for large wavenumber disturbances ($k \gg \beta_\rho$) in gradient-stabilized Rayleigh-Taylor instability:

$$\omega \approx \sqrt{2\, g\, At\, \beta_\rho} , \tag{64}$$

in which $At$ is the Atwood number. Turning now to shock-driven growth, we use the other term in Eq. 62. The weak shock is approximated [19] by a velocity jump $V$ induced by an impulsive pressure gradient $(1/\overline{\rho})\partial p\delta(t)/\partial y$ . Then $V = (\partial p/\partial y)/\overline{\rho}$ and

$$a_y = bV , \tag{65}$$

and

$$R_{yy} = b\bar{\rho}V^2 \,, \tag{66}$$

which agrees with Saffman and Meiron's result for initial turbulence kinetic energy after a weak shock contacts a density discontinuity, here modeled by a finite value of $b$.

When considering a combined Kelvin Helmholtz-Rayleigh-Taylor instability, the equations become somewhat more complicated [20]. From Eq. 62 and the time differential of Eq. 56, a fourth-order equation for $R_{yy}$ emerges:

$$\frac{D^4 R_{yy}}{Dt^4} = \left(3\omega_{RT}^2 + \frac{2}{3}C_{2R}(1 - C_{2R})\left(\frac{\partial \bar{u}}{\partial y}\right)^2\right)\frac{D^2 R_{yy}}{Dt^2} - 2\omega_{RT}^4 R_{yy} \,, \tag{67}$$

where $\omega_{RT}$ is given by Eq. 63. We will restrict the discussion to cases in which the density and pressure gradients have the same sign, the classically stable Rayleigh-Taylor case. Then $\omega_{RT}^2 < 0$ and the combined growth rate is given by

$$\begin{aligned}\omega_{\text{TOTAL}}^2 = \frac{1}{2}&\left(3\omega_{RT}^2 + \frac{2}{3}C_{2R}(1 - C_{2R})\left(\frac{\partial \bar{u}}{\partial y}\right)^2\right) \\ &\pm \frac{1}{2}\sqrt{\left(3\omega_{RT}^2 + \frac{2}{3}C_{2R}(1 - C_{2R})\left(\frac{\partial \bar{u}}{\partial y}\right)^2\right)^2 - 8\omega_{RT}^4} \,,\end{aligned} \tag{68}$$

which will have a real portion if $3\,|\omega_{RT}^2| < \frac{2}{3}C_{2R}(1 - C_{2R})\left(\frac{\partial \bar{u}}{\partial y}\right)^2$. If the density and velocity gradients have the same characteristic wavenumber $k_M$, then we expect growth for cases where, for $g$ and $\Delta\rho$ taken as positive,

$$k_M(\Delta u)^2 > \frac{9}{2}\frac{\Delta\rho}{\rho}g\frac{1}{C_{2R}(1 - C_{2R})} \,. \tag{69}$$

## 5. COMPARISON TO TWO-FIELD MODELS

Two-field descriptions of instability-driven turbulence and mixing hold some advantages over the approach taken thus far in this paper, e.g., the ability to describe interpenetration naturally by keeping two separate velocity fields, and the marking of the mixture

fraction at any point, among others. Further, the two means of analyzing mixtures are equivalent in some simple, yet interesting cases. The two-field continuum flow equations can take on many forms, depending on the amount of detail that the researcher wishes to capture. Here, for present purposes, one of the simplest forms of these equations, written for two microscopically incompressible fields, will suffice.

The model equations of Section 3 should include the capability of describing the interpenetration processes of two-field flow. To define the concepts of mean and fluctuating part in the two-field context, we consider the system composed of particles or droplets dispersed within a continuous surrounding fluid.

Two-field flow theory would allow for fluctuations from particle to particle and from point to point within the fluid. The dynamics of the system is described by field variables at several levels of specificity.

First, there are subscripted variables pertaining to the individual fields. The field densities $\rho_k$, $k = 1, 2$, are constants. The characteristic function $\beta_k(\mathbf{x}, t)$ satisfies $\beta_k = 1$ for regions of x-space occupied by the $k^{th}$ field and $\beta_k = 0$ elsewhere, so that $\sum_k \beta_k = 1$. The velocity $v_k(\mathbf{x}, t)$ of the $k^{th}$ field is defined where $\beta_k = 1$ and $\beta_k(\mathbf{x}, t)v_k(\mathbf{x}, t)$ is defined for all $\mathbf{x}$ (within the physical region occupied by any field).

