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A NEW MULTIFLUID TURBULENT-MIX MODEL

Charles W. Cranfill

Abstract

Equations are proposed for a new multifluid turbulent-mix model intended to simulate fluid flows near unstable material interfaces. The model is based on the usual decomposition of the fluid properties into mean and fluctuating parts whose evolution equations are obtained from the Navier-Stokes equations. Correlations among the fluctuating parts produce turbulent contributions to the bulk fluid properties. The innovation is to divide the turbulent contributions into ordered and disordered parts, where the ordered parts are obtained from the average drift motions produced by a set of multifluid interpenetration equations, while the disordered parts are obtained from a set of single-fluid turbulence equations. The problem of closing the multifluid and single-fluid sets of equations is solved by coupling them together in such a way that they close each other. The resulting energy cascade is from bulk kinetic to ordered drift kinetic to disordered turbulent kinetic to thermal internal energy.

The new model exhibits both the early-time convective and the late-time diffusive drift motions seen in numerical and experimental investigations of the evolution of interfacial instabilities. The division of the turbulent contributions into ordered and disordered parts provides a more natural formalism for deriving the equations than has been given for similar mix models that have been proposed. The new model incorporates several simplifying assumptions designed to minimize the extra computational work required, so it is suitable for implementation in multidimensional hydrodynamics codes.

1. INTRODUCTION.

Fluid systems containing multiple materials exhibit mix generated by bouyancy- and shear-driven instabilities at the material interfaces. The instabilities are seeded by small asymmetries in the flow conditions and produce features with a wide range of spatial scale sizes. Computational limitations currently prevent multidimensional hydrodynamics codes from resolving spatial features with scale sizes smaller than about one percent of the total scale size of the flow being simulated, so some sort of phenomenological model is needed to estimate the effects of unresolved spatial features on the bulk flow. For the purposes of the present work, the unresolved spatial features are considered to produce turbulent contributions to the bulk fluid properties. The contributions to be modeled are a turbulent energy reservoir which delays changes in the temperature, a turbulent stress which modifies the equation of state and viscosity, and turbulent fluxes which enhance the transfer of mass and energy across the material interfaces.

Theoretical and experimental investigations have long ago determined the time evolution of small-amplitude perturbations at a material interface experiencing a steady acceleration (Rayleigh-Taylor case)¹⁻³, an impulsive acceleration (Richtmyer-Meshkov case)^{4,5}, or a steady velocity shear (Kelvin-Helmholtz case)³. There are four unstable situations: (1) a steady acceleration directed toward the heavier material causes small perturbations to grow exponentially with time; (2) an impulsive acceleration directed toward the heavier material causes small perturbations to grow linearly with time; (3) an impulsive acceleration directed toward the lighter material causes small perturbations to shrink, change sign, and then grow linearly with time; (4) a steady velocity shear causes small perturbations to grow exponentially with time. For any of these unstable situations, a perturbation initialized with a single Fourier mode grows without changing shape so long as its amplitude remains much smaller than its wavelength. As its amplitude becomes a significant fraction of its wavelength, the perturbation changes shape to form a characteristic pattern with spikes of the heavier material moving through bubbles of the lighter material. The shear between the spikes and the bubbles then produces a secondary Kelvin-Helmholtz instability which causes the spikes to roll over into an increasingly chaotic pattern. This roll over proceeds to convert the material interpenetration from an early-time ordered convection into a late-time disordered diffusion. More recent numerical and experimental investigations⁶⁻⁸ have shown that the conversion from convective to diffusive material interpenetration is even more pronounced for perturbations initialized with multiple Fourier modes.

Two very different types of mix models have been formulated to describe the material interpenetration across unstable interfaces: Andronov, *et al.*,⁶ proposed a purely diffusive single-fluid turbulence model, while Youngs⁷ proposed a purely convective multifluid interpenetration model. Both models give reasonable agreement with the growth rates of the mix-layer thicknesses observed in Rayleigh-Taylor and Richtmyer-Meshkov experiments. However, the models give quite different predictions in some situations. For example, only the convective model predicts that demixing will occur if the sign of the acceleration is reversed during a

Rayleigh-Taylor experiment. But the demixing that actually occurs must depend on the amount of disordered motion that has evolved in the mix layer, and neither model correctly estimates that amount.

Both single-fluid turbulence⁹⁻¹⁷ and multifluid interpenetration¹⁸⁻²¹ models have been developed to a high level of sophistication in their respective purely diffusive and purely convective forms. To reproduce both the early-time convective and the late-time diffusive drift motions exhibited by fluid flows near unstable material interfaces, a few mix models which combine the single-fluid and multifluid descriptions have been proposed.²²⁻²⁴ The central innovation of the present work is to provide a more natural formalism for deriving the equations for such a combined multifluid turbulent-mix model by dividing the turbulent contributions to the bulk fluid properties into ordered convective and disordered diffusive parts. It has been shown previously that summing the multifluid interpenetration equations over the mixture constituents produces bulk fluid equations with turbulent contributions given explicitly as sums of the multifluid drift motions.²⁵ The new mix model proposed in this report interprets these sums as the ordered convective parts of the turbulent contributions and subtracts them from the total turbulent contributions to give the disordered diffusive parts.

