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Derivation, Modelling and Solution of the Conditionally Averaged Two-Phase Flow Equations

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Abstract

This report outlines the development of a general purpose, robust and stable numerical algorithm for the solution of industrial two-phase flow problems. Particular attention is paid to the issues of phase-inversion and complete phase separation; these being two of the most difficult problems to handle numerically. The derivation, using conditional averaging, of the two-phase equations is outlined followed by the manipulation necessary to cast the equations in a form suitable for numerical solution. The discretised form of the equations is presented in the code independent finite-volume notation of Weller [1] followed by the solution algorithm. Two-phase modelling, in particular turbulence closure, is not covered in detail except where it influences the numerical algorithm. The models used here are standard and obtained from the literature; altered where necessary to obey a stricter set of physical constraints. No attempt has been made to demonstrate the accuracy of these developments.

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Nomenclature

Normal symbols represent scalar quantities and boldface symbols represent vector and tensor quantities. Generally boldface roman symbols represent vector and bolface Greek symbols represent tensor quantities, but this rule is not adhered to religously. Dimensions and units are given in terms of the full SI set, *i.e.* mass (M) in kg, length (L) in meters (m), time (t) in seconds (s), temperature (T) in Kelvin (K), moles (m) in moles (mol), current (c) in Amperes (A) and luminous intensity (I) in candela (cd).

Roman Symbols

Symbol	Description	Dimensions	Units
A	Coefficient (*e.g.* for drag model)	?	?
C	Dimensionless coefficient (*e.g.* for drag model)	-	-
D	Diffusive transport term	1/t	1/s
$\mathcal{D}$	Diffusivity	L^2/t	m^2
$\mathbf{g}$	Acceleration due to gravity	L/t^2	m/s^2
I	Indicator function	-	-
$\mathbf{I}$	Identity matrix	-	-
k	Turbulence kinetic energy	L^2/t^2	J/kg
l	Turbulence integral length scale	L	m
$\mathbf{M}$	Interfacial momentum transfer rate	$M/(L^2t^2)$	$kg/(m^2s^2)$
$\mathbf{n}$	Unit normal	-	-
p	Pressure	M/Lt^2	Pa
$\mathbf{P}$	Tensor property of any rank	-	-
$\mathbf{Q}$	Tensor property of any rank	-	-
$\mathbf{R}$	Reynolds stress	L^2/t^2	m^2/s^2
S	Surface	L^2	m^2
S	Interface propagation speed	L/t	m/s
t	Time	t	s
$\mathbf{U}$	Velocity	L/t	m/s
$\mathbf{x}$	Spatial position	L	m

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Greek Symbols

Symbol	Description	Dimensions	Units
α	Volume fraction	-	-
ε	Turbulence kinetic energy dissipation rate	L^2/t^3	J/kgs
μ	Dynamic viscosity	M/Lt	Ns/m^2
ν	Kinematic viscosity	M^2/t	m^2/s
ρ	Density	M/L^3	kg/m^3
Σ	Surface area per unit volume	1/L	1/n
$\boldsymbol{\sigma}$	Stress tensor	M/Lt^2	Pa
$\boldsymbol{\tau}$	Deviatoric part of the stress tensor	M/Lt^2	Pa
Ξ	Total surface "wrinkling"	-	-

Subscripts

$\mathbf{Q}_a$	Value of $\mathbf{Q}$ in phase a
$\mathbf{Q}_b$	Value of $\mathbf{Q}$ in phase b
$\mathbf{Q}_c$	Value of $\mathbf{Q}$ in continuous phase
$\mathbf{Q}_d$	Value of $\mathbf{Q}$ in dispersed phase
$\mathbf{Q}_I$	Interface
$\mathbf{Q}_\varphi$	Value of $\mathbf{Q}$ in phase φ
$\mathbf{Q}_r$	Relative Value of $\mathbf{Q}$ between two phases
$\mathbf{Q}_s$	Surface
$\mathbf{Q}_t$	Turbulent

Superscripts

$\mathbf{Q}^T$	Transpose
$\mathbf{Q}'$	Integration parameter
$\mathbf{Q}'$	Fluctuation with respect to ensemble average
$\mathbf{Q}''$	Fluctuation with respect to density weighted ensemble average
$\mathbf{Q}^\sharp$	Fluctuation with respect to interface average

Oversymbols

$\overline{\mathbf{Q}}$	Ensemble average
$\overline{\mathbf{Q}}_\varphi$	Conditional ensemble average in phase φ
$\widetilde{\mathbf{Q}}$	Density weighted ensemble average in phase φ
$\widetilde{\mathbf{Q}}_\varphi$	Conditional density weighted ensemble average
$\widehat{\mathbf{Q}}$	Interface average
$\dot{\mathbf{Q}}$	Rate of change

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1 Introduction

Following extensive testing of the two-phase algorithm developed at Imperial College for the BRITE II project, serious deficiencies became apparent. These manifest themselves as poor convergence behaviour, numerical instabilities and restrictions in range of operation. Initially it appeared that these problems might be remedied through minor adjustments of the algorithm and numerical schemes. The ease with which such alternatives may be implemented in FOAM allowed a very large number of strategies to be tested in a relatively short time. However, these trials did not support such an optimistic view of the algorithm, rather it demonstrated the need for a significant redevelopment of the approach.