Second, one computes averages of these field data, either ensemble averages, or space averages over control volumes small compared to significant macroscopic length scales, but large compared to droplet size and separation scales. The volume fractions $\alpha_k$ are defined by

$$\alpha_k(x,t) = \overline{\beta_k(x,t)}\,, \quad 0 \le \alpha_k(\mathbf{x},t) \le 1 \tag{70}$$

and obey $\sum_k \alpha_k = 1$. Then an averaged velocity $u_k(x,t)$ is defined for each field and all $\mathbf{x}$ by

$$\alpha_k(x,t)\ \mathbf{u}_k(x,t) = \overline{\beta_k(\mathbf{x},t)v_k(\mathbf{x},t)}\,. \tag{71}$$

Other averaged individual field data, such as internal energy $I_k$ are defined similarly.

Next, "mixture" variables that characterize the system of fields as a single fluid are defined by sums over $k$, weighted by the characteristic functions $\beta_k$ (unaveraged mixture variables) or by the volume fractions $\alpha_k$ (averaged mixture variables). In this way, we arrive at analogs of the turbulence averages, denoted with overbars or tildes, and the turbulence fluctuations, denoted by primed variables:

$$\rho = \sum_k \beta_k \rho_k \,, \quad \bar{\rho} = \sum_k \alpha_k \rho_k \,, \quad \rho' = \rho - \bar{\rho} \,, \tag{72}$$

$$\mathbf{u} = \sum_k \beta_k \mathbf{v}_k \,, \quad \bar{\mathbf{u}} = \sum_k \alpha_k \mathbf{u}_k \,, \quad \mathbf{u}_k' = \mathbf{u}_k - \bar{\mathbf{u}} \,, \tag{73}$$

and

$$\tilde{\mathbf{u}} = \frac{\sum_k \alpha_k \rho_k \mathbf{u}_k}{\sum_k \alpha_k \rho_k} \,, \quad \tilde{I} = \frac{\sum_k \alpha_k \rho_k I_k}{\sum_k \alpha_k \rho_k} \,, \text{ etc.} \tag{74}$$

The evolution equations for the interacting averaged field variables are developed in detail by Ishii [6], starting from the statements of conservation of mass, momentum, and total energy for each field. We have

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = 0 \,, \tag{75}$$

$$\frac{\partial \alpha_k \rho_k \mathbf{u}_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k) = -\alpha_k \nabla P + K_D \bar{\rho} (\mathbf{u}_{k'} - \mathbf{u}_k) \,, \tag{76}$$

$$\begin{aligned} \frac{\partial \alpha_k \rho_k I_k}{\partial t} + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k I_k) &= -P \left( \frac{\partial \alpha_k}{\partial t} + \nabla \cdot \alpha_k \mathbf{u}_k \right) \\ &+ R_T \bar{\rho} C_{vm} (T_{k'} - T_k) + K_D \bar{\rho} (\mathbf{u}_{k'} - \mathbf{u}_k) \cdot (\bar{\mathbf{u}} - \mathbf{u}_k) \,. \end{aligned} \tag{77}$$

These equations represent averages over realizations of flows at high Reynolds number, and viscous stress terms are ignored. $P$ is the spatially averaged pressure of the surrounding field. $C_{vm}$ is an effective specific heat of the mixture. $R_T$ is a heat-exchange function and $K_D$ is a momentum-exchange function (inverse drag time scale); they result from modeling of the interactions at field interfaces. For present purposes, we need not specify how their

time and space variations are determined. $T_k$ is the temperature of the $k^{th}$ field and subscript $k'$ refers to the field other than the $k^{th}$ field. We wish to demonstrate a close relationship between these equations and the turbulent transport equations of Section 3.9.