Like the mix models referred to previously,^{6,7,22-24} the new model is intended as an engineering model to be implemented in multidimensional hydrodynamics codes. Since such codes already strain the computational resources available, the new model incorporates several simplifying assumptions to achieve the desired convective and diffusive drift motions with minimal increase in the computational work required. While these assumptions should be reasonable approximations for many fluid flows of interest, they are not essential and could be relaxed to describe more complicated flows, but this would entail a substantial increase in the computational work required.

The new model consists of three coupled sets of equations, which are derived and discussed in Sections 2-4 and are briefly described here:

1. The bulk fluid equations are derived by decomposing the fluid properties into mean and fluctuating parts and spatially averaging the Navier-Stokes equations over suitable volume elements. Averages involving the thermal stress and heat flux are simplified by ignoring fluctuations in the pressure and temperature of the fluid. The turbulent contributions appear as correlations among the fluctuating quantities and are assumed to be composed of ordered convective and disordered diffusive parts, which are to be determined respectively from multifluid interpenetration and single-fluid turbulence equations.
2. The multifluid interpenetration equations are derived by assuming that the material constituents of the mixture are separated into distinct spatial subvolumes called chunks and averaging the fluctuating parts of the Navier-Stokes equations accordingly. All constituents are assumed to have the same pressure and temperature, so evolution equations are required only for the mass and momentum densities of each constituent. The stress forces are simplified by assuming that the viscous stress generated by the unresolved spatial gradients in the thin boundary layers separating the chunks can be modeled as a phenomenological surface-frictional drag. The resulting relative drift motion of each constituent is driven by shear and buoyancy accelerations, is resisted by the frictional drag, and approaches a concentration-gradient diffusion in the quasisteady limit. Summing various combinations of the multifluid drift motions over the constituents produces the ordered convective parts of the turbulent quantities. The dependence of the stress forces on the disordered diffusive parts of the turbulent quantities couples these equations to the single-fluid turbulence equations.
3. The single-fluid turbulence equations are derived by summing the multifluid interpenetration equations over the constituents and subtracting the results from the bulk fluid equations. The disordered diffusive parts of the turbulent stress and energy fluxes are given by gradient approximations, so evolution equations are required only for the turbulent kinetic energy density and its dissipation rate, both of which are assumed to be apportioned among the constituents according to their volume fractions. The resulting growth of the disordered diffusive parts of the turbulent quantities is driven by the dissipation of the multifluid drift kinetic energies. This dependence on the drift motions couples these equations to the multifluid interpenetration equations.

The resulting equations defining the new multifluid turbulent-mix model are summarized in a form suitable for implementation in multidimensional hydrodynamics codes in Section 5.

2. BULK FLUID EQUATIONS.

In general, a fluid is characterized at each position $\vec{r}$ and time t by specifying its mass density m , momentum density $m\vec{v}$, energy density $me = \frac{1}{2}mv^2 + m\theta$, thermal stress Ψ , and heat flux $\vec{\chi}$. The time evolution of the fluid densities is then governed by the conservation equations:

$$0 = \frac{\partial}{\partial t}m + \vec{\nabla} \cdot (m\vec{v}) = \frac{\partial}{\partial t}(m\vec{v}) + \vec{\nabla} \cdot (m\vec{v}^2 + \Psi) = \frac{\partial}{\partial t}(me) + \vec{\nabla} \cdot (me\vec{v} + \Psi \cdot \vec{v} + \vec{\chi}). \quad (1)$$

The thermal stress and heat flux are usually approximated by the Navier-Stokes constitutive relations:

$$\Psi = P\delta + \Pi, \quad \Pi = -\eta(\vec{\nabla} \circ \vec{v} - \frac{2}{3}\vec{\nabla} \cdot \vec{v}\delta), \quad \vec{\chi} = -\kappa\vec{\nabla}T, \quad (2)$$

where δ is the unit dyadic, Π is the viscous stress, the pressure P and temperature T are related to m and θ through the equations of state, and the viscosity η and conductivity κ are assumed to be known functions of P , T , and the atomic properties of the fluid. Eqs. (1) & (2) are called the Navier-Stokes equations.

In a region of instability, the fluid properties can be separated into mean and fluctuating parts, where the means are gotten by some averaging procedure. Three averages are commonly used, depending on the source of the fluctuations of interest:

1. An ensemble average is appropriate for fluctuations due to uncertainties in the initial or boundary values of the fluid properties;
2. A time average is appropriate for fluctuations due to unresolved temporal variations in the fluid properties;
3. A volume average is appropriate for fluctuations due to unresolved spatial variations in the fluid properties.

The fluctuations of interest in the present analysis are due to unresolved spatial features generated by instabilities at material interfaces, so a volume average (over suitable volume elements) is most appropriate.