The ultimate aim of this work is to create a general and stable two-phase flow solution algorithm for complex industrial application. A frequent problem encountered is that of phase-inversion, for which it is not reasonable to assume either phase is continuous, but that either may dominate in different regions of the same flow; under extreme (but not uncommon) conditions either phase may not be present at all in some regions of the domain. This is a particularly difficult problem to handle numerically and requires special consideration. The failure of the BRITE II algorithm for industrial application appears in part to be a consequence of not considering these issues explicitly. Careful consideration of the phase-inversion problem has lead to an unusual set of numerical practices and algorithm elements which, when combined, form a robust, general and extensible approach to two-phase flow. This report describes all of the elements necessary to handle phase inversion but not complete separation as this creates very large density gradients which require special pressure interpolation practices on collocated grids.

The issues covered in this report are predominantly numerical, however, some of the analysis raises questions about the appropriateness of some of the models developed within the BRITE II project and by others; these points are covered in more detail. The issue of turbulence closure is avoided to a large extent as it does not impinge significantly on the major numerical problems. For completeness the derivation of the conditionally averaged multi-phase flow equations is first outlined. This is followed by the manipulation necessary to cast these equations in a form suitable for numerical solution. The algorithm is then described in sufficient detail for implementation in a general purpose CFD code. The advantages of the proposed approach over previous methods is outlined but also explaining possible limitations. The report concludes with proposals for further developments.

2 Conditional Averaging

The techniques associated with conditional averaging are not as well known as those used in Reynolds averaging so before proceeding to conditionally average the equations for multi-phase flow a short summary of the techniques is presented. This work is a development of that previously published in [2] which is based on the work of Dopazo [3]. A more complete description of the application of conditional averaging to incompressible two-phase flow with

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particular emphasis on modelling and turbulence closure is presented in the PhD thesis of Hill [4].

Conditional averaging is applied to multi-phase flow by considering the phases to be separated by an infinitesimally thin interface. Equations are conditionally averaged by multiplying by an indicator function I_φ, which is 1 in phase φ and 0 in the other phases, and then applying a conventional averaging technique, density weighted or otherwise. This approach is a simple extension of that applied to intermittent turbulent flows by Dopazo [3], but using an indicator function rather than the intermittency function, and allowing the phase interface to propagate. In the present work conditional averaging will be applied by conditioning the equations with the indicator function and then applying density-weighted ensemble averaging for generality. This is appropriate for compressible flow with large phase density fluctuations but in the incompressible limit the equations revert to the standard non-density weighted forms and some simplification is possible. It is felt that the use of density weighted ensemble averaging does not add significantly to the complexity of the derivation and may prove useful in the future when this work is extended to compressible multi-phase flow.

The terms resulting from conditional averaging are manipulated and simplified by applying formulae presented in [3] and outlined below, replacing terms involving the indicator function with equivalent terms involving the phase volume fraction α_φ. A subscript φ is used to denote the conditional average of a property in that phase.

2.1 Formulae for Conditional Averaging

The indicator function $I_\varphi(\mathbf{x}, t)$ is defined as

$$I_\varphi(\mathbf{x}, t) = \begin{cases} 1 & \text{if point } (\mathbf{x}, t) \text{ is in phase } \varphi, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

The phase volume fraction α_φ is calculated as the probability of point $(\mathbf{x}, t)$ being in phase φ *i.e.*

$$\alpha_\varphi = \overline{I_\varphi}(\mathbf{x}, t) \tag{2}$$

where the overbar denotes the ensemble average. It is also useful to define the phase mass fraction (which is equivalent to the density weighted volume fraction) $\widetilde{\alpha_\varphi}$ through the identity

$$\overline{\rho}\widetilde{\alpha_\varphi} \equiv \overline{\rho}_\varphi \alpha_\varphi. \tag{3}$$

Now let $\mathbf{Q}(\mathbf{x}, t)$ be any fluid property, scalar or tensor of any rank, then the conditional average of $\mathbf{Q}$, $\overline{\mathbf{Q}}_\varphi$ is defined by

$$\overline{I_\varphi \mathbf{Q}} = \alpha_\varphi \overline{\mathbf{Q}}_\varphi. \tag{4}$$

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Similarly the density weighted conditional average of $\mathbf{Q}$, $\widetilde{\mathbf{Q}_\varphi}$, is defined by

$$\overline{I_\varphi \rho \mathbf{Q}} = \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{Q}_\varphi}. \tag{5}$$

2.1.1 Conditional Fluctuations

The most convenient definition of conditional fluctuation is as the difference between the instantaneous and conditional average of the property, that is

$$\mathbf{Q}'_\varphi \equiv \mathbf{Q} - \overline{\mathbf{Q}}_\varphi. \tag{6}$$

This definition is chosen so that the conditional average of the conditional fluctuation is zero. Similarly, the density-weighted conditional fluctuation is defined as

$$\mathbf{Q}''_\varphi \equiv \mathbf{Q} - \widetilde{\mathbf{Q}_\varphi}, \tag{7}$$

but, as for the standard density weighted ensemble average, the average of this fluctuation is not zero unless it is density weighted.

