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Author(s): Schwarzkopf, John Dennis
Horwitz, Jeremy A.

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BHR Equations Re-derived with Immiscible Particle Effects

Jeremy A. Horwitz[a], John D. Schwarzkopf[b]

Abstract

Compressible and variable density turbulent flows with dispersed phase effects are found in many applications ranging from combustion to cloud formation. These types of flows are among the most challenging to simulate. While the exact equations governing a system of particles and fluid are known, computational resources limit the scale and detail that can be simulated in this type of problem. Therefore, a common method is to simulate averaged versions of the flow equations, which still capture salient physics and is relatively less computationally expensive. Besnard et al. [1] developed such a model for variable density miscible turbulence, where ensemble-averaging was applied to the flow equations to yield a set of filtered equations. Besnard et al. further derived transport equations for the Reynolds stresses, the turbulent mass flux, and the density-specific volume covariance, to help close the filtered momentum and continuity equations. We re-derive the exact BHR closure equations which include integral terms owing to immiscible effects. Physical interpretations of the additional terms are proposed along with simple models. The goal of this work is to extend the BHR model to allow for the simulation of turbulent flows where an immiscible dispersed phase is non-trivially coupled with the carrier phase.

Disclaimer: This document represents the beginnings of deriving a second moment equation for evaporating or burning particles in compressible or variable density turbulent flow. The exact equations are illustrated and documented assumptions have been made to provide modeled forms. The purpose of this document is to share initial thoughts and concepts with the community in order to further develop these models. This document is a work in progress.

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[a] Student at 2013 Computational Physics Student Summer Workshop.

[b] Mentor for the 2013 Computational Physics Student Summer Workshop

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Introduction

Variable density turbulent flows with dispersed phases are ubiquitous in engineering applications ranging from combustion in automobile and aircraft engines to environmental applications such as cloud formation. In flows involving multiple materials, we identify the continuous material which has the largest contribution to the system's dynamics as the carrier phase and discrete materials having higher order contributions to the flow dynamics as dispersed phases. Such identification is typically suitable when the carrier phase volume fraction is much larger than all dispersed phase volume fractions. However, in many flows even at low dispersed phase volume fraction, dispersed phase dynamics may have a contribution comparable to that of the carrier phase dynamics. In such cases, the presence of a dispersed phase may non-trivially couple with carrier phase dynamics to produce more complicated flow physics. When the dispersed phase material is immiscible with respect to the carrier phase (i.e. the phases do not mix at the molecular level), additional physics including the treatment of boundary conditions (slip, penetration, sources of mass, interfacial tension e.g.) must be accounted for since these effects may have a significant contribution to the total system's dynamics. Specifically, the addition of rigid particles to a turbulent fluid flow may either increase dissipation of turbulent kinetic energy (TKE) or enhance production of TKE depending on the particle size relative to the turbulent integral scale [13]. As the volume fraction increases, particles can no longer be treated as independent. In this regime, turbulent dissipation owing to particle-fluid interaction is accompanied by particle dissipation owing to particle-particle interaction in the form of collisions [10]. In regions where multiple particles are separated by scales comparable to or smaller than the un-laden Kolmogorov scale, the laden-dissipation length scales may be altered [16]. In flows involving droplets or bubbles, there may exist mass transfer between the dispersed and carrier phase in the form of evaporation or condensation. Mass transfer in turn affects production of TKE and turbulent mass flux (as we will show). When density variations and/or compressibility in the carrier phase is significant, additional production in the Reynolds stress equation may occur. Therefore, the combination of compressibility and dispersed phase coupling with the carrier phase makes simulating compressible and variable density turbulent flows with immiscible dispersed phases especially challenging. Particularly, the range of length scales in practical flows of this type makes direct numerical simulation (DNS) unviable.

A breakthrough in modeling variable density multicomponent turbulent flows came in 1992 when Besnard et al. [1] applied ensemble averaging to the instantaneous mass, momentum, and energy equations and derived exact transport equations for the Reynolds stresses, the turbulent mass flux, the density-specific volume covariance, and the turbulent heat flux. These exact equations were valid for compressible turbulence involving multiple miscible fluid components. The turbulent mass flux and density specific covariance transport equations were derived as a means for closing the Reynolds stress equation. With suitable closure models for the remaining terms in the Reynolds stress equation (dissipation, triple-correlation, pressure-strain, transport terms), as well as for the unclosed terms in the remaining transport equations, this system of equations are collectively referred to as the BHR model which is capable of capturing compressible single phase multicomponent effects for many flows [2]. Introduction of the BHR equations is postponed to the discussion section.

Independently, a large body of work exists on incompressible particle-laden flows where the carrier phase is treated as a single uniform material. In 1850, Stokes [4] first derived the drag on a spherical particle moving at a constant speed in a steady fluid in what would later be identified as the low-Reynolds number or creeping flow limit. From the Oseen equations, Kaplun and Lagerstrom as well as Proudman and Pearson derived a second-order correction to the non-dimensional drag coefficient corresponding to the Stokes solution [6][c]. In 1888, Basset [5] used successive approximations to derive the equation of motion for a spherical particle beginning from rest and falling slowly due to gravity in a viscous fluid. Batchelor [6] discusses the role of oscillating boundary layers on mean fluid element motion and shows that a mean drift of fluid elements or small particles will exist if there are spatial gradients in either amplitude or phase of the flow away from a domain boundary. Unsteady effects and curvature in the flow velocity are accounted for in the particle equation of motion derived by Maxey and Riley [7]. Later, Maxey [8] examined the motion of particles in a turbulent flow and showed that inertial particles should experience a net flux into regions of low vorticity and high strain-rate. Squires and Eaton [9] performed a DNS of particle-laden turbulence and observed the preferential concentration effect predicted by Maxey [8]. Sundaram and Collins [10] observed enhanced turbulent dissipation due to particle presence where the peak transient dissipation increased with particle Stokes number. Burton and Eaton [11] performed a fully-resolved DNS of a turbulent flow over a single particle and compared the force on the particle with a similar expression to that derived in [7]. The dominant contribution to the particle-drag is shown to be the steady Stokes drag and all other drag effects are small for almost all times. The discrepancy between the theoretical drag and calculated drag suggests the particle-force is more complicated in instances where the particle diameter is of order Kolmogorov scale or greater [11].

The challenge of studying particle-laden turbulence may be eclipsed by the difficulties in understanding flows with droplets and bubbles. In such flows, the dispersed phase is no longer rigid and may deform subject to the stresses exerted by both the carrier phase as well as the dispersed phase when the volume fraction of the latter is not small. At material interfaces between disparate immiscible molecular species, interfacial tension will play a dominate role in flow dynamics in the neighborhood of the interface when the appropriate non-dimensional parameter is not large (Weber, Capillary, Bond number e.g.). Attempts to model surface tension have had some success, (see [12] for early work on the subject). However, simulating surface tension and interfacial dynamics remain a challenging subject. We will not address this topic further except to mention in our results where such a model would be present. In the case of deformable droplets surrounded by a gaseous carrier phase of the same material, (e.g. water droplets in water-vapor) mass-transfer between the two phases may exist under the appropriate thermodynamic conditions. Hereto, we will not present an adequate review except to point out in our discussion section which terms are owing to mass transfer effects and to briefly discuss simple models which may capture the salient aspects.

Having briefly examined some of the relevant literature and additional physics present in variable density turbulent flows with immiscible dispersed phases, we state the objective of this work. In this paper, we present an extension to the equations first derived by Besnard et al. [1]. After a brief discussion of volume averaging, we present the exact volume-averaged continuity, momentum, Reynolds stress, turbulent mass-flux, and density-specific volume covariance

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[c] References for Oseen, Kaplun and Lagerstrom as well as Proudman and Pearson are found in [6].

equations. These equations are identical to those first derived in [1] by the process of ensemble averaging, except here there are explicit integral effects accounting for the variation of flow properties at the time-dependent boundaries separating the continuous with the dispersed phase(s). The resulting equations will be valid for compressible variable density turbulence with a distinct dispersed phase. Additional physics (evaporation, interfacial deformation) are explicit in the integral expressions. The additional immiscible phase effects represent a perturbation on mean-flow quantities. In the limit of zero-volume fraction of the dispersed phase, the BHR-equations are recovered. The integral expressions owing to the dispersed phase represent additional un-closed terms in the mean-flow equations. Our discussion of these terms is centered around classifying the new terms based on their expected contribution to the flow dynamics. That is, we attempt to classify the salient physics for each new term and present hypotheses as to their respective contribution to the carrier phase (production, transport, dissipation, etc.) Based on the hypothesized effect, we suggest simple models to close the new terms. In our discussion, the terms "particles" and "dispersed phase elements" will be used interchangeably. Additional physics (mass-transfer, interfacial deformation) will be presented as a superimposed effect built into the predominant effect of the dispersed phase on the carrier. The carrier-dispersed phase coupling then will be owing to satisfaction of appropriate boundary conditions at the interface between the respective materials.