The correlation functions studied in the first part of this paper can be expressed, in the two-field system, in terms of sums weighted by the volume fractions:

$$R_{ij} = \sum_k \alpha_k \rho_k (u_k - \hat{u})_i (u_k - \hat{u})_j \ , \tag{79}$$

$$\mathbf{a} = -\sum_k \alpha_k (\mathbf{u}_k - \hat{\mathbf{u}}) = \hat{\mathbf{u}} - \overline{\mathbf{u}} \ , \tag{80}$$

$$\mathbf{S} = \sum_k \alpha_k \rho_k (\mathbf{u}_k - \hat{\mathbf{u}}) \left( I_k - \hat{I} \right) \ , \tag{81}$$

$$b = -\sum_k \alpha_k (\rho_k - \overline{\rho}) \left( \frac{1}{\rho_k} - \overline{\left(\frac{1}{\rho}\right)} \right) = -1 + \sum_k \frac{\alpha_k}{\rho_k} \sum_n \alpha_n \rho_n \ . \tag{82}$$

$$w = \frac{\sum_k \alpha_k (\rho_k - \overline{\rho}) (I_k - \overline{I})}{\overline{\rho}} = -\sum_k \alpha_k \left( I_k - \hat{I} \right) = \hat{I} - \overline{I} \ . \tag{83}$$

In general, to form any correlation (which, previously, we had associated with turbulence), one averages the departures from the mean, either mass-weighted or uniformly weighted, over the number of materials. Another example of a correlation of fluctuations is

$$\overline{\mathbf{u}'\mathbf{u}'} = \sum_k \alpha_k (\mathbf{u}_k - \overline{\mathbf{u}})(\mathbf{u}_k - \overline{\mathbf{u}}) \ .$$

These relationships hold for any number of fields, but we are most interested in a two-field description because of the additional relationships that apply. Thus, for two fields, we have:

$$\overline{\rho} = \alpha_1 \rho_1 + \alpha_2 \rho_2 \ , \tag{84}$$

$$\mathbf{a} = \frac{\alpha_1\alpha_2(\rho_1 - \rho_2)(\mathbf{u}_1 - \mathbf{u}_2)}{\overline{\rho}}\,, \tag{85}$$

$$b = \overline{\rho}\left(\frac{\alpha_1}{\rho_1} + \frac{\alpha_2}{\rho_2}\right) - 1 = \frac{\alpha_1\alpha_2(\rho_1 - \rho_2)^2}{\rho_1\rho_2}\,, \tag{86}$$

$$w = \frac{\alpha_1\alpha_2(\rho_1 - \rho_2)(I_1 - I_2)}{\overline{\rho}}\,, \tag{87}$$

$$R_{ij} = \frac{\alpha_1\alpha_2\rho_1\rho_2(\mathbf{u}_1 - \mathbf{u}_2)_i(\mathbf{u}_1 - \mathbf{u}_2)_j}{\overline{\rho}} = \frac{a_i a_j\overline{\rho}}{b}\,, \tag{88}$$

and

$$\mathbf{S} = \frac{\alpha_1\alpha_2\rho_1\rho_2(\mathbf{u}_1 - \mathbf{u}_2)(I_1 - I_2)}{\overline{\rho}} = \frac{\mathbf{a}w}{b}\,\overline{\rho}\,. \tag{89}$$

In this model, evolution equations for **R** and **S** are not needed and only the **a**, $b$, and $w$ equations need to be examined.

From the two-field equations and the two-field definitions outlined above, an equation for **a** follows:

$$\begin{aligned}\frac{\partial\overline{\rho}\mathbf{a}}{\partial t} + \nabla\cdot\overline{\rho}\mathbf{a}\overline{\mathbf{u}} + \overline{\rho}(\mathbf{a}\cdot\nabla)\overline{\mathbf{u}} + \overline{\mathbf{u}'\mathbf{u}'}\cdot\nabla\overline{\rho} + \nabla\cdot\overline{\rho}\mathbf{a}\mathbf{a}\left(1 - \frac{1}{B} + \frac{1}{b}\right) = \\ b\nabla\overline{P} - K_D^*\mathbf{a}\overline{\rho}\,,\end{aligned} \tag{90}$$

where $B = \sum_k \alpha_1\alpha_2(\rho_1 - \rho_2)^2/\overline{\rho}^2 = \overline{\rho'^2}/\overline{\rho}^2 = b\rho_1\rho_2/\overline{\rho}^2$ and $K_D^* = K_D\overline{\rho}^2/(\alpha_1\alpha_2\rho_1\rho_2)$. By comparing this equation to (28), the turbulence equation for **a**, and to (29) we can infer a new modeling for the correlation $\overline{\rho'\mathbf{u}'\mathbf{u}'}$:

$$\overline{\rho' u_i' u_j'} = \overline{\rho} a_i a_j\left(1 - \frac{1}{B} + \frac{1}{b}\right)\,. \tag{91}$$

This gives a wave-like flux term in the **a** equation, as opposed to the diffusive flux term that most modelers would use, following (22). For the model of Section 3, taken in the limiting case of two-field interpenetration, $\overline{\rho' u_i' u_j'}$ should reduce to the right side of (91), which the gradient closure (diffusive flux) would not.