2.1.2 Conditionally Averaging Products

Let $\mathbf{P}(\mathbf{x}, t)$ be another fluid property, scalar or tensor of any rank, then from Eqs. (4 and 6)

$$\overline{I_\varphi \mathbf{P}\mathbf{Q}} = \alpha_\varphi \overline{\mathbf{P}}_\varphi \overline{\mathbf{Q}}_\varphi + \alpha_\varphi \overline{\mathbf{P}'_\varphi \mathbf{Q}'_\varphi} \tag{8}$$

and from Eqs. (5 and 7)

$$\overline{I_\varphi \rho \mathbf{P}\mathbf{Q}} = \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{P}_\varphi} \widetilde{\mathbf{Q}_\varphi} + \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{P}''_\varphi \mathbf{Q}''_\varphi} \tag{9}$$

2.1.3 Conditionally Averaging Differential Operations

Since differentiation and ensemble averaging commute

$$\overline{\nabla I_\varphi \mathbf{Q}} = \nabla(\overline{I_\varphi \mathbf{Q}}) = \nabla(\alpha_\varphi \overline{\mathbf{Q}}_\varphi) \tag{10}$$

and

$$\overline{\frac{\partial I_\varphi \mathbf{Q}}{\partial t}} = \frac{\partial(\overline{I_\varphi \mathbf{Q}})}{\partial t} = \frac{\partial(\alpha_\varphi \overline{\mathbf{Q}}_\varphi)}{\partial t}. \tag{11}$$

Now consider the mean of $I_\varphi \nabla \mathbf{Q} = \nabla(I_\varphi \mathbf{Q}) - (\nabla I_\varphi)\mathbf{Q}$ over the control volume δV. Note ∇I_φ is non-zero only at the interface, where it has the absolute value of the Dirac delta function and the direction of the unit normal $\mathbf{n}_\varphi$ to the interface, pointing into phase φ. Then

$$\overline{I_\varphi \nabla \mathbf{Q}} = \nabla(\overline{I_\varphi \mathbf{Q}}) - \lim_{\delta V \to 0} \overline{\frac{1}{\delta V} \int_{S(\mathbf{x}, t)} \mathbf{n}_\varphi \mathbf{Q}(\mathbf{x}, t)\, dS} \tag{12}$$

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where $S(\mathbf{x},t)=0$ is the equation for the interface. The interface average $\widehat{\mathbf{Q}}$ of a property $\mathbf{Q}$ is defined as the surface integral per unit volume divided by the surface area per unit volume Σ :

$$\widehat{\mathbf{Q}} \equiv \frac{\lim_{\delta V\to 0}\overline{\frac{1}{\delta V}\int_{S(\mathbf{x},\,t)}\mathbf{Q}(\mathbf{x},\,t)\,dS}}{\Sigma} \tag{13}$$

where

$$\Sigma \equiv \lim_{\delta V\to 0}\overline{\frac{a}{\delta V}\int_{S(\mathbf{x},t)} dS}. \tag{14}$$

Eqn. (12) may now be re-written as

$$\overline{I_\varphi \nabla \mathbf{Q}} = \nabla(\alpha_\varphi \overline{\mathbf{Q}}_\varphi) - \widehat{\mathbf{n}_\varphi \mathbf{Q}}\Sigma. \tag{15}$$

Also

$$\overline{I_\varphi \nabla \bullet \mathbf{Q}} = \nabla \bullet (\alpha_\varphi \overline{\mathbf{Q}}_\varphi) - \widehat{\mathbf{n}_\varphi \bullet \mathbf{Q}}\Sigma \tag{16}$$

and

$$\overline{I_\varphi \frac{\partial \mathbf{Q}}{\partial t}} = \frac{\partial \alpha_\varphi \overline{\mathbf{Q}}_\varphi}{\partial t} + \widehat{\mathbf{Q}\mathbf{n}_\varphi \bullet \mathbf{U}_s}\Sigma \tag{17}$$

where $\mathbf{U}_s$ is the velocity of the interface.

Useful identities are obtained by considering the simple case of $Q=1$, then from Eqn. (15)

$$\widehat{\mathbf{n}_\varphi}\Sigma = \nabla \alpha_\varphi \tag{18}$$

and from Eqn. (17)

$$\frac{\partial \alpha_\varphi}{\partial t} = -\widehat{\mathbf{n}_\varphi \bullet \mathbf{U}_s}\Sigma \tag{19}$$

The second identity is of particular importance in conditional averaging, it being the evolution equation for the mean interface distribution, which will be referred to as the interface transport equation. Although it would appear that an independent equation for the interface may be obtained from Eqn. (19) for both phases on either side of the interface, it is apparent that the equations are equivalent. For the present purpose this is as far as the analysis of the interface equation need be taken although it might be a useful in conjunction with the surface area density equation [5] as a starting point for the development of a model for bubble size distribution *etc.*.

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3 Turbulent Multi-Phase Flow Equations

In what follows, the conditional averaging techniques outlined above are applied to the basic transport equations representing turbulent multi-phase flow. Although the current interest is in two-phase flow, at this stage in the analysis the generality of multi-phase flow does not require greater complexity.