Discussion

Review of Volume Averaging

Before extending the BHR equations to include immiscible effects, we briefly review the method of volume averaging to understand how dispersed phased effects will enter the governing equations. We begin by considering the arbitrary control volume containing multiple materials shown in Figure 1. Here, the striped (blue) region represents the carrier phase which may have a spatially

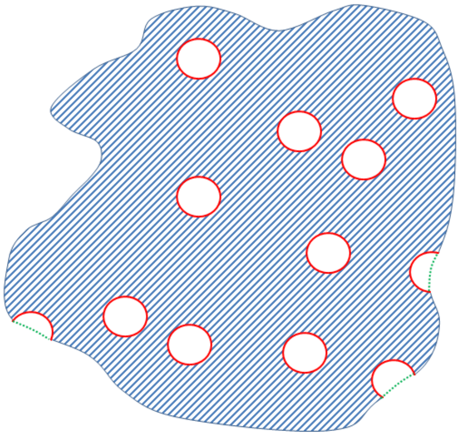

Figure 1: Arbitrary control volume containing carrier phase (stripes) and dispersed phase (circles/semi-circles).

varying density field owing to compressible effects or problem specification. It is important to note here that the carrier-phase fluids are treated as *miscible* so that any immiscible effects (distinguished by a surface) are treated as a separate phase with respect to the carrier fluid. The circular (spherical in 3D) elements represent the dispersed phase where the carrier-dispersed phase boundary is represented in red. It should be noted there is no loss in generality in assuming the dispersed phase is made up of identical spherical particles. So long as the *implemented* model is able to distinguish between members of the dispersed phase, the following analysis is valid for dispersed elements of arbitrary shapes and material properties. Having established an open control volume containing multiple materials, we define the average of some arbitrary flow quantity B in (1) viz. [3]:

$$\bar{B} = \frac{1}{V}\int_{V_c} B dV = \frac{V_c}{V}\frac{1}{V_c}\int_{V_c} B dV = \alpha_c \langle B \rangle \tag{1}$$

Here, $\bar{B}$ is read as the volume or bulk average of B, V is the total volume contained within the boundaries of the control volume (shown in Figure 1), V_c is the carrier-phase volume contained within the control volume specified in Figure 1, α_c is the carrier-phase volume fraction (often times referred to as the void fraction, $\alpha_c \equiv V_c/V$), and $\langle B \rangle$ is interpreted as the carrier-phase, or simply the phase, average of B. Having defined a volume average, it is now possible to decompose a carrier phase flow quantity B in terms of a phase average and a deviating part viz.

$$B = \langle B \rangle + B' \tag{2}$$

Here, B' is the read as the deviation of B from the carrier phase average $\langle B \rangle$. By construction, the volume average of the fluctuating term in (2) is zero, viz.:

$$\overline{B'} = \frac{1}{V}\int_{V_c} B' dV = 0 \tag{3}$$

The above expression implies that the carrier phase volume over which statistics are taken must be large enough such that the sum of the deviations is zero, as depicted in Figure 2.

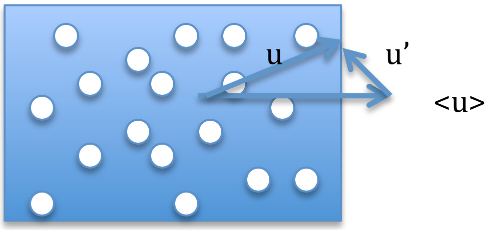

Figure 2: A control volume containing N particles (and/or turbulence) such that a statistical average is formed within the carrier phase. The carrier phase volume must be larger than the limiting volume of the fluid yet small enough to make use of differential operators.

As discussed in [1], it is often desirable to express mean quantities weighted by the local carrier-phase density. The Favre average [3] is formed by:

$$\tilde{B} \equiv \frac{\overline{\rho_c B}}{\bar{\rho}_c} = \frac{1}{\alpha_c \langle \rho_c \rangle V} \int_{V_c} \rho_c B dV = \frac{\langle \rho_c B \rangle}{\langle \rho_c \rangle} \tag{4}$$

Here, $\tilde{B}$ is referred as the Favre, mass, or density-weighted average of B and ρ_c is the carrier-phase density. The Favre average allows us to define an alternate decomposition for B:

$$B = \tilde{B} + B'' \tag{5}$$

As a consequence, the Favre average of the fluctuating term in (4) is zero, that is:

$$\overline{\rho_c B''} = \frac{1}{V} \int_{V_c} \rho_c B'' dV = 0 \tag{6}$$

The instantaneous carrier-phase velocity, denoted as u_i, can be decomposed into mean and deviation terms such as $u_i = \tilde{u}_i + u_i'' = \langle u_i \rangle + u_i'$, where the former is the Favre decomposition and the latter is the Reynolds. The average turbulent mass weighted turbulence velocity $a_i \equiv -\langle u_i'' \rangle = \langle \rho_c' u_i' \rangle / \langle \rho \rangle$ relates respective mean definitions of *velocity*[d] to each other and independently, the respective velocity fluctuation definitions viz.:

$$\tilde{u}_i = \langle u_i \rangle + a_i \tag{7}$$

$$u_i'' = u_i' - a_i \tag{8}$$

The bulk (1) and Favre average (4) notation will be used throughout where preference for one notation over the other is given based on convenience, noting that it is possible to switch between notations by equation (2) and (5). Having defined a volume average, it remains to specify how this average will commute with derivatives. This commutation rule will become necessary once the averaging procedure is applied to the carrier-phase equations of motion. The commutative rule for the bulk average of spatial and temporal derivatives is given in (9) and (10) respectively:

$$\overline{\frac{\partial B}{\partial x_i}} = \frac{\partial \bar{B}}{\partial x_i} - \frac{1}{V} \int_S B n_i dS \tag{9}$$

where S is the total particle surfaces within the control volume (shown by the red lines in Figure 1). In addition, the phase average of the gradient of a property can be written as:

$$\langle \frac{\partial B}{\partial x_i} \rangle = \frac{\partial \langle B \rangle}{\partial x_i} + \frac{\langle B \rangle}{\alpha_c} \frac{\partial \alpha_c}{\partial x_i} - \frac{1}{V_c} \int_S B n_i dS \tag{9a}$$

The bulk volume average of the temporal derivative is written as

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[d] That is, (7) and (8) hold for the velocity means and fluctuations, but *not* for an arbitrary flow quantity B.

$$\overline{\frac{\partial B}{\partial t}} = \frac{\partial \bar{B}}{\partial t} + \frac{1}{V}\int_S B(\mathrm{v}_i n_i + \dot{r})dS \qquad (10)$$

and the phase average of the temporal derivative can be written as:

$$\langle\frac{\partial B}{\partial t}\rangle = \frac{\partial \langle B\rangle}{\partial t} + \frac{\langle B\rangle}{\alpha_c}\frac{\partial \alpha_c}{\partial t} + \frac{1}{V_c}\int_S B(\mathrm{v}_i n_i + \dot{r})dS \qquad (10a)$$

The integral terms in (9) and (10) are consequences of Leibnitz's integral theorem [3] (the reader is referred to Crowe [3] for more details on the derivation of (9) and (10).) The integrals in (9) and (10) are taken over the total surface boundary between dispersed and continuous phases, as shown in Figure 1, and assume that the particle size (and the wake effect) is smaller than the control volume. These integrals are understood as the summation of surface integrals over all dispersed phase elements. In essence, the commutative rule in (9) and (10) allows the commutation of derivative and averaging operators at the cost of accounting for the variation of B along the dispersed phase boundary, and the fact that the dispersed phase boundaries are time dependent as the particles may move around within, enter, or exit the control volume. However, the boundary of the control volume itself is fixed and therefore makes no additional integral contribution in (9) and (10). Therefore, S in (9) and (10), which refers to the red surfaces in Figure 1 emphasizes that the only dispersed phase surfaces or fractions thereof within the *interior* of the control volume contribute to the surface integrals.

Notice there is an additional term in (9a) that arises when phase averaging is used, it is non-zero in general as can be shown using continuity, that is, the volume fraction obeys the material equation, such as

$$\frac{\partial}{\partial t}\alpha_c\langle\rho\rangle + \frac{\partial}{\partial x_j}\alpha_c\langle\rho\rangle u_j = \chi$$

$$\frac{\partial}{\partial t}\alpha_c\langle\rho\rangle + \langle\rho\rangle u_j\frac{\partial}{\partial x_j}\alpha_c + \alpha_c\frac{\partial}{\partial x_j}\langle\rho\rangle u_j = \chi$$

$$\frac{\langle\rho\rangle u_j}{\alpha_c}\frac{\partial \alpha_c}{\partial x_j} = -\frac{1}{\alpha_c}\frac{\partial}{\partial t}\alpha_c\langle\rho\rangle - \frac{\partial}{\partial x_j}\langle\rho\rangle u_j + \frac{\chi}{\alpha_c}$$

$$\frac{1}{\alpha_c}\frac{\partial \alpha_c}{\partial x_j} = -\frac{1}{\langle\rho\rangle u_j\alpha_c}\frac{\partial}{\partial t}\alpha_c\langle\rho\rangle - \frac{1}{\langle\rho\rangle u_j}\frac{\partial}{\partial x_j}\langle\rho\rangle u_j + \frac{1}{\langle\rho\rangle u_j}\frac{\chi}{\alpha_c}$$

where χ is the continuity residual owing to mass transfer. Evidently, the second term on the right hand side of (9a) is non-zero in general and must be retained in the derivation. In the limit of no dispersed phase, α_c is unity everywhere so that this extra term disappears and the commutation rules for phase and bulk average as well as the averages themselves become identical. Note that if α_c is zero, there is no continuous phase so that the entire dispersed phase may be treated as a single phase. In this case, the phase and bulk averages would be equivalent. Alternatively, if there are two separate phases, the bulk and phase averages are only well defined if α_c is close to unity in most regions of the flow, a dilute flow assumption. A similar term to that appearing in (9a) also appears on the right hand side of (10a).