Let angle brackets denote the average, and define the quantities

$$\begin{aligned} \rho &= \langle m \rangle, \quad \rho\vec{u} = \langle m\vec{v} \rangle, \quad \rho i = \langle m\theta \rangle, \quad P = \langle \Psi \rangle, \quad \vec{q} = \langle \vec{\chi} \rangle, \quad \vec{v}' = \vec{v} - \vec{u}, \quad \vec{w} = \langle \vec{v}' \rangle, \\ \rho k &= \langle \frac{1}{2}mv'^2 \rangle, \quad \vec{R} = \langle m\vec{v}'^2 \rangle, \quad \vec{s} = \langle m\theta\vec{v}' \rangle, \quad \vec{\sigma} = \langle \frac{1}{2}mv'^2\vec{v}' \rangle, \quad \vec{\pi} = \langle \Pi \cdot \vec{v}' \rangle, \\ \Pi' &= -\eta(\vec{\nabla} \circ \vec{v}' - \frac{2}{3}\vec{\nabla} \cdot \vec{v}'\delta), \quad Q = \langle \Pi' \rangle, \quad \rho\epsilon = -\langle \Pi' : \vec{\nabla}\vec{v}' \rangle. \end{aligned} \quad (3)$$

Then averaging the Navier-Stokes Eqs. (1) & (2) gives the bulk fluid equations, which can be written in terms of the convective time derivative $\frac{d}{dt} = \frac{\partial}{\partial t} + \vec{u} \cdot \vec{\nabla}$ as follows:

$$0 = \frac{d}{dt}\rho + \rho\vec{\nabla} \cdot \vec{u}, \quad (4)$$

$$0 = \rho \frac{d}{dt}\vec{u} + \vec{\nabla} \cdot (\vec{R} + P), \quad (5)$$

$$0 = \rho \frac{d}{dt}i + \vec{\nabla} \cdot (\vec{s} + \vec{q}) + (\vec{P} + Q) : \vec{\nabla}\vec{u} + P\vec{\nabla} \cdot \vec{w} - \rho\epsilon, \quad (6)$$

$$0 = \rho \frac{d}{dt}k + \vec{\nabla} \cdot (\vec{\sigma} + \vec{\pi}) + (\vec{R} - Q) : \vec{\nabla}\vec{u} + (\vec{\nabla}P) \cdot \vec{w} + \rho\epsilon, \quad (7)$$

$$P = P\delta + Q - \langle \eta \rangle (\vec{\nabla} \circ \vec{u} - \frac{2}{3}\vec{\nabla} \cdot \vec{u}\delta), \quad \vec{q} = -\langle \kappa \rangle \vec{\nabla}T. \quad (8)$$

Averages involving the thermal stress and heat flux have been simplified by ignoring the fluctuating parts of P and T . The turbulent contributions to the energy density ρk , the stress $\vec{R}$, and the energy fluxes $\vec{s}$ and $\vec{\sigma} + \vec{\pi}$ are explicitly present as correlations among the fluctuating parts of the fluid properties. Note that $(\vec{R} - Q) : \vec{\nabla}\vec{u}$ provides compression and shear sources for ρk , $(\vec{\nabla}P) \cdot \vec{w}$ provides a bouyancy source for ρk , and $\rho\epsilon$ provides a dissipation of ρk into ρi . The energy thus cascades from bulk kinetic to turbulent kinetic to thermal internal energy.

In Sections 3 & 4 the turbulent quantities are divided into ordered convective and disordered diffusive parts, and a prescription for determining those parts is presented which combines the multifluid and single-fluid approaches to turbulent-mix modeling.

3. MULTIFLUID INTERPENETRATION EQUATIONS.

The conservation Eqs. (1) can be manipulated to give evolution equations for the fluctuating parts of the fluid motions. These equations can be written in terms of the mass density ratio $x = m/\rho$ as follows:

$$0 = \rho \frac{d}{dt} x + \vec{\nabla} \cdot (\rho x \vec{v}'), \quad (9)$$

$$0 = \rho \frac{d}{dt} (x \vec{v}') + \rho x \vec{v}' \cdot \vec{\nabla} \vec{u} + \vec{\nabla} \cdot (\rho x \vec{v}'^2 + \Psi) + \rho x \frac{d}{dt} \vec{u}, \quad (10)$$

$$0 = \rho \frac{d}{dt} (x \theta) + \vec{\nabla} \cdot (\rho x \theta \vec{v}') + \vec{\nabla} \cdot \Psi + \vec{\nabla} \cdot (\vec{u} + \vec{v}'), \quad (11)$$

$$0 = \rho \frac{d}{dt} (\frac{1}{2} x v'^2) + \rho x \vec{v}'^2 : \vec{\nabla} \vec{u} + \vec{\nabla} \cdot (\frac{1}{2} \rho x v'^2 \vec{v}') + (\vec{\nabla} \cdot \Psi + \rho x \frac{d}{dt} \vec{u}) \cdot \vec{v}'. \quad (12)$$

The definitions in Eqs. (3) can be used to show that the average of Eq. (9) vanishes identically, while the averages of Eqs. (10)–(12) produce Eqs. (5)–(7), respectively.