If a gradient approximation for **a** is derived from the balance in Eq. 49 for **a** between the decay term ( $C'_{1a}\bar{\rho}\epsilon\mathbf{a}/k$) and the density gradient production term $(R_{in}/\bar{\rho})(\partial\bar{\rho}/\partial x_n)$, then

$$a_i = -C'_{1a}\frac{K}{\epsilon\bar{\rho}^2}R_{in}\frac{\partial\bar{\rho}}{\partial x_n} . \tag{92}$$

We expect that (92) will best approximate **a**, as a constraint equation relating data at a common time, in the fully developed turbulence limit when production and dissipation are in balance. Furthermore, one may show, from the two-field description expressed in terms of single-field variables with $\rho_1$ and $\rho_2$ as constants, that (expressing $\alpha_1$, $\alpha_2$ in terms of $\bar{\rho}$, $\rho_1$, $\rho_2$, and here **A** in terms of $\bar{\rho}$, $\rho_1$, $\rho_2$, and $\mathbf{u}_1 - \mathbf{u}_2$)

$$\mathbf{a}\left(1 - \frac{1}{B} + \frac{1}{b}\right) = \frac{\partial\mathbf{A}}{\partial\bar{\rho}} .$$

Then, substituting into Eqs. 91 92, symmetrizing the expression and approximating $\partial\mathbf{A}/\partial x_n$ by $(\partial\mathbf{A}/\partial\bar{\rho})(\partial\bar{\rho}/\partial x_n)$, the approximation to $\overline{\rho'\mathbf{u}'\mathbf{u}'}$ emerges as

$$\overline{\rho' u'_i u'_j} = -C_{Da}\frac{K}{\epsilon\bar{\rho}}\left(R_{in}\frac{\partial}{\partial x_n}A_j + R_{jn}\frac{\partial}{\partial x_n}A_i\right) , \tag{93}$$

which is different, and perhaps better, than the form in (22). Also, the decay term in the newly-derived **a** equation could be modeled as

$$K^*_D\mathbf{a}\bar{\rho} \approx C'_{1a}\frac{\mathbf{a}\sqrt{\mathbf{a}\cdot\mathbf{a}}\,\bar{\rho}}{L_{turb}} = C'_{1a}\frac{\mathbf{a}|\mathbf{a}|\bar{\rho}\epsilon}{K^{3/2}} . \tag{94}$$

By extending the analysis for other turbulence quantities, we get, for the evolution of $b$,

$$\frac{\partial b}{\partial t} + (\bar{\mathbf{u}}\cdot\nabla)b + \frac{b+1}{\bar{\rho}}\nabla\cdot\bar{\rho}\mathbf{a} + \bar{\rho}\nabla\cdot\overline{\mathbf{u}'\left(\frac{1}{\rho}\right)'} = 0 . \tag{95}$$

if $\nabla\cdot\mathbf{u}' = 0$. This leads to a revised model for the term we were calling diffusion-like, which is

$$\overline{\mathbf{u}'\left(\frac{1}{\rho}\right)'} = -\frac{\mathbf{a}b}{\bar{\rho}B} . \tag{96}$$

Now we write an equation for $B = \overline{\rho'^2}/\overline{\rho}^2$. The turbulence equation for this is, again assuming incompressible turbulence,

$$\frac{\partial \overline{\rho}^2 B}{\partial t} + \nabla \cdot (\overline{\mathbf{u}}\,\overline{\rho}^2 B) + \overline{\rho}^2 B \nabla \cdot \overline{\mathbf{u}} + 2\overline{\rho}\mathbf{a} \cdot \nabla \overline{\rho} + \nabla \cdot \overline{\rho'^2 \mathbf{u}'} = 0\,. \tag{97}$$