In Equations (10) and (10a), v_i is the velocity of the center of mass of any given particle and $\dot{r}$ is the radius rate-of-change of the particle surface w.r.t. its center of mass. While variation in B along dispersed phase surfaces is necessary for the integral term in (9) to be non-zero, the integral term in (10) may be non-zero when B is constant along the surface since $\dot{r}$ need not be constant on S. Note, v_i is constant on S by definition. We may state this observation more generally and concisely: the integral of *any* mean flow quantity along a dispersed phase surface is zero[e] viz.:

$$\int_S \langle B\rangle n_i dS = \langle B\rangle \int_S n_i dS = 0 \tag{11}$$

The veracity of (11) comes from the definition of the volume average. Upon applying the averaging operator to a flow quantity, the averaged quantity becomes independent of the volume of integration. On the closure of the region of integration, the averaged quantity is invariant so that the averaged quantity must therefore be invariant over each dispersed phase surface. Spatial variations in mean quantities are then understood as varying from one control volume to the next, in the limit as the control volume is reduced to a size much smaller than the average length-scale over which macroscopic flow quantities change, but large compared to the characteristic dimension of dispersed phase elements. The above equation (11) leads to the additional conclusion that immiscible/integral effects are owing to fluctuations[f] viz.:

$$\int_S Bn_i dS = \int_S (\bar{B} + B')n_i dS = \int_S B' n_i dS$$

$$= \int_S \left(\tilde{B} + B''\right)n_i dS = \int_S B'' n_i dS = \int_S B' n_i dS \tag{12}$$

This concludes the necessary discussion of volume averaging. In the next section, we present the results of applying volume averaging to the flow equations to yield the BHR equations with explicit integral effects owing to the dispersed phase. We conclude this section by providing a list of useful identities which are used throughout the to derive the transport equations for the compressible and variable density turbulence quantities. For any carrier phase quantities A and B we have:

$$\overline{B'} = \overline{\rho_c B''} = 0 \tag{a}$$

$$\overline{AB} = \bar{A}\bar{B} + \overline{A'B'} \tag{b}$$

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[e] The integration must be performed over a closed surface contour and the surface unit normal [15].

[f] Mean flow quantities may be present in dispersed phase integrals, but only when combined with other fluctuating quantity(s).

$$\overline{A'B} = \overline{A'B'} \tag{c}$$

$$\overline{A''} = -\overline{\rho' A'}/\bar{\rho}_c \tag{d}$$

$$\overline{\frac{\partial \bar{A}}{\partial x_i}} = \frac{\partial \bar{A}}{\partial x_i} \tag{e}$$

$$\overline{\frac{\partial \tilde{A}}{\partial x_i} B''} = \frac{\partial \tilde{A}}{\partial x_i} \overline{B''} \tag{f}$$

$$\overline{\frac{\partial \bar{A}}{\partial x_i} B'} = 0 \tag{g}$$

and for the arbitrary fluid variable C:

$$\overline{\frac{\partial \bar{A}}{\partial x_i} B'C'} = \frac{\partial}{\partial x_i}(\bar{A}\,\overline{B'C'}) - \bar{A}\frac{\partial}{\partial x_i}(\overline{B'C'}) \tag{h}$$

where (a)-(d) are given in [1], and (e)-(h) were found during the present investigation.

BHR Equations with Immiscible Effects

We now present the exact volume-averaged equations for continuity, momentum, Reynolds stress, turbulent mass-flux, and density-specific volume covariance and discuss their salient aspects. In the following equations, we will observe that as the continuous phase volume fraction α_c goes to unity, surface elements will shrink to null so that all dispersed phase effects will vanish. In addition, all phase-averages will become volume-averages since the carrier-phase will occupy an entire control volume. The reduced equations will then be identical to those derived by Besnard et al. [1].

Volume-Averaged Continuity Equation with Immiscible Effects

The volume-averaged continuity equation is given as (13):

$$\frac{\partial}{\partial t}[\alpha_c\langle\rho_c\rangle] + \frac{\partial}{\partial x_i}[\alpha_c\langle\rho_c\rangle\tilde{u}_i] = \frac{1}{V}\int_S \rho_c w dS = \chi \tag{13}$$

where *w* is the penetration velocity or the velocity of the mass ejected from the particle surface. Equation (13) agrees with the expression derived in Crowe [3]. Evidently, the volume-averaged continuity equation differs from the BHR-equation by a single term in the form of a mass source denoted as χ. The mass source depends only on the carrier-phase density evaluated along the surface[g] of each particle as well as the mass-transfer velocity w which is owing to condensation, evaporation or reaction effects. The motion of particles into and out of the control volume as well as their respective deformations are captured in the void faction (α_c). As particles of constant size, number and mass move about within a control volume over some time Δt, the net mass of the fluid is unchanged. However, if the particle changes in size or mass, or if the number of particles change, this affects the void fraction which in turn affects the fluid mass within the control volume. The term on the RHS of (13) suggests that *net* sources of mass between the dispersed and carrier-phase may affect the averaged continuity equation. The term net is used here to emphasize competing effects, that is, nothing in χ suggests that this term must be a source and in practice it may be a sink of mass from the carrier-phase (e.g. condensation). The net effect of χ on any given control volume can be found by performing the integration in (13) on each particle surface, or fraction there-of within a given control volume and then summing these contributions. Such an integral evaluation would likely be done using a numerical integration procedure. This procedure would require knowledge of the geometry of each dispersed surface (which may vary from one particle to the next in poly-disperse flows) and a method for determining the mass-transfer rate at a sample of points along each respective dispersed phase surface. When the details of S are complicated or when the calculation of w on S is impractical, a simple model to account for the bulk effect of the mass-source may be preferred. Crowe [3] shows that the integral in (13) over a spherical particle is simply the mass-transfer rate at the surface:

$$\chi_{model} = -\frac{1}{V}\sum_{k} \dot{m}_k \qquad (14)$$

The summation in (14) is performed over the k-particles contained at least partially within a given control volume, and $\dot{m}_k$ is the mass rate-of-change of the k^{th} particle.

Volume-Averaged Momentum Equation with Immiscible Effects

The volume-averaged momentum equation is presented in (15):

$$\frac{\partial}{\partial t}\alpha_c\langle\rho_c\rangle\tilde{u}_i + \frac{\partial}{\partial x_j}\alpha_c\langle\rho_c\rangle\tilde{u}_i\tilde{u}_j = -\frac{\partial}{\partial x_j}\alpha_c\langle\rho_c\rangle\tilde{R}_{ij} - \frac{\partial\langle p\rangle}{\partial x_i} + \frac{\partial\langle\tau_{ij}\rangle}{\partial x_j} + \alpha_c\langle\rho_c\rangle g_i + C_i \qquad (15)$$

The expression for the volume-averaged momentum equation (15) agrees with [3]. Here, p is the pressure, τ_{ij} is the deviatoric stress tensor, $\tilde{R}_{ij} = \langle\rho_c u_i''u_j''\rangle/\langle\rho_c\rangle$ is the generalized Reynolds stress which shall henceforth be referred to as the Reynolds stress, g_i is the gravitational acceleration, and C_i is the total contribution of dispersed phase effects on the mean momentum equation and is given in (16):

$$C_i = \frac{1}{V}\int_S \left(\rho_c u_i w + p n_i - \tau_{ij} n_j\right) dS \qquad (16)$$

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[g] Since the carrier-phase density may be ill-defined at material boundaries, the density here is understood as a limit taking into account carrier-phase density in the neighborhood of the boundary.

The dispersed phase effects in (16) may be categorized into two groups: the first term in the integrand of (16) is owing to mass-transfer effects between the dispersed and carrier phase while the remaining terms are owing to variation in stress exerted over each dispersed phase surface. C_i may therefore be decomposed into a thrust contribution owing to mass-transfer, and a drag contribution owing to stress at the particle surface. Of course, lift components may be present in the latter contribution; the term drag is used with the understanding that the net effect of a particle on the carrier phase is that of flow impedance, and the sense of the resulting drag will likely have some component orthogonal to a particle's instantaneous velocity vector. Therefore, upon decomposition of C_i into the sum of momentum transfer due to mass exchange, steady and unsteady drag effects, we have without approximation:

$$C_i = F_{me} + F_{drag} \tag{17}$$

If each particle is non-deformable (i.e. $\dot{r}$ is zero[h]), and the thrust contribution is negligible (i.e. evaporation or burn rate is constant along the particle surface) then the momentum due to mass exchange can be modeled viz. [3]:

$$F_{me} \approx -\frac{1}{V}\sum_k \mathrm{v}_{i,k}\dot{m}_k \tag{18}$$

Such a model is expected to be a reasonable approximation when the dispersed phase elements are small compared with flow scales, so that the details of each particle's geometry are unimportant. Similarly, if the dispersed phase elements are much smaller than relevant flow scales, specifically the turbulent Kolmogorov scales [11], the drag term in (17) may be modeled via a relationship similar to that derived by Maxey and Riley [7] viz.:

$$F_{drag} \approx F_{d,model} = F_{grav} + F_{visc,st} + F_{hist} + F_{added} + F_{p,visc} \tag{19}$$

where F_{grav} is the gravitational force, $F_{visc,st}$ is the steady Stokes drag which may be modified for finite Reynolds number and Mach number effects [11, 17, 18], and the remaining terms are unsteady effects due to history, added mass, and combined pressure gradient and viscous stresses respectfully. When the particle Reynolds number is small, and the particle to carrier phase density is high, the Stokes term will be the primary contribution to the drag and the remaining terms will be small except during rapid motions or highly unsteady conditions. Additionally, deformable particles have the ability to store strain-energy at their boundary with the carrier-phase. The model for the pressure and viscous terms in (16) would then also require treatment of interfacial tension effects using [12] for example.