When the fluctuating motions are caused by fluid instabilities at material interfaces, it is appropriate to consider the multifluid description of a mixture whose material constituents are separated into distinct subvolumes called chunks. Consistent with the desire to formulate a mix model exhibiting both convective and diffusive drift motions with a minimum of extra computational work, several assumptions will be introduced. While these assumptions are not essential, they greatly simplify the multifluid description and should be reasonable approximations for many fluid flows of interest.

First, it is assumed that any unresolved spatial gradients in the fluid properties are confined to thin boundary layers separating the chunks, so a concentration function $c_j(\vec{r}, t)$ can be defined to have the values 1 or 0 for positions respectively inside or outside chunks of the j -th material. Then the average volume fraction, mass fraction, specific drift momentum, specific thermal energy, pressure, viscous stress, viscosity, and conductivity of that material are

$$\begin{aligned} f_j &= \langle c_j \rangle, \quad x_j = \langle c_j x \rangle, \quad x_j \bar{w}_j = \langle c_j x \vec{v}' \rangle, \quad x_j \theta_j = \langle c_j x \theta \rangle, \\ f_j P_j &= \langle c_j P \rangle, \quad f_j \Pi_j = \langle c_j \Pi \rangle, \quad f_j \eta_j = \langle c_j \eta \rangle, \quad f_j \kappa_j = \langle c_j \kappa \rangle. \end{aligned} \quad (13)$$

It is further assumed that the average fluctuating viscous stress of each material is given by a gradient approximation:

$$f_j \Pi'_j = \langle c_j \Pi' \rangle = -f_j \eta_j (\vec{\nabla} \circ \vec{w}_j - \frac{2}{3} \vec{\nabla} \cdot \vec{w}_j \delta), \quad f_j \Pi_j = -f_j \eta_j [\vec{\nabla} \circ (\vec{u} + \vec{w}_j) - \frac{2}{3} \vec{\nabla} \cdot (\vec{u} + \vec{w}_j) \delta]. \quad (14)$$

The sums of these quantities over all constituents must satisfy

$$\begin{aligned} \sum_j f_j &= \sum_j x_j = 1, \quad \sum_j x_j \bar{w}_j = 0, \quad \sum_j f_j \bar{w}_j = \vec{w}, \quad \sum_j x_j \theta_j = i, \\ \sum_j f_j (P_j \delta + \Pi_j) &= P, \quad \sum_j f_j \Pi'_j = Q, \quad \sum_j f_j \eta_j = \langle \eta \rangle, \quad \sum_j f_j \kappa_j = \langle \kappa \rangle. \end{aligned} \quad (15)$$

The turbulent quantities $\vec{w}$ and Q are thus considered to have only ordered convective parts, given as sums of the multifluid drift motions. All other turbulent quantities are considered to have both ordered convective and disordered diffusive parts, represented by the respective subscripts "o" and "d":

$$\begin{aligned} \rho k_o &= \sum_j \frac{1}{2} \rho x_j w_j^2, \quad R_o = \sum_j \rho x_j \bar{w}_j^2, \quad \bar{s}_o = \sum_j \rho x_j \theta_j \bar{w}_j, \\ \bar{\sigma}_o &= \sum_j \frac{1}{2} \rho x_j w_j^2 \bar{w}_j, \quad \bar{\pi}_o = \sum_j f_j \Pi_j \cdot \bar{w}_j, \quad \rho \epsilon_o = -\sum_j f_j \Pi'_j : \vec{\nabla} \bar{w}_j, \end{aligned} \quad (16)$$

$$\begin{aligned} \rho k_d &= \sum_j \rho x_j k_{dj}, \quad R_d = \sum_j f_j R_{dj}, \quad \bar{s}_d = \sum_j f_j \bar{s}_{dj}, \\ \bar{\sigma}_d &= \sum_j (\rho x_j k_{dj} \bar{w}_j + f_j R_{dj} \cdot \bar{w}_j + f_j \bar{\sigma}_{dj}), \quad \bar{\pi}_d = \sum_j f_j \bar{\pi}_{dj}, \quad \rho \epsilon_d = \sum_j \rho x_j \epsilon_{dj}. \end{aligned} \quad (17)$$

Expressions for the disordered diffusive parts are given in Section 4.

Next, it is assumed that the mixture is in an equilibrium with all materials having the same pressure, P , and temperature, T , so the f_j and θ_j can be determined from the equations of state without solving a separate evolution equation for the thermal energy of each material. The equations of state can be expressed in a form giving the pressure and temperature of each material as functions of mass density and specific thermal energy, whereupon the equilibrium conditions to be inverted become

$$P_j(m_j, \theta_j) = P(\rho, i, x_1, x_2, \dots), \quad T_j(m_j, \theta_j) = T(\rho, i, x_1, x_2, \dots), \quad m_j = \rho x_j / f_j. \quad (18)$$

For given values of ρ , i , and the x_j , these equations along with the constraints $\sum_j f_j = 1$ and $\sum_j x_j \theta_j = i$ uniquely determine the values of P , T , and the f_j and θ_j .