From the two-field description, written in terms of single-field variables, $B$ evolves according to

$$\begin{aligned} \frac{\partial \overline{\rho}^2 B}{\partial t} &+ \nabla \cdot (\overline{\mathbf{u}}\,\overline{\rho}^2 B) + \overline{\rho}^2 B \nabla \cdot \overline{\mathbf{u}} + 2\overline{\rho}\mathbf{a} \cdot \nabla \overline{\rho} \\ &+ \nabla \cdot \left(\overline{\rho}^2 B \mathbf{a}\left(1 - \frac{1}{B} + \frac{1}{b}\right)\right) = 0\,, \end{aligned} \tag{98}$$

which implies that the triple correlation in Eq. 97 should be modeled as

$$\overline{\rho'^2 \mathbf{u}'} = \overline{\rho} B \mathbf{a}\left(1 - \frac{1}{B} + \frac{1}{b}\right)\,. \tag{99}$$

A similar treatment of the $w$ equation gives

$$\overline{\rho' \mathbf{u}' T'} = \overline{\rho} w \mathbf{a}\left(1 - \frac{1}{B} + \frac{1}{b}\right)\,, \tag{100}$$

which also reduces properly in the fully-developed turbulence limit. The potential decay terms (cf. Eqs. 53 and 77) in the two-field version of this equation can be written as

$$-R_T^* \overline{\rho} C_{vm} \frac{\alpha_1 \alpha_2 (\rho_1 - \rho_2)(T_1 - T_2)}{\overline{\rho}}$$

$$+ K^* \overline{\rho} \frac{\alpha_2^2 \rho_2 - \alpha_1^2 \rho_1}{\alpha_1 \alpha_2 (\rho_1 - \rho_2)} \frac{\alpha_1^2 \alpha_2^2 (\rho_1 - \rho_2)^2 (\mathbf{u}_1 - \mathbf{u}_2) \cdot (\mathbf{u}_1 - \mathbf{u}_2)}{\overline{\rho}^2}$$

where $R_T^* = R_T \overline{\rho}^2 / (\alpha_1 \alpha_2 \rho_1 \rho_2)$. These two expressions can be transformed into single-field variables, to become

$$-R_T^* \overline{\rho} w$$

and

$$K^* \overline{\rho}\left(\frac{1}{b} - \frac{1}{B}\right) \mathbf{a} \cdot \mathbf{a}\,.$$

These can be identified with two terms in the original w equation, namely

$$-\overline{\rho}\,\overline{\left(\frac{1}{\rho}\right)'\nabla\cdot(\kappa\nabla T')} \approx -C_{1w}\overline{\rho}\frac{\epsilon}{K}w$$

and

$$\overline{\rho}\,\overline{\left(\frac{1}{\rho}\right)'\left(p'\frac{\partial\overline{u}_n}{\partial x_n} - \tau'_{mn}\frac{\partial\overline{u}_m}{\partial x_n}\right)} - b\overline{\rho}\epsilon\,,$$

respectively, though the second correspondence is less clear.

For the mass concentration equations, a similar formal parallel holds. Applying Eq. 15 for the mass-averaged concentration of material 1 at high Peclet numbers for mass transfer, ($D \to 0$),

$$\frac{\partial\overline{\rho}\tilde{c}_1}{\partial t} + \nabla\cdot\overline{\rho}\tilde{c}_1\tilde{\mathbf{u}} + \nabla\cdot\overline{\rho c_1''\mathbf{u}''} = 0\,. \tag{101}$$

From the two-field description as a point of departure, the mass fraction for field 1, in the region occupied by field $k$ is $c_{1k} = \delta_{1k}$. The associated single-field variables, unaveraged and mass averaged, respectively, are $c_1 = \sum_k \beta_k c_{1k} = \beta_1$ and

$$\tilde{c}_1 = \sum_k \overline{\beta_k\rho_k c_{1k}}/\overline{\rho} = \alpha_1\rho_1/\overline{\rho}\,. \tag{102}$$

Observe that $\tilde{c}_1 + \tilde{c}_2 = 1$ and $c''_{1k} = c_{1k} - \tilde{c}_1$ is the negative of $c''_{2k}$ Rewriting the unknown correlation in (101) in terms of two-field variables, we get

$$\overline{\rho c_1''\mathbf{u}''} = \overline{\rho c_1\mathbf{u}''} = \alpha_1\rho_1(\mathbf{u}_1 - \tilde{\mathbf{u}}) = \frac{\alpha_1\alpha_2\rho_1\rho_2}{\overline{\rho}}(\mathbf{u}_1 - \mathbf{u}_2)\,. \tag{103}$$