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[h] Surely $\dot{r}$ will be coupled to mass transfer effects since gain or loss of mass over long enough times will result in a measurable change in the volume of a dispersed phase element, and as a consequence, the position of its surface w.r.t. to its center of mass. Therefore, we must assume the timescale over which r changes is much greater than other relevant timescales (mass-transfer and flow timescales). When this assumption fails, i.e. burning or combustion, an additional term in the summation in (18) of the form $\dot{r}_k\dot{m}_k$ will become necessary. However, we may expect the time-scale over which mass changes to be small since the particle mass scales as the third power of its radius (the volume). For, small particles, their mass decreases sharply as the radius decreases. To compare time-scales then, it is necessary to compare the radial dependence of $\dot{r}$ with r.

Reynolds Stress Equation with Immiscible Effects

The Reynolds stress in (15) needs a closure model, and algebraic models will not work for dispersed phase flows. The exact equation for the Reynolds stresses, including immiscible effects is derived from $\overline{u_\imath \cdot NS_\jmath + u_\jmath \cdot NS_\imath} - \left(\tilde{u}_i \cdot \overline{NS_j} + \tilde{u}_j \cdot \overline{NS_i}\right)$ and the result is shown in (20):

$$\frac{\partial}{\partial t}\left(\alpha_c\langle\rho_c\rangle\tilde{R}_{ij}\right) + \frac{\partial}{\partial x_k}\left(\alpha_c\langle\rho_c\rangle\tilde{u}_k\tilde{R}_{ij}\right) = \tag{20}$$

$$\underbrace{-\alpha_c\langle\rho_c\rangle\tilde{R}_{jk}\frac{\partial\tilde{u}_i}{\partial x_k} - \alpha_c\langle\rho_c\rangle\tilde{R}_{ik}\frac{\partial\tilde{u}_j}{\partial x_k} + a_i\frac{\partial\bar{p}}{\partial x_j} + a_j\frac{\partial\bar{p}}{\partial x_i} - a_i\frac{\partial\bar{\tau}_{jk}}{\partial x_k} - a_j\frac{\partial\bar{\tau}_{ik}}{\partial x_k}}_{\text{Production}}$$

$$\text{Transport}\left\{\begin{aligned} & -\frac{\partial}{\partial x_k}\,\alpha_c\langle\rho_c u_i'' u_j'' u_k''\rangle - \frac{\partial}{\partial x_j}\alpha_c\langle p' u_i'\rangle - \frac{\partial}{\partial x_i}\,\alpha_c\langle p' u_j'\rangle \\ & \qquad + \frac{\partial}{\partial x_k}\,\alpha_c\langle u_i'\tau_{jk}'\rangle + \frac{\partial}{\partial x_k}\,\alpha_c\langle u_j'\tau_{ik}'\rangle \end{aligned}\right.$$

$$\underbrace{+\,\alpha_c\,\langle p'\frac{\partial u_j'}{\partial x_i}\rangle + \alpha_c\,\langle p'\frac{\partial u_i'}{\partial x_j}\rangle}_{\text{Pressure-Strain}} \underbrace{-\,\alpha_c\,\langle\tau_{jk}'\frac{\partial u_i'}{\partial x_k}\rangle - \alpha_c\,\langle\tau_{ik}'\frac{\partial u_j'}{\partial x_k}\rangle}_{\text{Dissipation}}$$

$$\underbrace{+\,E_{ij} + P_{ij} + T_{ij}}_{\text{Dispersed Phase}}$$

and,

$$E_{ij} = \frac{1}{V}\int_S \rho_c w u_i'' u_j''\,dS \tag{21}$$

$$\begin{aligned} P_{ij} = {} & \frac{1}{V}\int_S u_i P n_j\,dS + \frac{1}{V}\int_S u_j P n_i\,dS - \langle P\rangle\frac{1}{V}\int_S u_i n_j\,dS - \langle P\rangle\frac{1}{V}\int_S u_j n_i\,dS \\ & -\tilde{u}_i\frac{1}{V}\int_S P n_j\,dS - \tilde{u}_j\frac{1}{V}\int_S P n_i\,dS \end{aligned} \tag{22}$$

$$\begin{aligned} T_{ij} = {} & -\frac{1}{V}\int_S u_i\tau_{jk} n_k\,dS - \frac{1}{V}\int_S u_j\tau_{ik} n_k\,dS + \langle\tau_{jk}\rangle\frac{1}{V}\int_S u_i n_k\,dS \\ & +\langle\tau_{ik}\rangle\frac{1}{V}\int_S u_j n_k\,dS + \tilde{u}_i\frac{1}{V}\int_S \tau_{jk} n_k\,dS + \tilde{u}_j\frac{1}{V}\int_S \tau_{ik} n_k\,dS \end{aligned} \tag{23}$$

If the density of the carrier fluid is taken to be constant and no mass-transfer takes place at surfaces separating the carrier and dispersed phases, the Reynolds stress equation (20) agrees with the expression derived in [3]. In the absence of immiscible effects all-together, (20) will reduce to the expression originally derived in [1]. The unclosed production, transport, and pressure-strain terms in (20) may be closed using direct models discussed in [2]. The turbulent mass-flux, $\langle \rho_c \rangle a_i$, is also unclosed; its closure comes via a transport equation discussed in the next section. The dissipation term in (20) may be closed using a compressible analog to the dissipation equation derived in [14]. Then, as with the momentum equation, the dispersed phase contribution to the Reynolds stress may be categorized as owing to mass-transfer effects (21) and stress effects (22), (23). Equations (22) and (23) are significant since they establish that rigid, non-evaporating particles may still contribute as a source of Reynolds stress. The mass-transfer term (21) may be re-written in a more convenient form for modeling. Without approximation, we have:

$$E_{ij} = \frac{1}{V}\int_S \rho_c w u_i'' u_j'' \, dS = \frac{1}{V}\int_S \left[\rho_c w (u_i' - a_i)(u_j' - a_j)\right] dS$$

$$= \frac{1}{V}\int_S \left[\rho_c w \left(u_i' u_j' - a_j u_i' - a_i u_j' + a_i a_j\right)\right] dS \tag{24}$$

The last term in (24) can be modeled using (14) as

$$a_i a_j \tfrac{1}{V}\textstyle\int_S \rho_c w \, dS = -\, a_i a_j \tfrac{1}{V}\sum_k \dot{m}_k \tag{24a}$$

Using (18), the two middle terms in (24) can be modeled assuming that the net thrust on the particles is negligible, e.g.,

$$-a_j \tfrac{1}{V}\textstyle\int_S \rho_c w u_i' \, dS \;\approx a_j \tfrac{1}{V}\sum_k \mathrm{v}_{i,k}\dot{m}_k - a_j \bar{u}_i \tfrac{1}{V}\sum_k \dot{m}_k \tag{24b}$$

$$-a_i \tfrac{1}{V}\textstyle\int_S \rho_c w u_j' \, dS \;\approx a_i \tfrac{1}{V}\sum_k \mathrm{v}_{j,k}\dot{m}_k - a_i \bar{u}_j \tfrac{1}{V}\sum_k \dot{m}_k \tag{24c}$$

and the remaining term in (24) is also related to mass transfer and thrust effects and can be modeled as:

$$\begin{aligned}
&\frac{1}{V}\int_S \left[\rho_c w\left(\{\mathrm{v}_i + \widehat{w} n_i - \bar{u}_i\}\{\mathrm{v}_j + \widehat{w} n_j - \bar{u}_j\}\right)\right] dS = \\
&\qquad \mathrm{v}_i \mathrm{v}_j \, \frac{1}{V}\int_S \rho_c w \, dS + \mathrm{v}_i \frac{1}{V}\int_S \rho_c w \widehat{w} n_j \, dS + \mathrm{v}_j \frac{1}{V}\int_S \rho_c w \widehat{w} n_i \, dS \\
&\qquad + \frac{1}{V}\int_S \rho_c w \widehat{w}^2 \, \delta_{ij} dS - \mathrm{v}_i \bar{u}_j \, \frac{1}{V}\int_S \rho_c w \, dS - \mathrm{v}_j \bar{u}_i \, \frac{1}{V}\int_S \rho_c w \, dS \\
&\qquad - \bar{u}_i \, \frac{1}{V}\int_S \rho_c w \widehat{w} n_j \, dS - \bar{u}_j \, \frac{1}{V}\int_S \rho_c w \widehat{w} n_i \, dS + \bar{u}_i \bar{u}_j \, \frac{1}{V}\int_S \rho_c w \, dS
\end{aligned} \tag{24d}$$