3.1 Conditionally Averaged Continuity Equation

In addition to the interface equation presented in Section 2.1.3, the conditionally averaged continuity equation is required in the derivation and simplification of other transport equation. The continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \mathbf{U}) = 0 \tag{20}$$

is conditionally averaged by multiplying by the indicator function I_φ, ensemble averaginging and simplifying using Eqs. (16 and 17), resulting in

$$\frac{\partial \alpha_\varphi \overline{\rho}_\varphi}{\partial t} + \widehat{\rho \mathbf{n}_\varphi \bullet \mathbf{U}_s}\Sigma + \nabla \bullet (\alpha_\varphi \overline{\rho_\varphi \mathbf{U}_\varphi}) - \widehat{\rho \mathbf{n}_\varphi \bullet \mathbf{U}}\Sigma = 0. \tag{21}$$

Eqn. (21) may be further simplified by combining the two surface average terms and applying density weighted averaging to the $\rho\mathbf{U}$ correlation leading to

$$\frac{\partial \alpha_\varphi \overline{\rho}_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}_\varphi}) = \widehat{\rho \mathbf{n}_\varphi \bullet (\mathbf{U} - \mathbf{U}_s)}\Sigma \tag{22}$$

The difference between the interface velocity $\mathbf{U}_s$ and the fluid velocity $\mathbf{U}$ at the interface is of course the interface propagation velocity which may be expressed in terms of the interface propagation speed S_φ, due to phase mass transfer and the interface normal $\mathbf{n}_\varphi$ as $S_\varphi \mathbf{n}_\varphi$. Applying this simplification, the final form of the conditionally averaged continuity equation is

$$\frac{\partial \alpha_\varphi \overline{\rho}_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi) = -\widehat{\rho_\varphi S_\varphi}\Sigma \tag{23}$$

3.2 Conditionally Averaged Momentum Equation

The momentum equation for a compressible fluid under the influence of gravity may be written

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \bullet (\rho \mathbf{U}\mathbf{U}) = -\nabla \bullet \boldsymbol{\sigma} + \rho \mathbf{g}. \tag{24}$$

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The total stress tensor $\boldsymbol{\sigma}$ is traditionally decomposed into an isotropic part $\mathbf{I}p$, where p is the static pressure, and a deviatoric part $\boldsymbol{\tau}$ such that $\boldsymbol{\sigma} = \mathbf{I}p + \boldsymbol{\tau}$, in which case the momentum equation becomes

$$\frac{\partial \rho \mathbf{U}}{\partial t} + \nabla \bullet (\rho \mathbf{U}\mathbf{U}) = -\nabla p - \nabla \bullet \boldsymbol{\tau} + \rho \mathbf{g}. \tag{25}$$

For a Newtonian fluid $\boldsymbol{\tau} = -2\mu\,\mathrm{dev}(\mathrm{symm}(\nabla \mathbf{U})) = -\mu(\nabla \mathbf{U} + \nabla \mathbf{U}^T - \frac{2}{3}\mathbf{I}\nabla \bullet \mathbf{U})$ although this assumption need not be made here as it does not affect the development of the solution algorithm and so the general form is maintained.

The conditionally averaged momentum equation is derived in a manner analogous to the continuity equation, multiplying Eqn. (25) by the indicator function I_φ, averaging, simplifying using Eqs. (17, 16, 15 and 8) and applying density weighting to the averages of correlations, Eqn. (9), resulting in

$$\begin{aligned}\frac{\partial \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi}{\partial t} + \widehat{\rho \mathbf{U}\mathbf{n}_\varphi \bullet \mathbf{U}_s}\Sigma + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi \widetilde{\mathbf{U}}_\varphi) + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}''_\varphi \mathbf{U}''_\varphi}) - \widehat{\rho \mathbf{U}\mathbf{n}_\varphi \bullet \mathbf{U}}\Sigma \\ = -\nabla(\alpha_\varphi \overline{p}_\varphi) + \widehat{\mathbf{n}_\varphi p}\Sigma - \nabla \bullet (\alpha_\varphi \overline{\boldsymbol{\tau}}_\varphi) + \widehat{\mathbf{n}_\varphi \bullet \boldsymbol{\tau}}\Sigma + \alpha_\varphi \overline{\rho}_\varphi \mathbf{g}\end{aligned} \tag{26}$$

The l.h.s. of Eqn. (26) can be simplified by combining the two interface average terms, noting that $S_\varphi \mathbf{n}_\varphi = \mathbf{U}_s - \mathbf{U}$. The density weighted phase Reynolds stress $\widetilde{\mathbf{U}''_\varphi \mathbf{U}''_\varphi}$ will be denoted $\widetilde{\mathbf{R}}_\varphi$ as the details of the turbulence closure will not be covered here.

$$\begin{aligned}\frac{\partial \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi \widetilde{\mathbf{U}}_\varphi) + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{R}}_\varphi) + \widehat{\rho \mathbf{U} S_\varphi}\Sigma \\ = -\nabla(\alpha_\varphi \overline{p}_\varphi) + \widehat{\mathbf{n}_\varphi p}\Sigma - \nabla \bullet (\alpha_\varphi \overline{\boldsymbol{\tau}}_\varphi) + \widehat{\mathbf{n}_\varphi \bullet \boldsymbol{\tau}}\Sigma + \alpha_\varphi \overline{\rho}_\varphi \mathbf{g}\end{aligned} \tag{27}$$