Thus, the material fluxes can be re-expressed in terms of single-field variables as

$$\overline{\rho c_1\mathbf{u}''} = -\overline{\rho c_2\mathbf{u}''} = \overline{\rho}\mathbf{a}\sqrt{\frac{\tilde{c}_1\tilde{c}_2}{b}}\,\mathrm{sign}(\rho_1 - \rho_2)\,. \tag{104}$$

If a is again taken in its fully developed turbulence limit $\left(a_i = -C^*_{1a}\left(K/\epsilon\overline{\rho}^2\right)R_{in}\left(\partial\overline{\rho}/\partial x_n\right)\right)$ as in Eq. 92, then, after re-expressing $\alpha_1$, $\alpha_2$, and hence $\tilde{c}_1\tilde{c}_2$, in terms of $\overline{\rho}$, $\rho_1$, $\rho_2$,

$$\overline{\rho}a_i\sqrt{\frac{\tilde{c}_1\tilde{c}_2}{b}}\,\mathrm{sign}(\rho_1 - \rho_2) = -C^*_{1a}\frac{K}{\epsilon\overline{\rho}}R_{in}\frac{\partial\overline{\rho}}{\partial x_n}\overline{\rho}\frac{\partial\tilde{c}_1}{\partial\overline{\rho}} = -C^*_{1a}\frac{K}{\epsilon}R_{in}\frac{\partial\tilde{c}_i}{\partial x_n}\,. \tag{105}$$

which agrees with (43), to within an adjustable constant. Thus, we have demonstrated the relationship of the unmodeled turbulence equations to the two-field equations and, as a result, suggested some new closures for variable-density turbulence models that capture both the ordered and fully turbulent limits.

## 6. SIMPLER MODELS

Implementation of such models in multidimensional hydrodynamics codes can become extremely tedious and the resulting run times can become unreasonable. (Therefore, it is of significant interest to develop and program simpler models in order to gain experience with them and, if they can be demonstrated to be deficient in crucial areas, then improved at a later time.) One of the simplifications we have used with some success in the CAVEAT code [1] retains a transport equation for the trace of the Reynolds stress tensor ($\frac{1}{2}R_{nn} = \bar{\rho}K$) and makes use of the Boussinesq (gradient) approximation for specifying the components of the Reynolds stress tensor in terms of $K$ and $\epsilon$. Then

$$\frac{\partial \bar{\rho}K}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n K) + R_{mn}\frac{\partial \tilde{u}_m}{\partial x_n} = a_n \frac{\partial \bar{P}}{\partial x_n} + \frac{\partial}{\partial x_n}\left(\mu_t \frac{\partial K}{\partial x_n}\right) - \bar{\rho}\epsilon \,, \tag{106}$$

$$R_{ij} = -\mu_t\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}(\nabla \cdot \tilde{\mathbf{u}})\right) + \frac{2}{3}\delta_{ij}\bar{\rho}K \,, \tag{107}$$

$$\mu_t = C_\mu \bar{\rho}\frac{K^2}{\epsilon} \,. \tag{108}$$

Furthermore, keeping only the most important production terms, the decay term and a simpler turbulent diffusion term from the a equation (cf. Eq. 49), results in a more manageable model expression:

$$\begin{aligned}\frac{\partial \bar{\rho}a_i}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n a_i) + \bar{\rho}a_n\frac{\partial \bar{u}_i}{\partial x_n} &= b\left(\frac{\partial \bar{P}}{\partial x_i} - \frac{\partial}{\partial x_n}\bar{\tau}_{ni}\right) \\ &- \frac{R_{in}}{\bar{\rho}}\frac{\partial \bar{\rho}}{\partial x_n} + C_{Da}\frac{\partial}{\partial x_n}\left(\frac{\bar{P}K^2}{\epsilon}\frac{\partial a_i}{\partial x_n}\right) - C_{1a}\frac{\bar{\rho}\epsilon}{K}a_i \,.\end{aligned} \tag{109}$$