where $\widehat{w} = \dot{r} + w.$ If $\dot{r}$ is taken to be approximately zero and the terms related to particle thrust can be neglected, (24d) may be expressed in modeled form using expressions analogous to (14) and (18). Substituting Eqs. (24a) – (24d) into (24), we have the beginning of a model for the contribution to the Reynolds stresses owing to mass-transfer from the dispersed phase (25):

$$E_{ij} \approx E_{ij,model} =$$

$$-a_i a_j \frac{1}{V}\sum_k \dot{m}_k + a_j \frac{1}{V}\sum_k (\mathrm{v}_{i,k} - \bar{u}_i)\dot{m}_k + a_i \frac{1}{V}\sum_k (\mathrm{v}_{j,k} - \bar{u}_j)\dot{m}_k$$

$$-\frac{1}{V}\sum_k (\mathrm{v}_{i,k}\mathrm{v}_{j,k} + \bar{u}_i\bar{u}_j)\dot{m}_k + \mathrm{v}_i\bar{u}_j \frac{1}{V}\sum_k \dot{m}_k + \mathrm{v}_j\bar{u}_i \frac{1}{V}\sum_k \dot{m}_k$$

$$+(\mathrm{v}_i - \bar{u}_i)\frac{1}{V}\int_S \rho_c w^2 n_j \, dS + (\mathrm{v}_j - \bar{u}_j)\frac{1}{V}\int_S \rho_c w^2 n_i \, dS + \frac{1}{V}\int_S \rho_c w^3 \delta_{ij} \, dS \qquad (25)$$

We now turn our attention to modeling the pressure and viscous work terms in (22) and (23). According to Crowe et al. [3], the particle surfaces (*S*) within a control volume are split into boundary surfaces (S_b) and internal surfaces (S_{si}), such as

$$\int_S B\,dS = \int_{S_b} B\,dS + \int_{S_{si}} B\,dS$$

and the boundary particles can be approximated by the severed surfaces (S_s) [see green dashed lines in Figure 1, and (11)], such as

$$\int_{S_b} n_i\,dS = -\int_{S_s} n_i\,dS$$

To start, we decompose the pressure into an average and deviation and assume that the pressure deviation along a severed surface is zero and the average pressure along the surface of the particle internal to the control volume is constant. Utilizing Eq. (11) and $u_i = \{\mathrm{v}_i + (\dot{r} + w)n_i\}$ at the particle surface, P_{ij_Si} for the particles internal to the control volume is then (where it was assumed that $\langle P \rangle$ is constant over the surfaces)

$$P_{ij\_S_i} = (v_i - \tilde{u}_i)\frac{1}{V}\int_{S_{si}} P' n_j\,dS + (v_j - \tilde{u}_j)\frac{1}{V}\int_{S_{si}} P' n_i\,dS + 2\frac{1}{V}\int_{S_{si}} P'(\dot{r} + w)n_i n_j\,dS$$

Along the severed surfaces, $\langle P \rangle$ varies and the integral is approximated by (Crowe et al. 2012)

$$-\frac{1}{V}\int_{S_s} B n_j\,dS = -\frac{\partial \alpha_d B}{\partial x_j}$$

Utilizing this, the severed surface integrals produce P_{ij_Ss}

$$P_{ij\_S_s} = -\alpha_d\left\{\widehat{v}_i + (\dot{r} + w)n_i\right\}\frac{\partial\langle P\rangle}{\partial x_j} - \alpha_d\left\{\widehat{v}_j + (\dot{r} + w)n_j\right\}\frac{\partial\langle P\rangle}{\partial x_i} + \tilde{u}_i\frac{\partial}{\partial x_j}\left(\alpha_d\langle P\rangle\right) + \tilde{u}_j\frac{\partial}{\partial x_i}\left(\alpha_d\langle P\rangle\right)$$

where $\widehat{v}_i$ is the mass averaged particle velocity. Combining terms, such that $P_{ij} = P_{ij\_Si} + P_{ij\_Ss}$ and Eq. (22) is then

$$P_{ij} = (v_i - \tilde{u}_i)\frac{1}{V}\int_{S_{si}} \delta P n_j\,dS + (v_j - \tilde{u}_j)\frac{1}{V}\int_{S_{si}} \delta P n_i\,dS + 2\frac{1}{V}\int_{S_{si}} \delta P(\dot{r} + w)n_i n_j\,dS$$

$$-\alpha_d\left\{\widehat{v}_{\boldsymbol{i}} + (\dot{r} + w)n_i\right\}\frac{\partial\langle P\rangle}{\partial x_j} - \alpha_d\left\{\widehat{v}_j + (\dot{r} + w)n_j\right\}\frac{\partial\langle P\rangle}{\partial x_i} + \tilde{u}_i\frac{\partial}{\partial x_j}\left(\alpha_d\langle P\rangle\right) + \tilde{u}_j\frac{\partial}{\partial x_i}\left(\alpha_d\langle P\rangle\right)$$

A similar approach can be taken for the shear terms (T_{ij}) in Eq. (23), giving

$$T_{ij}=-\left(v_i-\tilde{u}_i\right)\frac{1}{V}\int\limits_{S_{si}}\tau'_{jk}n_k\,dS-\left(v_j-\tilde{u}_j\right)\frac{1}{V}\int\limits_{S_{si}}\tau'_{ik}n_k\,dS-\frac{1}{V}\int\limits_{S_{si}}\tau'_{jk}\left(\dot{r}+w\right)n_in_k\,dS-\frac{1}{V}\int\limits_{S_{si}}\tau'_{ik}\left(\dot{r}+w\right)n_jn_k\,dS$$
$$+\alpha_d\left\{\widehat{v}_i+\left(\dot{r}+w\right)n_i\right\}\frac{\partial\left\langle\tau_{jk}\right\rangle}{\partial x_k}+\alpha_d\left\{\widehat{v}_j+\left(\dot{r}+w\right)n_j\right\}\frac{\partial\left\langle\tau_{ik}\right\rangle}{\partial x_k}-\tilde{u}_i\frac{\partial}{\partial x_k}\left(\alpha_d\left\langle\tau_{jk}\right\rangle\right)-\tilde{u}_j\frac{\partial}{\partial x_k}\left(\alpha_d\left\langle\tau_{ik}\right\rangle\right)$$

Combining terms shows

$$P_{ij}+T_{ij}=-\left(v_i-\tilde{u}_i\right)\frac{1}{V}\int\limits_{S_{si}}\left(-P'n_j+\tau'_{jk}n_k\right)dS-\left(v_j-\tilde{u}_j\right)\frac{1}{V}\int\limits_{S_{si}}\left(-P'n_i+\tau'_{ik}n_k\right)dS$$
$$+2\frac{1}{V}\int\limits_{S_{si}}P'\left(\dot{r}+w\right)n_in_j\,dS-\frac{1}{V}\int\limits_{S_{si}}\tau'_{jk}\left(\dot{r}+w\right)n_in_k\,dS-\frac{1}{V}\int\limits_{S_{si}}\tau'_{ik}\left(\dot{r}+w\right)n_jn_k\,dS$$
$$-\alpha_d\left\{\widehat{v}_i+\left(\dot{r}+w\right)n_i\right\}\frac{\partial\langle P\rangle}{\partial x_j}-\alpha_d\left\{\widehat{v}_j+\left(\dot{r}+w\right)n_j\right\}\frac{\partial\langle P\rangle}{\partial x_i}+\alpha_d\left\{\widehat{v}_i+\left(\dot{r}+w\right)n_i\right\}\frac{\partial\left\langle\tau_{jk}\right\rangle}{\partial x_k}+\alpha_d\left\{\widehat{v}_j+\left(\dot{r}+w\right)n_j\right\}\frac{\partial\left\langle\tau_{ik}\right\rangle}{\partial x_k}$$
$$+\tilde{u}_i\frac{\partial}{\partial x_j}\left(\alpha_d\langle P\rangle\right)+\tilde{u}_j\frac{\partial}{\partial x_i}\left(\alpha_d\langle P\rangle\right)-\tilde{u}_i\frac{\partial}{\partial x_k}\left(\alpha_d\left\langle\tau_{jk}\right\rangle\right)-\tilde{u}_j\frac{\partial}{\partial x_k}\left(\alpha_d\left\langle\tau_{ik}\right\rangle\right)$$

(26)

The first two terms in the right hand side represent the turbulent work due to the particles, where

$$-\left(v_i-\tilde{u}_i\right)\sum_k\frac{1}{V}\int\limits_{S_{si}}\left(-P'n_j+\tau'_{jk}n_k\right)dS=\sum_k\left(\tilde{u}_i-v_{i,k}\right)F_{j,k}\qquad(27)$$

where $F_{j,k}$ is interpreted as the net fluid force in the j^{th} direction on the k^{th} particle owing to pressure *and* viscous stresses. This force acts over the entire surface of the particle within the control volume. Therefore, a suitable expression for $F_{j,k}$, which can include wake or particle Reynolds and Mach number effects, is found in (19). The next three terms are turbulent work due to mass transfer between the carrier phase and the particle and are zero if there is no mass transfer. The remaining terms are related to pressure and shear gradients across the control volume within the flow and they are negligible in dilute flows.