Finally, it is assumed that the viscous stress generated by the unresolved spatial gradients in the thin boundary layers separating the chunks can be modeled as a phenomenological surface-frictional drag. The average stress forces for the j -th material can then be written

$$(\vec{\nabla} \cdot (c_j \rho x \vec{v}^{1/2} + c_j \Psi) - \Psi \cdot \vec{\nabla} c_j) = \vec{\nabla} \cdot (\rho x_j \vec{w}_j^2 + f_j \mathbf{R}_{dj} + f_j \mathbf{I}_j) + f_j \vec{\nabla} P + \omega \rho x_j \vec{w}_j. \quad (19)$$

The phenomenological drag frequency ω is discussed at the end of this section.

With the above assumptions, the multifluid description requires evolution equations only for the mass fraction and specific drift momentum of each material. These equations are obtained by multiplying Eqs. (9) & (10) by c_j and averaging. If molecular diffusion is ignored, then $\frac{d}{dt} c_j + \vec{v}' \cdot \vec{\nabla} c_j = 0$, and the multifluid interpenetration equations for the j -th material become

$$0 = \rho \frac{d}{dt} x_j + \vec{\nabla} \cdot (\rho x_j \vec{w}_j), \quad (20)$$

$$0 = \rho \frac{d}{dt} (x_j \vec{w}_j) + \rho x_j \vec{w}_j \cdot \vec{\nabla} \vec{u} + \vec{\nabla} \cdot (\rho x_j \vec{w}_j^2 + f_j \mathbf{R}_{dj} + f_j \mathbf{I}_j) + f_j \vec{\nabla} P + \omega \rho x_j \vec{w}_j + \rho x_j \frac{d}{dt} \vec{u}. \quad (21)$$

The presence of the disordered diffusive part $\mathbf{R}_{dj}$ of the turbulent stress couples these equations to the single-fluid turbulence equations derived in Section 4. According to Eq. (5), the pressure gradient can be written

$$\vec{\nabla} P = -\vec{\nabla} \cdot (\mathbf{R} + \mathbf{P} - P\delta) - \rho \frac{d}{dt} \vec{u}. \quad (22)$$

At early times, the stresses are small and the drift motion is a convective acceleration which can be shown to reproduce the effects of the Rayleigh-Taylor, Richtmyer-Meshkov, and Kelvin-Helmholtz instabilities described in Section 1:

$$\frac{d}{dt} (x_j \vec{w}_j) \simeq (f_j - x_j) \frac{d}{dt} \vec{u} - x_j \vec{w}_j \cdot \vec{\nabla} \vec{u}. \quad (23)$$

At late times, the transients die out and the stresses become disordered and equilibrated among the constituents of the mixture, so the drift motion approaches a concentration-gradient diffusion:

$$\rho x_j \vec{w}_j \simeq -\omega^{-1} (\mathbf{R}_d + \mathbf{P} - P\delta) \cdot \vec{\nabla} f_j. \quad (24)$$

Thus, the correct early-time convection can be achieved through the choice of the initial value of f_j , while the correct late-time diffusion can be achieved through the choice of the form for ω (see below).

Dotting Eq. (21) with $\vec{w}_j$ and summing over all constituents gives an evolution equation for the ordered convective part of the turbulent kinetic energy density:

$$0 = \rho \frac{d}{dt} k_o + \vec{\nabla} \cdot (\vec{\sigma}_o + \vec{\pi}_o) + (\mathbf{R}_o - \mathbf{Q}) : \vec{\nabla} \vec{u} + (\vec{\nabla} P) \cdot \vec{w} + \rho \phi_o + 2\omega \rho k_o + \rho \varepsilon_o, \quad (25)$$

$$\rho \phi_o = \sum_j \vec{\nabla} \cdot (f_j \mathbf{R}_{dj}) \cdot \vec{w}_j. \quad (26)$$

The similarity between Eqs. (25) & (7) justifies the interpretation of the sums of multifluid drift motions in Eqs. (16) as the ordered convective parts of the turbulent quantities. Note that $\rho \phi_o$ provides an additional buoyancy source for ρk_o , $2\omega \rho k_o$ provides a dissipation of ρk_o into ρk_d , and $\rho \varepsilon_o$ provides a dissipation of ρk_o into ρi . This suggests that the energy now cascades from bulk kinetic to ordered drift kinetic to disordered turbulent kinetic to thermal internal energy.

The phenomenological drag frequency ω can be written as the ratio of a characteristic speed and an effective dissipation length for the turbulent fluctuations. The use of a single drag frequency for all constituents of the mixture is consistent with the use in Section 4 of a single-fluid turbulence model to determine the disordered diffusive parts of the turbulent quantities. The drag frequency used in the multifluid interpenetration model of Youngs⁷ is equivalent to

$$\omega_o = \frac{2}{3} C_{\omega o} \sqrt{k_o} / \ell_o, \quad \frac{d}{dt} \ell_o = \sqrt{k_o} + \ell_o \vec{\nabla} \cdot \vec{u}, \quad (27)$$

while the drag frequency used in the single-fluid turbulence model of Andronov, *et al.*,⁶ is equivalent to

$$\omega_d = \frac{2}{3} C_{\omega d} \sqrt{k_d} / \ell_d, \quad \ell_d = k_d \sqrt{k_d} / \varepsilon_d, \quad (28)$$

where $C_{\omega o}$ and $C_{\omega d}$ are constants adjusted to fit experiments. A form for the drag frequency consistent with both these choices is given in Section 4.