The proposed $\epsilon$ equation is the same as derived previously (cf. Eq. 51), as is the concentration equation (cf. Eq. 54):

$$\frac{\partial \overline{\rho}\epsilon}{\partial t} + \frac{\partial}{\partial x_n}(\overline{\rho}\tilde{u}_n\epsilon) + C_{1\epsilon}\frac{\epsilon}{K}R_{mn}\frac{\partial \tilde{u}_m}{\partial x_n} = C_{3\epsilon}\frac{\epsilon}{K}a_n\frac{\partial \overline{P}}{\partial x_n} + C_{D\epsilon}\frac{\partial}{\partial x_n}\left(\frac{\overline{P}K^2}{\epsilon}\frac{\partial \epsilon}{\partial x_n}\right)$$

$$- C_{2\epsilon}\frac{\epsilon^2\overline{\rho}}{K} - C_{4\epsilon}\overline{\rho}\epsilon\frac{\partial \tilde{u}_n}{\partial x_n}\,, \tag{110}$$

$$\frac{\partial \overline{\rho}\tilde{c}_i}{\partial t} + \frac{\partial}{\partial x_n}(\overline{\rho}\tilde{u}_n\tilde{c}_i) = \frac{\partial}{\partial x_n}\left(\overline{\rho}D\frac{\partial}{\partial x_n}\tilde{c}_i\right) + C_{Dc}\frac{\partial}{\partial x_m}\left(\frac{K}{\epsilon}R_{mn}\frac{\partial \tilde{c}_i}{\partial x_n}\right)\,. \tag{111}$$

Further, $b$ can be computed from its own transport equation or, if we assume that there is no interspecies diffusion, so that the $b$ equation has no decay term, the two-field expression for $b$ should be accurate:

$$b = \frac{\alpha_1\alpha_2(\rho_1 - \rho_2)^2}{\rho_1\rho_2}\,. \tag{112}$$

In practice, in a computational cell, $\alpha_1$, $\alpha_2$, $\rho_1$, and $\rho_2$ would be determined from the two criteria of (1) pressure equilibrium between components, and (2) either adiabatic work exchange or temperature equilibrium between materials. Finally, the turbulent heat flux, in accordance with this simplified approach, is given by diffusion of the internal energy, as

$$S_i = -C_{DI}\frac{K}{\epsilon}R_{in}\frac{\partial \tilde{I}}{\partial x_n}\,. \tag{113}$$

This model can be considered a natural extension of $K - \epsilon$ models and the modeling methodology to variable-density flows.

Another type of model would use the two-field (or multifield) flow equations (75–77) for the stable part of the flow, together with the turbulent transport equations of Section 3 to represent the multifield instabilities. In this context, the stable part of the flow has been referred to as "ordered," while the unstable part may be called "disordered." Closures should then be modeled so that they vanish in the pure multifield limit, rather than approaching their multifield limits as given in this section. The type of turbulence

model to be used to augment the description of ordered motion could also provide the drag length scale [6] for the phenomenological momentum exchange coefficient:

$$L_T = \frac{K^{3/2}}{\epsilon} . \tag{114}$$

The Reynolds stress and turbulence dissipation equations in the disordered portion of the model are taken from standard turbulence models (e.g., that of Launder, Reece, and Rodi [16]), but we suppose that the energy lost from the ordered motion ($-2K^{\bullet}\frac{a_i a_j \bar{\rho}}{b} = -2K^{\bullet}R_{ij}^{\mathrm{ord}}$) acts as a source to disordered energy, not heat:

$$\begin{aligned}
&\frac{\partial R_{ij}^d}{\partial t} + \frac{\partial}{\partial x_n}(\tilde{u}_n R_{ij}^d) + R_{in}^d \frac{\partial \tilde{u}_j}{\partial x_n} + R_{jn}^d \frac{\partial \tilde{u}_i}{\partial x_n} - 2K_D^{\bullet}\frac{\bar{\rho} a_i a_j}{b} \\
&= C_{DR}\frac{\partial}{\partial x_m}\left[\frac{K}{\epsilon}\sum{}' R_{in}\frac{\partial}{\partial x_n}\frac{R_{mj}}{\bar{\rho}}\right] \\
&- C_{1R}\left(R_{ij}^d - \frac{1}{3}\delta_{ij}R_{nn}^d\right) - C_{2R}\left(\Phi_{ij} - \frac{1}{3}\delta_{ij}\Phi_{nn}\right) \\
&- C_{4R}\left(\frac{2K_D^{\bullet}\bar{\rho}}{b}\right)\left(a_i a_j - \frac{1}{3}\delta_{ij}a_n a_n\right) - \frac{2}{3}\delta_{ij}\bar{\rho}\epsilon ,
\end{aligned} \tag{115}$$