In the limit of single phase multicomponent flow, i.e., $\alpha_c\to 1$ (meaning no dispersed immiscible phase), $dS\to 0$ and $\left\langle\rho_c\right\rangle\to\bar{\rho}=\rho_m$, where ρ_m is the mixture density, the BHR equation for single-phase multicomponent fluids can be recovered.

Turbulent Mass Flux Equation with Immiscible Effects

We now present the transport equation for the turbulent mass flux $\bar{\rho}a_i$, or density-velocity covariance, a_i. Our definition of the a_i remains consistent with Besnard et al. (1992), but in the volume average sense for the carrier phase is defined as:

$$a_i = \frac{\langle \rho'_c u'_i \rangle}{\langle \rho_c \rangle} = -\langle u''_i \rangle.$$

The exact equation for the turbulent mass flux, including immiscible effects is derived from $\overline{NS}_i - \alpha_c \langle \rho_c \rangle \langle \frac{Du_i}{Dt} = \frac{1}{\rho}\frac{\partial \sigma_{ij}}{\partial x_j} \rangle$, where $\sigma_{ij} = -P\delta_{ij} + \tau_{ij}$. The transport equation with explicit integral terms accounting for immiscible dispersed phase effects (28):[i]

$$\begin{aligned} \frac{\partial}{\partial t}\alpha_c \langle \rho_c \rangle a_i + \frac{\partial}{\partial x_j}\alpha_c \langle \rho_c \rangle a_i \tilde{u}_j \\ = -b\frac{\partial}{\partial x_j}\left(\alpha_c \langle \sigma_{ij} \rangle\right) - \alpha_c \langle \rho_c \rangle a_j \frac{\partial \langle u_i \rangle}{\partial x_j} - \tilde{R}_{ij}\frac{\partial}{\partial x_j}\alpha_c \langle \rho_c \rangle + \alpha_c \langle \rho_c \rangle \frac{\partial a_i a_j}{\partial x_j} \\ - \alpha_c \langle \rho_c \rangle \langle u'_i \frac{\partial}{\partial x_j} u'_j \rangle - \alpha_c \langle \rho_c \rangle \langle v' \frac{\partial}{\partial x_j}\sigma'_{ij} \rangle - \alpha_c \langle \rho_c \rangle \frac{\partial}{\partial x_j}\frac{\langle \rho' u'_i u'_j \rangle}{\langle \rho_c \rangle} + B_i \end{aligned} \tag{28}$$

where $b = -\langle \rho'_c v'_c \rangle$ is the density-specific volume covariance and B_i represents the particle effects is given as (29):

$$B_i = b\frac{1}{V}\int_S \sigma_{ij} n_j dS + \frac{1}{V}\int_S \rho'_c u_i w dS + \langle \rho \rangle \frac{1}{V}\int_S u_j \tilde{u}_i n_j dS - \langle u_i \rangle \chi \tag{29}$$

Neglecting immiscible effects (i.e. $dS \to 0$ and $\alpha_c \to 1$), (28) agrees with the miscible a_i equation first derived in [1] except for an additional dilatation term, which was assumed to be small and therefore neglected in the original derivation. Models for the unclosed triple-product and specific-volume-stress divergence terms in (28) are discussed in [2]. Terms in (29) may be modeled using the following techniques:

1) the stress tensor in (29) may be expressed as

$$b\frac{1}{V}\int_S \sigma_{ij} n_j dS = -b\frac{1}{V}\int_{S_s} \langle \sigma_{ij} \rangle n_j dS + b\frac{1}{V}\int_{S_{si}} \sigma'_{ij} n_j dS$$

where the first term is modeled as

$$-b\frac{1}{V}\int_{S_s} \langle \sigma_{ij} \rangle n_j dS = -b\frac{\partial}{\partial x_j}\left(\alpha_d \langle \sigma_{ij} \rangle\right)$$

and the second term is modeled as

$$b\frac{1}{V}\int_{S_{si}} \sigma'_{ij} n_j dS = b\frac{1}{V}\sum_k F_{i,k}$$

2) the second term is related to thrust effects and can be re-written as

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[i] During the derivation of (28), it was assumed that the spatial and temporal changes in the volume fraction were negligible. This implies a homogeneous mixture of particles and assumes that the particles do not transition from dilute to dense regions. An example of where this assumption could be invalid is in flows with preferential concentration, where small particles congregate in regions of high strain. To account for significant variations in volume fraction, one needs to include the following in the right hand side of (28): $+\langle \rho \rangle \langle u_i \rangle \frac{\partial \alpha_c}{\partial t} + \langle \rho \rangle \tilde{u}_i \tilde{u}_j \frac{\partial \alpha_c}{\partial x_j} - \langle \rho \rangle \tilde{u}_j a_i \frac{\partial \alpha_c}{\partial x_j} + \langle \rho \rangle \langle u''_j u''_i \rangle \frac{\partial \alpha_c}{\partial x_j}$.

$$+\frac{1}{V}\int_S \rho_c' u_i w dS = +\frac{1}{V}\int_{S_{si}} \rho_c\{\mathrm{v}_i + (\dot{r} + w)n_i\} w dS - \langle\rho_c\rangle \frac{1}{V}\int_{S_{si}} \{\mathrm{v}_i + (\dot{r} + w)n_i\} w dS$$

which can be simplified by assuming that the mass flux due to evaporation or chemical reactions is uniform over the particle surface, and the rate of change of particle radius is negligible, then

$$+\frac{1}{V}\int_S \rho_c' u_i w dS = -\frac{1}{V}\sum_k \mathrm{v}_{i,k}\dot{m}_k - \langle\rho_c\rangle \mathrm{v}_i \frac{1}{V}\int_{S_{si}} w dS$$

3) the third term is

$$+\langle\rho\rangle\frac{1}{V}\int_S u_j\tilde{u}_i n_j dS = +\langle\rho\rangle\tilde{u}_i\frac{1}{V}\int_{S_{si}}\{\mathrm{v}_j + (\dot{r} + w)n_j\}n_j dS = +\langle\rho\rangle\tilde{u}_i \frac{1}{V}\int_{S_{si}}(\dot{r} + w)dS$$

where $n_j n_j = 1$, because it was assumed that these terms apply only in the outward normal direction on an assumed spherical surface. Note that the severed surface effects are null.

4) the last term can be modeled simply using Eq. (14), such as

$$-\langle u_i\rangle\chi = \langle u_i\rangle\frac{1}{V}\sum_k \dot{m}_k$$

Collecting terms, the beginning of a model for B_i is then

$$\begin{aligned} B_i = &-b\frac{\partial}{\partial x_j}\left(\alpha_d\langle\sigma_{ij}\rangle\right) + b\frac{1}{V}\sum_k F_{i,k} - \frac{1}{V}\sum_k \mathrm{v}_{i,k}\dot{m}_k - \langle\rho_c\rangle\mathrm{v}_i\frac{1}{V}\int_{S_d} w dS \\ &+ \langle\rho\rangle\tilde{u}_i\frac{1}{V}\int_{S_d}(\dot{r} + w)dS + \langle u_i\rangle\frac{1}{V}\sum_k \dot{m}_k \end{aligned} \qquad (29a)$$

Assuming uniform ejection velocity across the particle surface and that the $\dot{r}$ terms can be neglected under the assumptions previously discussed, (28) can be modeled as

$$\begin{aligned} &\frac{\partial}{\partial t}\alpha_c\langle\rho_c\rangle a_i + \frac{\partial}{\partial x_j}\alpha_c\langle\rho_c\rangle a_i\tilde{u}_j \\ &\quad = -b\frac{\partial\langle\sigma_{ij}\rangle}{\partial x_j} - \alpha_c\langle\rho_c\rangle a_j\frac{\partial\langle u_i\rangle}{\partial x_j} - \tilde{R}_{ij}\frac{\partial}{\partial x_j}\alpha_c\langle\rho_c\rangle + \alpha_c\langle\rho_c\rangle\frac{\partial a_i a_j}{\partial x_j} \\ &\quad - \alpha_c\langle\rho_c\rangle\left\langle u_i'\frac{\partial}{\partial x_j}u_j'\right\rangle - \alpha_c\langle\rho_c\rangle\left\langle v'\frac{\partial}{\partial x_j}\sigma_{ij}'\right\rangle - \alpha_c\langle\rho_c\rangle\frac{\partial}{\partial x_j}\frac{\langle\rho' u_i' u_j'\rangle}{\langle\rho_c\rangle} + b\frac{1}{V}\sum_k F_{i,k} \\ &\quad - \frac{1}{V}\sum_k \mathrm{v}_{i,k}\dot{m}_k + \langle u_i\rangle\frac{1}{V}\sum_k \dot{m}_k + \langle\rho\rangle(\tilde{u}_i - \mathrm{v}_i)\frac{1}{V}\sum_k w_k A_k \end{aligned} \qquad (30)$$

where the particle velocity $\mathrm{v}_{i,k}$ may be found through particle-tracking, $F_{i,k}$ is the net combination of pressure and viscous drag on the k^{th} particle within the control volume and may be modeled using (19), $\dot{m}_k$ is the mass-transfer rate and $w_k A_k$ is the volume flow rate of the ejected mass of the k^{th} particle, which may be determined via an appropriate model.