4. SINGLE-FLUID TURBULENCE EQUATIONS.

Subtracting Eq. (25) from Eq. (7) gives an evolution equation for the disordered diffusive part of the turbulent kinetic energy density:

$$0 = \rho \frac{d}{dt} k_d + \vec{\nabla} \cdot (\vec{\sigma}_d + \vec{\pi}_d) + \mathbf{R}_d : \vec{\nabla} \vec{u} - \rho \phi_d - 2\omega \rho k_o + \rho \varepsilon_d. \quad (29)$$

This equation forms the basis for constructing a single-fluid turbulence model. Comparing the definitions in Eqs. (3), (16), & (17) shows that the contributions from the j -th material to the disordered diffusive parts of the turbulent quantities are given by

$$\begin{aligned} \rho x_j k_{dj} &= \langle c_j \frac{1}{2} \rho x |\vec{v}' - \vec{w}_j|^2 \rangle, \quad f_j \mathbf{R}_{dj} = \langle c_j \rho x (\vec{v}' - \vec{w}_j)^2 \rangle, \quad f_j \vec{s}_{dj} = \langle c_j \rho x \theta (\vec{v}' - \vec{w}_j) \rangle, \\ f_j \vec{\sigma}_{dj} &= \langle c_j \frac{1}{2} \rho x |\vec{v}' - \vec{w}_j|^2 (\vec{v}' - \vec{w}_j) \rangle, \quad f_j \vec{\pi}_{dj} = \langle c_j \mathbf{II} \cdot (\vec{v}' - \vec{w}_j) \rangle, \\ \rho x_j \varepsilon_{dj} &= -\langle c_j \mathbf{II}' : \vec{\nabla} (\vec{v}' - \vec{w}_j) \rangle. \end{aligned} \quad (30)$$

Consistent with the desire to determine these quantities with a minimum of extra computational work, several assumptions will be introduced. While these assumptions are not essential, they greatly simplify the turbulence description and should be reasonable approximations for many fluid flows of interest.

First, it is assumed that the disordered diffusive parts of the turbulent kinetic energy density and its dissipation rate are apportioned among the constituents of the mixture according to their volume fractions:

$$\rho x_j k_{dj} = f_j \rho k_d, \quad \rho x_j \varepsilon_{dj} = f_j \rho \varepsilon_d. \quad (31)$$

This assumption reduces the turbulence description to a single-fluid model, which is consistent with the use in Section 3 of a single drag frequency for all constituents of the mixture.

Next, it is assumed that the disordered diffusive part of the turbulent stress of each constituent is given by a gradient approximation:

$$\mathbf{R}_{dj} = \frac{2}{3} \rho k_d \delta + \mathbf{\Gamma}_{dj}, \quad \mathbf{\Gamma}_{dj} = -\eta_d [\vec{\nabla} \circ (\vec{u} + \vec{w}_j) - \frac{2}{3} \vec{\nabla} \cdot (\vec{u} + \vec{w}_j) \delta], \quad \eta_d = C_{\eta d} \omega^{-1} (\frac{2}{3} \rho k_d), \quad (32)$$

where $C_{\eta d}$ is a constant adjusted to fit experiments. This so-called Boussinesq approximation produces a turbulent viscous stress $\mathbf{\Gamma}_{dj}$ having the same form as the real viscous stress $\mathbf{II}_j$ given in Eq. (14).

Finally, it is assumed that the disordered diffusive parts of the turbulent energy fluxes of each constituent are also given by gradient approximations:

$$\vec{s}_{dj} = -C_{id} (\partial i / \partial T)_\rho \omega^{-1} (\mathbf{R}_{dj} + \mathbf{II}_j) \cdot \vec{\nabla} T, \quad \vec{\sigma}_{dj} + \vec{\pi}_{dj} = -C_{kd} \omega^{-1} (\mathbf{R}_{dj} + \mathbf{II}_j) \cdot \vec{\nabla} k_d, \quad (33)$$

where C_{id} and C_{kd} are additional constants adjusted to fit experiments. This assumption reduces the turbulence description to a diffusion model.

The definitions in Eqs. (17) then give

$$\mathbf{R}_d = \frac{2}{3} \rho k_d \delta + \sum_j f_j \mathbf{\Gamma}_{dj}, \quad \mathbf{D}_d = \omega^{-1} (\mathbf{R}_d + \mathbf{P} - \mathbf{P} \delta), \quad (34)$$

$$\vec{s}_d = -C_{id} (\partial i / \partial T)_\rho \mathbf{D}_d \cdot \vec{\nabla} T, \quad \vec{\sigma}_d + \vec{\pi}_d = \rho k_d \vec{w} - C_{kd} \mathbf{D}_d \cdot \vec{\nabla} k_d + \sum_j f_j \mathbf{R}_{dj} \cdot \vec{w}_j. \quad (35)$$

Note that the diffusion tensor $\mathbf{D}_d$ is the same as the one occurring in Eq. (24), which describes the multifluid concentration-gradient diffusion at late times. Indeed, producing this diffusion tensor motivated the forms of the gradient approximations chosen for the turbulent energy fluxes.