The surface averaged correlation terms on the r.h.s. of Eqn. (27) may be decomposed into surface average and surface fluctuation correlations [2] *e.g.* $\widehat{\mathbf{n}_\varphi p}\Sigma = \widehat{p}\nabla\alpha_\varphi + \widehat{\mathbf{n}_\varphi p^\sharp}\Sigma$. The first term of this decomposition may then be combined with equivalent conditional mean term in the equation to create a separation between in-phase and surface effects. Applying this to Eqn. (27) gives

$$\begin{aligned}\frac{\partial \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi \widetilde{\mathbf{U}}_\varphi) + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{R}}_\varphi) = -\alpha_\varphi \nabla \overline{p}_\varphi - \alpha_\varphi \nabla \bullet \overline{\boldsymbol{\tau}}_\varphi + \alpha_\varphi \overline{\rho}_\varphi \mathbf{g} \\ + (\widehat{p} - \overline{p}_\varphi)\nabla\alpha_\varphi + \nabla\alpha_\varphi \bullet (\widehat{\boldsymbol{\tau}} - \overline{\boldsymbol{\tau}}_\varphi) + \widehat{\mathbf{n}_\varphi p^\sharp}\Sigma + \widehat{\mathbf{n}_\varphi \bullet \boldsymbol{\tau}^\sharp}\Sigma - \widehat{\rho \mathbf{U} S_\varphi}\Sigma.\end{aligned} \tag{28}$$

In the work of Hill [4] the interface terms on the r.h.s. of Eqn. (28) are grouped to form the interfacial momentum transfer term from phase φ :

$$\mathbf{M}_\varphi = (\widehat{p} - \overline{p}_\varphi)\nabla\alpha_\varphi + \widehat{\mathbf{n}_\varphi p^\sharp}\Sigma - \widehat{\mathbf{n}_\varphi \bullet \boldsymbol{\tau}}\Sigma \tag{29}$$

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and $\mathbf{M}_\varphi$ is subsequently modelled for bubbly flow. It is concluded in [4] that $\mathbf{M}_c = -\mathbf{M}_d$ where the subscripts c and d represent the continuous and dispersed phases respectively. But $\overline{p}_c \neq \overline{p}_d \therefore \mathbf{M}_c \neq -\mathbf{M}_d$ indicating that this particular grouping of terms is not appropriate. However, the approximation applied later in the derivation in which it assumed that the two phase pressures are equal to the phase fraction weighted averaged pressure does ensure that $\mathbf{M}_c = -\mathbf{M}_d$ with $\mathbf{M}_c$ and $\mathbf{M}_d$ defined according to Eqn. (29). This approach also treats the pressure and stress terms inconsistently, which is rather unsatisfactory considering that they are both part of same total stress tensor, the separation into a normal and deviatoric components being done for modelling convenience. Another possible grouping of terms in which both parts of the total stress tensor are treated equivalently is

$$\mathbf{M}_\varphi = (\widehat{p} - \langle p \rangle)\nabla\alpha_\varphi + \nabla\alpha_\varphi \bullet (\widehat{\boldsymbol{\tau}} - \langle \boldsymbol{\tau} \rangle) + \widehat{\mathbf{n}_\varphi p^\sharp}\Sigma + \widehat{\mathbf{n}_\varphi \bullet \boldsymbol{\tau}^\sharp}\Sigma \tag{30}$$

in which $\langle p \rangle$ and $\langle \boldsymbol{\tau} \rangle$ are functions of the conditional averaged properties of both phases and are hence the same for both phases. This approach guarantees that $\mathbf{M}_c = -\mathbf{M}_d$ which is essential for the modelling of two-phase flow. Combining Eqs. (28 and 30) results in

$$\frac{\partial \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}}_\varphi \widetilde{\mathbf{U}}_\varphi) + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{R}}_\varphi) = -\alpha_\varphi \nabla \overline{p}_\varphi - \alpha_\varphi \nabla \bullet \overline{\boldsymbol{\tau}}_\varphi + \alpha_\varphi \overline{\rho}_\varphi \mathbf{g} + (\langle p \rangle - \overline{p}_\varphi)\nabla\alpha_\varphi + \nabla\alpha_\varphi \bullet (\langle \boldsymbol{\tau} \rangle - \overline{\boldsymbol{\tau}}_\varphi) + \mathbf{M}_\varphi - \widehat{\rho \mathbf{U} S_\varphi}\Sigma. \tag{31}$$

Closure of Eqn. (31) requires models for the phase viscous stress tensor $\overline{\boldsymbol{\tau}}_\varphi$, the phase Reynolds stress $\widetilde{\mathbf{R}}_\varphi$, an averaging procedure to obtain $\langle p \rangle$ and $\langle \boldsymbol{\tau} \rangle$ from the phase values, the interfacial momentum transfer rate $\mathbf{M}_\varphi$ and the surface mass transfer term $\widehat{\rho \mathbf{U} S_\varphi}\Sigma$. This is the subject of the next section.