$$\begin{aligned}
&\frac{\partial \bar{\rho}\epsilon}{\partial t} + \frac{\partial}{\partial x_n}(\bar{\rho}\tilde{u}_n\epsilon) + C_{1\epsilon}\frac{\epsilon}{K}R_{mn}^d\frac{\partial \tilde{u}_m}{\partial x_n} = C_{D\epsilon}\frac{\partial}{\partial x_n}\left(\frac{\bar{\rho}K^2}{\epsilon}\frac{\partial \epsilon}{\partial x_n}\right) \\
&- C_{2\epsilon}\frac{\bar{\rho}\epsilon^2}{K} - C_{4\epsilon}\bar{\rho}\epsilon(\nabla\cdot\tilde{u}) ,
\end{aligned} \tag{116}$$

$$\Phi_{ij} = -\left(R_{in}^d\frac{\partial \tilde{u}_j}{\partial x_n} + R_{jn}^d\frac{\partial \tilde{u}_j}{\partial x_n}\right) . \tag{117}$$

The "$d$" superscript refers to only the disordered part of the turbulence and $K_D^{\bullet}$ can be modeled as in Eq. 94. Then the total Reynolds stress that enters the mean flow momentum equation is (cf. Eq. 13)

$$\mathbf{R}^{\mathrm{total}} = \mathbf{R}^d + \mathbf{R}^{\mathrm{ord}} = \mathbf{R}^d + \sum_k \alpha_k\rho_k(\mathbf{u}_k - \tilde{\mathbf{u}})(\mathbf{u}_k - \tilde{\mathbf{u}}) , \tag{118}$$

and equations for $\mathbf{a}$, $b$, and $c_i$ are not needed. An equation for the disordered part of the heat flux could be derived in an analogous fashion, with a source term

$$\xi = (K_D^* + R_T^*)\mathbf{S} + K_D^* \frac{\mathbf{a}}{b} R_{nn}^{ord} \tag{119}$$

arising from the decay of the ordered part of $\mathbf{S}$:

$$\frac{\partial S_i^d}{\partial t} + \frac{\partial}{\partial x_n}(\tilde{u}_n S_i^d) + R_{in}^d \frac{\partial \tilde{I}}{\partial x_n} + S_n^d \frac{\partial \tilde{u}_i}{\partial x_n} =$$

$$C_{DS}\frac{\partial}{\partial x_m}\left[\frac{K}{\epsilon}\left(R_{in}^d \frac{\partial}{\partial x_n}\left(\frac{S_m^d}{\bar{\rho}}\right) + R_{mn}^d \frac{\partial}{\partial x_n}\left(\frac{S_i^d}{\bar{\rho}}\right)\right)\right] \tag{120}$$

$$- C_{1S}\frac{\bar{\rho}\epsilon}{K} S_i^d + C_{2S} S_n^d \frac{\partial \tilde{u}_i}{\partial x_n} + (1 - C_{3S})\xi_i \, .$$

Then

$$\mathbf{S}^{total} = \mathbf{S}^d + \sum_k \alpha_k \rho_k (\mathbf{u}_k - \tilde{\mathbf{u}})\left(I_k - \tilde{I}\right) \, . \tag{121}$$

is the quantity needed for the mean internal energy equation.

## 7. SUMMARY

Starting from the Navier-Stokes equations written for a single field, we have derived and closed a set of transport equations appropriate for variable-density turbulence when the fluctuating velocities are far subsonic. This condition implies local pressure equilibrium among the different eddies and species over a distance small compared to mean-flow gradients. We have also taken a rather simple two-field model from the literature and demonstrated that our unclosed equations are formally equivalent to this model if the densities of the two fluids are constant. From this equivalence, new closures for turbulence quantities, such as triple correlations, emerge naturally. These new closure ideas have the ability to describe not only fully developed turbulence but also encompass the limit of purely ordered interpenetration of two incompressible materials. Therefore, these closures

may be superior to those commonly proposed for variable-density turbulence and their application to real problems should be explored.

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