With the above assumptions, the turbulence description requires evolution equations only for the disordered diffusive parts of the turbulent kinetic energy density and its dissipation rate. The first single-fluid turbulence equation is derived directly from Eq. (29):

$$0 = \rho \frac{d}{dt} k_d + \vec{\nabla} \cdot (\rho k_d \vec{w} - C_{kd} \mathbf{D}_d \cdot \vec{\nabla} k_d) + \rho \phi_d - 2\omega \rho k_o + \rho \varepsilon_d, \quad (36)$$

$$\rho \phi_d = \sum_j f_j \mathbf{R}_{dj} : \vec{\nabla} (\vec{u} + \vec{w}_j). \quad (37)$$

The dependence of $\rho \phi_d$ and ρk_o on the drift motions couples these equations to the multifluid interpenetration equations derived in Section 3. Note that $\rho \phi_d$ provides compression and shear sources for ρk_d , $2\omega \rho k_o$ provides a dissipation of ρk_o into ρk_d , and $\rho \varepsilon_d$ provides a dissipation of ρk_d into ρi . This confirms that the energy now cascades from bulk kinetic to ordered drift kinetic to disordered turbulent kinetic to thermal internal energy.

There remains the task of determining ε_d or some algebraically equivalent turbulent quantity such as the ω_d or ℓ_d defined in Eqs. (28) or the η_d defined in Eqs. (32). Evolution equations have been proposed in the turbulence literature^{10,11,16,17} for all these quantities (and some others), but ε_d has been the most popular choice for the second turbulent variable (giving the so-called $k\varepsilon$ models). Unfortunately, the turbulent kinetic energy dissipation rate is a rather nonintuitive quantity whose initialization is difficult to specify in fluid flows of interest, so Daly¹⁶ (among others) has suggested using an evolution equation for the effective turbulent dissipation length instead. This suggestion is particularly attractive for the purposes of the present work since it allows the alternative forms for the drag frequency given in Eqs. (27) & (28) to be made mutually consistent.

Accordingly, the second single-fluid turbulence equation is taken to be

$$0 = \rho \frac{d}{dt} \ell + \vec{\nabla} \cdot (\rho \ell \vec{w} - C_{ld} \mathbf{D}_d \cdot \vec{\nabla} \ell) - C_{lo} \rho (\ell \vec{\nabla} \cdot \mathbf{u} + \sqrt{k_o + k_d}), \quad (38)$$

and the dissipation rate and drag frequency are given by

$$\rho \varepsilon_d = \rho k_d \sqrt{k_o + k_d} / \ell, \quad \omega = \frac{2}{3} C_\omega \sqrt{k_o + k_d} / \ell. \quad (39)$$

Note that these equations are very similar to the length-scale treatment used in the combined multifluid turbulent-mix model of Youngs²⁴ and reproduce Eqs. (27) & (28) in the respective limits of purely ordered convective and purely disordered diffusive turbulence. Furthermore, in the latter limit Eqs. (36)–(39) can be combined to produce an equation for ε_d which is consistent with that given in the turbulence literature^{10,11,16,17} if the adjustable constants are assigned the following values:

$$C_{\eta d} \simeq .09 C_\omega, \quad C_{id} \simeq .09 C_\omega, \quad C_{kd} \simeq .09 C_\omega, \quad C_{ld} \simeq .0675 C_\omega, \quad C_{lo} \simeq .50, \quad C_\omega \simeq 7.8. \quad (40)$$

These values are only tentatively recommended since they are based on comparisons with models which treat turbulence as purely disordered diffusive. Final determination of the values of the adjustable constants must await detailed comparisons of the new multifluid turbulent-mix model with a wide range of experiments.

5. SUMMARY OF MODEL EQUATIONS.

For easy reference, the equations defining the new multifluid turbulent-mix model are summarized in a form suitable for implementation in multidimensional hydrodynamics codes in this section. These equations exhibit both the early-time convective and the late-time diffusive drift motions seen in numerical and experimental investigations of the evolution of interfacial instabilities, so the new model should give a reasonable description of the turbulent mixing in many fluid flows of interest. The simplifying assumptions incorporated in the new model could be relaxed to describe more complicated flows, but this would entail a substantial increase in the computational work required.

- Bulk fluid equations:

$$0 = \frac{d}{dt}\rho + \rho \vec{\nabla} \cdot \vec{u}, \quad (41)$$

$$0 = \rho \frac{d}{dt} \vec{u} + \vec{\nabla} \cdot (\mathbf{R}_o + \mathbf{R}_d + \mathbf{P}), \quad (42)$$

$$0 = \rho \frac{d}{dt} i + \vec{\nabla} \cdot (\vec{s}_o + \vec{s}_d + \vec{q}) + (\mathbf{P} + \mathbf{Q}) : \vec{\nabla} \vec{u} + P \vec{\nabla} \cdot \vec{w} - \rho(\epsilon_o + \epsilon_d), \quad (43)$$

$$\mathbf{P} = P\delta + \mathbf{Q} - \langle \eta \rangle (\vec{\nabla} \circ \vec{u} - \frac{2}{3} \vec{\nabla} \cdot \vec{u} \delta), \quad \vec{q} = -\langle \kappa \rangle \vec{\nabla} T. \quad (44)$$