4 Turbulent Two-Phase Flow Equation Closure

It is not necessary to give details of all the modelling necessary to close the conditionally averaged multi-phase equations of the previous section, but those parts which strongly influence the solution algorithm will be described. The first approximation to be applied is that the problems of interest are specifically two-phase rather than multi-phase. This allows some useful equation combinations to be exploited, *e.g.* the creation of an equation for the relative velocity between the phases. The greatest numerical difficulty encountered when attempting the solution of Eqn. (31) is the need for a pressure equation for each phase. These equations are elliptic in nature and strongly coupled, requiring some kind of coupled solution procedure. However, in incompressible flow the most important use of the pressure field to force the momentum solution to obey the continuity constraint. If, in two-phase flow, the pressure is used mainly to ensure overall continuity, phase-fraction being guaranteed by the solution of appropriate continuity equations, then only one pressure is required. Clearly this approximation reduces the number of variables in the system by one, which, if the system is

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to remain well posed, requires the removal of one of the equations. Typically the interface transport equations Eqn. (**??**) is neglected; the interface distribution being obtained from the continuity equations. Thus a useful approximation (used by most researchers in the field) is to assume that the two phase pressures are equal to the average pressure; but what average? The average commonly used for this purpose is the phase volume fraction mean: $\overline{p} = \alpha_b \overline{p}_b + \alpha_a \overline{p}_a$ and this will be used here. The same approximation cannot be applied to $\langle \boldsymbol{\tau} \rangle$ as the difference between the phase shear stresses is an important feature of the flow and therefore modelling is required. If it is assumed that all contributions from $\widehat{\boldsymbol{\tau}}$ are represented by the model for $\mathbf{M}_\varphi$ then $\langle \boldsymbol{\tau} \rangle = 0$. This is a very simple and convenient model but may not be adequate for all conditions, particularly flows in which the mean velocity gradients are comparable to those surrounding individual dispersed phase particles. A simple and general procedure for obtaining interface averages of the phase properties is proposed in [2] using which

$$\langle \boldsymbol{\tau} \rangle = \alpha_b \overline{\boldsymbol{\tau}}_a + \alpha_a \overline{\boldsymbol{\tau}}_b. \tag{32}$$

This model obeys important physical constraints but it has not yet been validated and it would be unwise to use it until adequate tests have been performed, for this reason the simple approach of neglecting $\langle \boldsymbol{\tau} \rangle$ will be used here.

For the moment interface mass transfer effects are neglected, although it is not expected that serious numerical difficulties will be encountered when they are included. Applying all these approximations to Eqs. (23 and 31) results in

$$\frac{\partial \alpha_\varphi \overline{\rho}_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}_\varphi}) = 0 \tag{33}$$

and

$$\frac{\partial \alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}_\varphi}}{\partial t} + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{U}_\varphi} \widetilde{\mathbf{U}_\varphi}) + \nabla \bullet \alpha_\varphi \overline{\boldsymbol{\tau}}_\varphi + \nabla \bullet (\alpha_\varphi \overline{\rho}_\varphi \widetilde{\mathbf{R}_\varphi}) = -\alpha_\varphi \nabla \overline{p} + \alpha_\varphi \overline{\rho}_\varphi \mathbf{g} + \mathbf{M}_\varphi. \tag{34}$$

4.1 Phase Intensive Momentum Equation

A major numerical difficulty is encountered when solving Eqn. (34) in regions where $\alpha_\varphi \to 0$. Various *ad hoc.* numerical tricks could be applied to avoid this problem, *e.g.* limiting α_φ such that $\alpha_\varphi \to \delta$ where $0 < \delta \ll 1$ or by forcing $lim_{\alpha_\varphi \to 0} \widetilde{\mathbf{U}_\varphi} = \widetilde{\mathbf{U}_\varphi}^*$ where $\widetilde{\mathbf{U}_\varphi}^*$ is some limiting value of $\widetilde{\mathbf{U}_\varphi}$ obtained from a model. None of these approaches are satisfactory and it would preferable to be able to solve Eqn. (34) directly even as $\alpha_\varphi \to 0$. This can be achieved if α_φ if factored out of the transport terms in Eqn. (34) and removed by subtracting $\widetilde{\mathbf{U}_\varphi}$ times Eqn. (33) and dividing by $\alpha_\varphi \overline{\rho}_\varphi$. The phase intensive momentum equation obtained by this procedure is

$$\frac{\partial \widetilde{\mathbf{U}_\varphi}}{\partial t} + \widetilde{\mathbf{U}_\varphi} \bullet \nabla \widetilde{\mathbf{U}_\varphi} + \nabla \bullet \left(\frac{\overline{\boldsymbol{\tau}}_\varphi}{\overline{\rho}_\varphi} + \widetilde{\mathbf{R}_\varphi} \right) + \frac{\nabla (\alpha_\varphi \overline{\rho}_\varphi)}{\alpha_\varphi \overline{\rho}_\varphi} \bullet \left(\frac{\overline{\boldsymbol{\tau}}_\varphi}{\overline{\rho}_\varphi} + \widetilde{\mathbf{R}_\varphi} \right) = -\frac{\nabla \overline{p}}{\overline{\rho}_\varphi} + \mathbf{g} + \frac{\mathbf{M}_\varphi}{\alpha_\varphi \overline{\rho}_\varphi}. \tag{35}$$

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Some interesting conclusions can be drawn from the form of Eqn. (35). The first is that

$$\lim_{\alpha_\varphi \to 0} \frac{\mathbf{M}_\varphi}{\alpha_\varphi \overline{\rho}_\varphi} \neq \infty, \tag{36}$$

and must be the case for both phases between which $\mathbf{M}_\varphi$ represents the transfer. For a two-phase system where $\mathbf{M}_a = -\mathbf{M}_b$,

$$\lim_{\alpha_a \to 0} \frac{\mathbf{M}_a}{\alpha_a \overline{\rho}_a} \neq \infty \quad \text{and} \quad \lim_{\alpha_b \to 0} \frac{\mathbf{M}_a}{\alpha_b \overline{\rho}_b} \neq \infty \tag{37}$$

which is a useful constraint on drag and lift modelling for both the dispersed bubble and droplet limits. The second is,

$$\text{given that} \quad \lim_{\alpha_\varphi \to 0} \widetilde{\mathbf{R}}_\varphi \neq \mathbf{0} \quad \text{then} \quad \lim_{\alpha_\varphi \to 0} \frac{\nabla \alpha_\varphi}{\alpha_\varphi} \neq \boldsymbol{\infty}. \tag{38}$$