Density-Specific Volume Covariance Equation with Immiscible Effects

Finally, we present the transport equation for the density-specific volume covariance b, including explicit and exact representation of the immiscible dispersed phase effects. The transport equation for *b* is found from manipulating the instantaneous mass continuity equation, such as $\rho_c \cdot MC - \langle \rho_c \rangle \cdot MC$, where *MC* is the mass continuity equation with $\rho_c = 1/\upsilon_c$ substituted. After decomposing and bulk averaging, the transport equation for *b* is shown as

$$\frac{\partial \alpha_c b}{\partial t} + \langle u_j \rangle \frac{\partial \alpha_c b}{\partial x_j} \\ = -\langle \upsilon_c \rangle \frac{\partial}{\partial x_j}\left(\alpha_c \langle \rho_c \rangle a_j\right) - \langle \rho_c \rangle \frac{\partial}{\partial x_j}\left(\alpha_c \langle \upsilon_c' u_j{}' \rangle\right) + 2\alpha_c \langle \rho_c \rangle \left\langle \upsilon_c' \frac{\partial u_j'}{\partial x_j} \right\rangle + H \qquad (31)$$

where the sum of the immiscible effects *H* is expressed as (32):

$$H = \langle \rho \rangle \frac{1}{V}\int_{S_d} \upsilon_c' u_j n_j \, dS + 2\langle \upsilon \rangle \frac{1}{V}\int_{S_d} \rho_c' u_j n_j \, dS + \frac{1}{V}\int_{S_d} \rho_c' \upsilon_c' \left(v_j n_j + \dot{r}\right) dS \\ +2\frac{1}{V}\int_{S_d} \rho_c' \upsilon_c' u_j n_j \, dS - 2\langle u_j \rangle \frac{1}{V}\int_{S_d} \rho_c' \upsilon_c' n_j \, dS \qquad (32)$$

In the limit of fully miscible turbulence, the immiscible effects in (31) are neglected and the resulting *b* equation is exactly the expression originally derived in [1]. Models for the specific volume-velocity correlation and dilatation terms in (31) are discussed in [2].

The immiscible effects shown in (32) suggest that if mass is uniformly ejected from the particle surface and the density and specific volume is constant along the particle surface, then $H = 0$ and there is no effect of mass transfer on the carrier phase *b*. However, non-uniform burn or evaporation can contribute to the carrier phase *b*. The carrier phase *b* can also be intensified through the stirring motion of continuous phase when particles are transported through a mixture of variable density fluids. Using the definition of the phase average decomposition, (32) is reformulated in terms of the instantaneous and mean quantities

$$H = (1-b)\frac{1}{V}\int_{S_d} w\,dS - \langle \rho_c \rangle \frac{1}{V}\int_{S_d} \upsilon_c w\,dS + 3\frac{1}{V}\int_{S_d} \dot{r}\,dS - 2\langle \rho_c \rangle \frac{1}{V}\int_{S_d} \upsilon_c \dot{r}\,dS - \langle \upsilon_c \rangle \frac{1}{V}\int_{S_d} \rho_c \dot{r}\,dS \\ \underbrace{-2\langle \rho_c \rangle \left(v_j - \langle u_j \rangle\right)\frac{1}{V}\int_{S_d} \upsilon_c n_j\,dS - \langle \upsilon_c \rangle \left(v_j - 2\langle u_j \rangle\right)\frac{1}{V}\int_{S_d} \rho_c n_j\,dS}_{\text{Effects of non-uniform burn or evaporation along the particle surface}} \qquad (33)$$

where $\langle \upsilon_c \rangle = (1+b)/\langle \rho_c \rangle$. If the evaporation or burn is uniform along the particle surface and the $\dot{r}$ terms can be neglected under the assumptions previously discussed, (33) reduces to

$$H = (1-b)\frac{1}{V}\int_{S_d} w\,dS - \langle \rho_c \rangle \frac{1}{V}\int_{S_d} \upsilon_c w\,dS = (1-b)\sum_k w_k A_k - \langle \rho_c \rangle \frac{1}{V}\int_{S_d} \upsilon_c w\,dS \qquad (34)$$

where the latter term needs a formulation for variation of the instantaneous specific volume along the particle surface.

A Simple Application

Consider a single component isothermal multiphase flow (i.e. water droplets traveling in water vapor). In order for the liquid to change phase, a driving mechanism must be present, such as an energy source or a local temperature gradient. An energy source applied to an isothermal system would simply break the molecular bonds and therefore the thermodynamic quality would increase. For this type of problem, the carrier phase *b* should be zero and the constraints are $\rho_c' = \nu_c' = 0$ and $b_0 = 0$ in the carrier phase. For this simplified problem, the evaporation is constant across the particle surface and therefore (33) is reduced to

$$H = (1-b)\frac{1}{V}\int_{S_d} w\,dS - \langle \rho_c \rangle \frac{1}{V}\int_{S_d} \nu_c w\,dS + 3\frac{1}{V}\int_{S_d} \dot{r}\,dS - \langle \nu_c \rangle \frac{1}{V}\int_{S_d} \rho_c \dot{r}\,dS - 2\langle \rho_c \rangle \frac{1}{V}\int_{S_d} \nu_c \dot{r}\,dS \qquad (35)$$

Since $\rho_c' = \nu_c' = 0$, this implies $\rho_c = \langle \rho_c \rangle$ and $\nu_c = \langle \nu_c \rangle$, which further reduces the equation to

$$H = 0 \qquad (36)$$

The above conclusion suggests that the ejected mass from the droplet does not generate *b* for this special case. Applying the same arguments to the droplet surface integrals in the turbulence mass flux (29a) shows

$$B_i = -\frac{1}{V}\sum_k \mathrm{v}_{i,k}\dot{m}_k - \langle \rho_c \rangle \mathrm{v}_i \frac{1}{V}\int_{S_d} w\,dS + \langle \rho_c \rangle \tilde{u}_i \frac{1}{V}\int_{S_d} (\dot{r} + w)\,dS + \langle u_i \rangle \frac{1}{V}\sum_k \dot{m}_k$$

Recalling that $\rho_c = \langle \rho_c \rangle$ and utilizing (14)

$$B_i = \frac{1}{V}\int_{S_d} \dot{r}\,dS \approx 0 \qquad (37)$$

for this special case. If $\dot{r}$ is negligible, this term has no effect on the turbulence mass flux, however if $\dot{r}$ is substantial (such as an explosion or rapid chemical reaction), then this term can alter the turbulence mass flux through the rapid expansion of the carrier phase into the region of the dispersed phase or vise-versa. This will not contribute to altering the turbulence kinetic energy unless a pressure gradient exists, nor will it contribute to the density-specific-volume covariance unless a density gradient in the carrier phase exits.

Modeled Form of the Equations for a Simplified Flow

In this section, we show a simplified set of the above mentioned second moment equations. Models for the instantaneous terms in (20), (28) and (31) are taken from [1], [2] and [3]. This set of equations can be applied to a mixture of miscible carrier phase fluids containing small to large density differences. We assume that the dispersed phase consists of particles or droplets that are immiscible with the carrier phase. In order to simplify the turbulence equations for the carrier phase, we also assume dilute flow conditions. The net force acting on the particle is assumed to be

$$F_{i,k} = \sum_k 3\pi\mu_c D_k f_k (u_{i,k} - v_{i,k})$$

where $f_k = C_D \mathrm{Re}_p / 24$ is the drag factor for the k^{th} particle, μ_c is the dynamic viscosity of the carrier phase, $v_{i,k}$ is the velocity of the particle, and $u_{i,k}$ is the local carrier phase velocity. Modifications for the drag coefficient for compressible flows can be found in [17] and [18]. Assuming no mass transfer between the dispersed and carrier phases, the closed form of the second moment equations for the carrier phase turbulence is then

1) Reynolds Stress Model

For the above mentioned conditions, $E_{ij} = 0$. Substituting (26) and (27) into (20) gives