- Ordered convective fluid properties:

$$\sum_j f_j = \sum_j x_j = 1, \quad \sum_j x_j \vec{w}_j = 0, \quad \sum_j f_j \vec{w}_j = \vec{w}, \quad \sum_j x_j \theta_j = i, \quad (45)$$

$$\sum_j f_j (P_j \delta + \mathbf{II}_j) = \mathbf{P}, \quad \sum_j f_j \mathbf{II}'_j = \mathbf{Q}, \quad \sum_j f_j \eta_j = \langle \eta \rangle, \quad \sum_j f_j \kappa_j = \langle \kappa \rangle,$$

$$\mathbf{II}'_j = -\eta_j (\vec{\nabla} \circ \vec{w}_j - \frac{2}{3} \vec{\nabla} \cdot \vec{w}_j \delta), \quad \mathbf{II}_j = -\eta_j [\vec{\nabla} \circ (\vec{u} + \vec{w}_j) - \frac{2}{3} \vec{\nabla} \cdot (\vec{u} + \vec{w}_j) \delta], \quad (46)$$

$$\rho k_o = \sum_j \frac{1}{2} \rho x_j w_j^2, \quad \mathbf{R}_o = \sum_j \rho x_j \vec{w}_j^2, \quad \vec{s}_o = \sum_j \rho x_j \theta_j \vec{w}_j, \quad \rho \epsilon_o = -\sum_j f_j \mathbf{II}'_j : \vec{\nabla} \vec{w}_j. \quad (47)$$

- Multifluid interpenetration equations:

$$0 = \rho \frac{d}{dt} x_j + \vec{\nabla} \cdot (\rho x_j \vec{w}_j), \quad (48)$$

$$0 = \rho \frac{d}{dt} (x_j \vec{w}_j) + \rho x_j \vec{w}_j \cdot \vec{\nabla} \vec{u} + \vec{\nabla} \cdot (\rho x_j \vec{w}_j^2 + f_j \mathbf{R}_{dj} + f_j \mathbf{II}_j) + f_j \vec{\nabla} P + \omega \rho x_j \vec{w}_j + \rho x_j \frac{d}{dt} \vec{u}, \quad (49)$$

$$P_j(m_j, \theta_j) = P(\rho, i, x_1, x_2, \dots), \quad T_j(m_j, \theta_j) = T(\rho, i, x_1, x_2, \dots), \quad m_j = \rho x_j / f_j. \quad (50)$$

- Disordered diffusive fluid properties:

$$\mathbf{R}_{dj} = \frac{2}{3} \rho k_d \delta + \mathbf{\Gamma}_{dj}, \quad \mathbf{\Gamma}_{dj} = -\eta_d [\vec{\nabla} \circ (\vec{u} + \vec{w}_j) - \frac{2}{3} \vec{\nabla} \cdot (\vec{u} + \vec{w}_j) \delta], \quad \eta_d = C_{\eta d} \omega^{-1} (\frac{2}{3} \rho k_d), \quad (51)$$

$$\mathbf{R}_d = \frac{2}{3} \rho k_d \delta + \sum_j f_j \mathbf{\Gamma}_{dj}, \quad \mathbf{D}_d = \omega^{-1} (\mathbf{R}_d + \mathbf{P} - P\delta), \quad \vec{s}_d = -C_{id} (\partial i / \partial T)_\rho \mathbf{D}_d \cdot \vec{\nabla} T. \quad (52)$$

- Single-fluid turbulence equations:

$$0 = \rho \frac{d}{dt} k_d + \vec{\nabla} \cdot (\rho k_d \vec{w} - C_{kd} \mathbf{D}_d \cdot \vec{\nabla} k_d) + \rho \phi_d - 2\omega \rho k_o + \rho \epsilon_d, \quad (53)$$

$$0 = \rho \frac{d}{dt} \ell + \vec{\nabla} \cdot (\rho \ell \vec{w} - C_{ld} \mathbf{D}_d \cdot \vec{\nabla} \ell) - C_{Lo} \rho (\ell \vec{\nabla} \cdot \vec{u} + \sqrt{k_o + k_d}), \quad (54)$$

$$\rho \phi_d = \sum_j f_j \mathbf{R}_{dj} : \vec{\nabla} (\vec{u} + \vec{w}_j), \quad \rho \epsilon_d = \rho k_d \sqrt{k_o + k_d} / \ell, \quad \omega = \frac{2}{3} C_\omega \sqrt{k_o + k_d} / \ell. \quad (55)$$

- Tentatively recommended values of the adjustable constants:

$$C_{\eta d} \simeq .09 C_\omega, \quad C_{id} \simeq .09 C_\omega, \quad C_{kd} \simeq .09 C_\omega, \quad C_{ld} \simeq .0675 C_\omega, \quad C_{Lo} \simeq .50, \quad C_\omega \simeq 7.8. \quad (56)$$

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