It is not immediately clear from the equations that this constraint will be obeyed, however, the $\frac{\nabla(\alpha_\varphi \overline{\rho}_\varphi)}{\alpha_\varphi \overline{\rho}_\varphi} \bullet (\frac{\overline{\boldsymbol{\tau}}_\varphi}{\overline{\rho}_\varphi} + \widetilde{\mathbf{R}}_\varphi)$ term in Eqn. (35) produces a divergent phase velocity field which has the effect of dispersing α_φ according to Eqn. (33) which should remove the singularity from the equation. Proof of this has not yet been obtained and further work is required.

4.2 Laminar Stress Modelling

For Newtonian incompressible flow the laminar stress term

$$\frac{\overline{\boldsymbol{\tau}}_\varphi}{\overline{\rho}_\varphi} = -\nu_\varphi 2 \,\mathrm{dev}\,(\mathrm{symm}(\nabla \widetilde{\mathbf{U}}_\varphi)) \tag{39}$$

$$= -\nu_\varphi (\nabla \widetilde{\mathbf{U}}_\varphi + \nabla \widetilde{\mathbf{U}}_\varphi^{\,T} - \frac{2}{3} \mathbf{I} \nabla \bullet \widetilde{\mathbf{U}}_\varphi). \tag{40}$$

4.3 Interfacial Momentum Transfer Modelling

The BRITE II project was predominantly concerned with low phase-fraction dispersed bubbly flow. Under these conditions it is convenient to decompose the interfacial momentum transfer rate into contributions from the bubble drag, lift, virtual mass and Basset forces. The Basset force is very much smaller than the drag and is usually neglected, however, the other three are important and were modelled in the BRITE II project as

$$\begin{aligned} \mathbf{M}_d &= C_d \tfrac{3}{4} \tfrac{\alpha_d \overline{\rho}_c}{d} |\widetilde{\mathbf{U}}_r| \widetilde{\mathbf{U}}_r && \text{drag} \\ &+ C_l \alpha_d \overline{\rho}_c \widetilde{\mathbf{U}}_r \times \nabla \times \widetilde{\mathbf{U}}_c && \text{lift} \\ &+ C_{vm} \alpha_d \overline{\rho}_c \left(\tfrac{d_c \widetilde{\mathbf{U}}_c}{dt} - \tfrac{d_d \widetilde{\mathbf{U}}_d}{dt} \right) && \text{virtual mass} \end{aligned} \tag{41}$$

where the relative velocity $\widetilde{\mathbf{U}}_r = \widetilde{\mathbf{U}}_c - \widetilde{\mathbf{U}}_d$. While these models are well posed for low phase-fraction flows, they cannot possibly handle phase inversion or simultaneously the bubble

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and droplet limits for example. In general, the interfacial momentum transfer rate will have contributions from all the two-phase flow regimes weighted according to probability density functions. Currently not enough is known about two-phase flow to be able to construct such a model so for the purpose of this study the simple mixture model

$$\begin{aligned}\mathbf{M}_a &= \tfrac{3}{4}\alpha_a\alpha_b(\alpha_b\tfrac{C_{d_a}\rho_b}{d_a}+\alpha_a\tfrac{C_{d_b}\rho_a}{d_b})|\widetilde{\mathbf{U}_r}|\widetilde{\mathbf{U}_r} && \text{drag}\\ &+ \alpha_a\alpha_b(\alpha_b C_{l_a}\rho_b+\alpha_a C_{l_b}\rho_a)\widetilde{\mathbf{U}_r}\times\nabla\times\widetilde{\mathbf{U}} && \text{lift}\\ &+ \alpha_a\alpha_b(\alpha_b C_{vm_a}\rho_b+\alpha_a C_{vm_b}\rho_a)\left(\tfrac{d_b\widetilde{\mathbf{U}_b}}{dt}-\tfrac{d_a\widetilde{\mathbf{U}_a}}{dt}\right) && \text{virtual mass}\end{aligned} \tag{42}$$

where

$$\frac{d_a\widetilde{\mathbf{U}_a}}{dt}=\frac{\partial\widetilde{\mathbf{U}_a}}{\partial t}+\widetilde{\mathbf{U}_a}\bullet\nabla\widetilde{\mathbf{U}_a} \tag{43}$$

and

$$\frac{d_b\widetilde{\mathbf{U}_b}}{dt}=\frac{\partial\widetilde{\mathbf{U}_b}}{\partial t}+\widetilde{\mathbf{U}_b}\bullet\nabla\widetilde{\mathbf{U}_b} \tag{44}$$

will be used which is capable of realistically (though not accurately) representing the full range of phase fraction. In the limit of $\alpha_a \to 0$ or $\alpha_a \to 1$ Eqn. (42) is equivalent to Eqn. (41), also this model obeys the constraint Eqn. (37) derived in Section 4.1. The lift and virtual mass coefficients in Eqn. (42) are assumed constant and supplied by the user, however, this is not a reasonable assumption for the most important effect: drag. There are many possible drag models which are valid for different two-phase systems and flow regimes, but for the purposes of this numerical study the simple and reliable solid particle model of Wallis [6] is chosen, which reads