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(\alpha_c\langle\rho_c\rangle\tilde{R}_{ij}\right) + \frac{\partial}{\partial x_k}\left(\alpha_c\langle\rho_c\rangle\tilde{u}_k\tilde{R}_{ij}\right) \\
&\quad = -\alpha_c\langle\rho_c\rangle\tilde{R}_{jk}\frac{\partial\tilde{u}_i}{\partial x_k} - \alpha_c\langle\rho_c\rangle\tilde{R}_{ik}\frac{\partial\tilde{u}_j}{\partial x_k} + a_i\frac{\partial\langle p\rangle}{\partial x_j} + a_j\frac{\partial\langle p\rangle}{\partial x_i} - a_i\frac{\partial\langle\tau_{jk}\rangle}{\partial x_k} \\
&\quad - a_j\frac{\partial\langle\tau_{jk}\rangle}{\partial x_k} + \alpha_c\langle\rho_c\rangle C_r\frac{\partial}{\partial x_m}\left(\frac{K}{\varepsilon}\tilde{R}_{mn}\frac{\partial\tilde{R}_{ij}}{\partial x_n}\right) \\
&\quad + \alpha_c\langle\rho_c\rangle C_{r2}\left(\tilde{R}_{jk}\frac{\partial\tilde{u}_i}{\partial x_k} + \tilde{R}_{ik}\frac{\partial\tilde{u}_j}{\partial x_k} - \frac{2}{3}\delta_{ij}\tilde{R}_{mn}\frac{\partial\tilde{u}_m}{\partial x_n}\right) \\
&\quad - \alpha_c C_{r3}\left(a_i\frac{\partial\langle p\rangle}{\partial x_j} + a_j\frac{\partial\langle p\rangle}{\partial x_i} - \frac{2}{3}\delta_{ij}a_m\frac{\partial\langle p\rangle}{\partial x_n}\right) \\
&\quad + \alpha_c C_{r4}\left(a_i\frac{\partial\langle\tau_{jk}\rangle}{\partial x_k} + a_j\frac{\partial\langle\tau_{ik}\rangle}{\partial x_k} - \frac{2}{3}\delta_{ij}a_m\frac{\partial\langle\tau_{nk}\rangle}{\partial x_k}\right) - \frac{2}{3}\delta_{ij}\alpha_c\langle\rho_c\rangle\varepsilon \\
&\quad + \frac{1}{V}\sum_k 3\pi\mu_c D_k f_k\left(u_{j,k} - \mathrm{v}_{j,k}\right)\left(\tilde{u}_i - \mathrm{v}_{i,k}\right) \\
&\quad + \frac{1}{V}\sum_k 3\pi\mu_c D_k f_k\left(u_{i,k} - \mathrm{v}_{i,k}\right)\left(\tilde{u}_j - \mathrm{v}_{j,k}\right)
\end{aligned}$$

where the gradient terms in (26) where neglected based on the dilute flow assumption along with the unsteady, added mass and pressure gradient forces that should be in (27). Models for the pressure-strain, transport and dissipation are taken from [1-3].

2) Turbulence Mass Flux Model

If there is no mass transfer between the dispersed and continuous phases, then (28) and (29a) reduce to

$$\begin{aligned}\frac{\partial \alpha_c\langle\rho_c\rangle a_i}{\partial t}+\frac{\partial \alpha_c\langle\rho_c\rangle\tilde{u}_j a_i}{\partial x_j}&\\ = -b\frac{\partial\langle\sigma_{ij}\rangle}{\partial x_j} - \tilde{R}_{ij}\frac{\partial \alpha_c\langle\rho_c\rangle}{\partial x_j} &+ \alpha_c\langle\rho_c\rangle\frac{\partial}{\partial x_j}\left(a_i a_j\right) - \alpha_c\langle\rho_c\rangle a_j\frac{\partial\langle u_i\rangle}{\partial x_j}\\ &+ \alpha_c\langle\rho_c\rangle C_a\frac{\partial}{\partial x_m}\left(\frac{K}{\varepsilon}\tilde{R}_{mn}\frac{\partial a_i}{\partial x_n}\right) - C_{a1}\alpha_c\langle\rho_c\rangle\frac{\varepsilon}{K}a_i + b\frac{1}{V}\sum_k 3\pi\mu_c D_k f_k\left(u_{i,k}-\mathrm{v}_{i,k}\right)\end{aligned}$$

where models for the transport and dissipation are taken from [1-3].

3) Density Specific Volume Covariance

For this special case, there is no contribution to b from the dispersed phase, so the transport equation is similar to [2]

$$\begin{aligned}\frac{\partial \alpha_c\langle\rho_c\rangle b}{\partial t}+\frac{\partial \alpha_c\langle\rho_c\rangle b\tilde{u}_i}{\partial x_i}&\\ = -2(b+1)a_i\frac{\partial \alpha_c\langle\rho_c\rangle}{\partial x_i} &+ 2\alpha_c\langle\rho_c\rangle a_i\frac{\partial b}{\partial x_i}\\ &+ (\alpha_c\langle\rho_c\rangle)^2 C_b\frac{\partial}{\partial x_m}\left(\frac{K}{\alpha_c\langle\rho_c\rangle\varepsilon}\tilde{R}_{mn}\frac{\partial b}{\partial x_n}\right) - C_{b1}\alpha_c\bar{\rho}_c\frac{\varepsilon}{K}b\end{aligned}$$

4) Turbulence Dissipation

The dissipation equation is found from assuming that the turbulence dissipation scales with the turbulence kinetic energy. Combining the work of [1] and [14], a dimensionally correct equation for the dissipation is then

$$\begin{aligned}\frac{\partial}{\partial t}(\alpha_c\langle\rho_c\rangle\varepsilon)+\frac{\partial}{\partial x_k}(\alpha_c\langle\rho_c\rangle\tilde{u}_k\varepsilon) &=\\ -C_{\varepsilon1}\alpha_c\langle\rho_c\rangle\frac{\varepsilon}{K}\tilde{R}_{km}\frac{\partial\tilde{u}_m}{\partial x_k} + C_{\varepsilon3}\alpha_c\frac{\varepsilon}{K}a_k\frac{\partial\langle p\rangle}{\partial x_k} &- C_{\varepsilon4}\alpha_c\frac{\varepsilon}{K}a_m\frac{\partial\langle\tau_{mk}\rangle}{\partial x_k} - C_{\varepsilon5}\alpha_c\langle\rho_c\rangle\frac{K^{3/2}}{\varepsilon}\frac{\partial\langle u_k\rangle}{\partial x_k}\\ &+ \alpha_c\langle\rho_c\rangle C_\varepsilon\frac{\partial}{\partial x_m}\left(\frac{K}{\varepsilon}\tilde{R}_{mn}\frac{\partial\varepsilon}{\partial x_n}\right) - \alpha_c C_{\varepsilon2}\langle\rho_c\rangle\frac{\varepsilon^2}{K} + C_{\varepsilon6}\frac{v_c^2}{V}\sum_k f_k\frac{|u_i-v_i|_k^2}{D_k}\end{aligned}$$

where the latter term is taken from [Crowe et al. 2011] and accounts for the production of dissipation due to particles. Although the above equations have not been applied, a suggested starting place for the above set of coefficients was taken from [2] and [3], and given as

C_{r1}	C_{r2}	C_{r3}	C_r	C_a	C_{a1}	C_b	C_{b1}	C_c	C_ε	$C_{\varepsilon1}$	$C_{\varepsilon2}$	$C_{\varepsilon3}$	$C_{\varepsilon4}$	$C_{\varepsilon5}$
0.3	0.6	1.8	0.22	0.18	3.0	0.18	2.0	0.18	0.15	1.44	1.92	1.2	0.95	-1.2

and $C_{\varepsilon6} = 0.0587C_{\varepsilon2}Re_p^{1.416}$.

Conclusions and Future Work

In this report, we extended the work of Besnard et al. [1] and Crowe [3] by deriving explicit integral source terms owing to immiscible particle effects for the volume-averaged continuity and momentum equations, as well as the Reynolds stress, turbulence mass-flux, and density-specific volume covariance transport equations. We then proposed models, where applicable, to close the integral terms using expressions analogous to those discussed in [3]. Incorporating models for the immiscible effects along with models [2] developed for the carrier-phase unclosed turbulent quantities, the resulting set of coupled non-linear PDEs forms a closed set of equations that may be simulated. These equations are valid for compressible multiphase turbulent flows where a definable interface separates the carrier phase fluid from discrete pieces of dispersed phase material (particles, droplets, bubbles). The models for the immiscible terms and the method of volume averaging itself are valid when the pieces of dispersed phase material are small in comparison with relevant flow scales and the particle volume fraction is low enough such that particle-particle interactions are scarce. Specifically, the particle force model proposed by Maxey and Riley [7] should be valid provided the dispersed phase is made up of rigid particles much smaller than the Kolmogorov scales [11]. Work is still needed to extend many of the terms in these equations to moderate particle Reynolds and Mach numbers. When the flow involves two phases of the same molecular component—water liquid and vapor for example—mass transfer effects may exist which require modeling.

Following Crowe's work [3], the immiscible integrals in the Reynolds stress and turbulent mass-flux equations may be decomposed into sources involving mass-transfer and stress effects. If the dispersed phase is comprised of evaporating or condensing material whose surface changes over much longer time scales than the characteristic rate of mass-transfer (i.e. $\dot{r} \ll w$), then only mass-transfer effects contribute to sources of density-specific volume covariance b. In the case of deformable droplets or bubbles, a model for $\dot{r}$ becomes necessary.

The dispersed phase effects on the Reynolds stress amount to turbulent work produced near the particle surface and within the wake. Mass transfer effects were also found to affect the Reynolds stress, however a model for these terms was not found. The net dispersed phase effects on the carrier phase turbulence mass flux owe to particle forces coupled to the density-specific-volume covariance and mass transfer effects. The effects on the density-specific-volume covariance is mainly caused by mass transfer.

In the present work, there was insufficient time to derive the immiscible effects for the turbulent heat flux originally derived in [1] and to fully understand the compressible effects on the turbulence dissipation equation. The latter, is presently an extension of the work of [1] and [3, 14], with the assumption that the turbulence dissipation scales with the turbulence energy. Future work should focus on extending the dissipation equation derived by Schwarzkopf et al. [14] for incompressible particle-laden flows to include both the effects of compressibility and mass-transfer. In this report, we have proposed simple models for the immiscible effects resulting from the volume averaging procedure. However, validation of these models is necessary to assess their applicability in various flow regimes.

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