$$C_d=\frac{24}{R_e}\left(1+0.15R_e^{0.687}\right)\qquad R_e\leq 10^3 \tag{45}$$

4.4 Phase Reynolds Stress Modelling

For the purposes of this work the phase Reynolds Stress $\widetilde{\mathbf{R}_\varphi}$ is modelled using the Boussinesq eddy viscosity concept giving

$$\begin{aligned}\widetilde{\mathbf{R}_\varphi}&=-\nu_{t_\varphi}2\,\mathrm{dev}\left(\mathrm{symm}(\nabla\widetilde{\mathbf{U}_\varphi})\right)+\frac{2}{3}\mathbf{I}\widetilde{k_\varphi}\\ &=-\nu_{t_\varphi}(\nabla\widetilde{\mathbf{U}_\varphi}+\nabla\widetilde{\mathbf{U}_\varphi}^T-\frac{2}{3}\mathbf{I}\nabla\bullet\widetilde{\mathbf{U}_\varphi})+\frac{2}{3}\mathbf{I}\widetilde{k_\varphi}\end{aligned} \tag{46}$$

where

$$\nu_{t_\varphi}=C_\mu\frac{\widetilde{k_\varphi}^2}{\widetilde{\varepsilon_\varphi}}. \tag{47}$$

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This model requires the phase turbulent kinetic energy $\widetilde{k_\varphi}$ and dissipation rate $\widetilde{\varepsilon_\varphi}$. In the BRITE II project transport equations were solved for these properties in the continuous phase and an algebraic model used to relate the dispersed phase Reynolds stress to that of the continuous phase. This approach is not completely satisfactory and is unable to handle complex phenomena such as phase inversion which is of particular interest here. In the expectation that developments in this area will again be based on the Boussinesq hypothesis, the momentum equations will retain the Reynolds stress term in this form, which when combined with the laminar stress term gives

$$\begin{aligned}\widetilde{\mathbf{R}_{\mathit{eff}_\varphi}} &= \widetilde{\mathbf{R}_\varphi} + \frac{\overline{\boldsymbol{\tau}}_\varphi}{\overline{\rho}_\varphi} = -\nu_{\mathit{eff}_\varphi} 2\,\mathrm{dev}\left(\mathrm{symm}(\nabla\widetilde{\mathbf{U}_\varphi})\right) + \frac{2}{3}\mathbf{I}\widetilde{k_\varphi} \\ &= -\nu_{\mathit{eff}_\varphi}(\nabla\widetilde{\mathbf{U}_\varphi} + \nabla\widetilde{\mathbf{U}_\varphi}^T - \frac{2}{3}\mathbf{I}\nabla\bullet\widetilde{\mathbf{U}_\varphi}) + \frac{2}{3}\mathbf{I}\widetilde{k_\varphi}\end{aligned} \tag{48}$$

where the effective viscosity is given by

$$\nu_{\mathit{eff}_\varphi} = \nu_\varphi + \nu_{t_\varphi} \tag{49}$$

Substituting the model Eqn. (48) into the phase intensive momentum equation Eqn. (35) results in

$$\frac{\partial\widetilde{\mathbf{U}_\varphi}}{\partial t} + \widetilde{\mathbf{U}_\varphi}\bullet\nabla\widetilde{\mathbf{U}_\varphi} + \nabla\bullet\widetilde{\mathbf{R}_{\mathit{eff}_\varphi}} + \frac{\nabla(\alpha_\varphi\overline{\rho}_\varphi)}{\alpha_\varphi\overline{\rho}_\varphi}\bullet\widetilde{\mathbf{R}_{\mathit{eff}_\varphi}} = -\frac{\nabla\overline{p}}{\overline{\rho}_\varphi} + \mathbf{g} + \frac{\mathbf{M}_\varphi}{\alpha_\varphi\overline{\rho}_\varphi}. \tag{50}$$

For numerical implementation of Eqn. (50) it is useful to decompose the Reynolds stress terms into a diffusive component and a correction $\widetilde{\mathbf{R}_{\mathit{eff}_\varphi}} = \overline{\mathbf{R}}^{\mathcal{D}}_{\mathit{eff}_\varphi} + \overline{\mathbf{R}}^{\mathcal{C}}_{\mathit{eff}_\varphi}$ where

$$\overline{\mathbf{R}}^{\mathcal{D}}_{\mathit{eff}_\varphi} = -\nu_{\mathit{eff}_\varphi}\nabla\widetilde{\mathbf{U}_\varphi} \tag{51}$$

and

$$\overline{\mathbf{R}}^{\mathcal{C}}_{\mathit{eff}_\varphi} = \widetilde{\mathbf{R}_{\mathit{eff}_\varphi}} + \nu_{\mathit{eff}_\varphi}\nabla\widetilde{\mathbf{U}_\varphi} \tag{52}$$

Modelling the Reynolds stress according to the Boussinesq eddy viscosity hypothesis Eqn. (48) leads to a Reynolds stress correction term of the form

$$\overline{\mathbf{R}}^{\mathcal{C}}_{\mathit{eff}_\varphi} = -\nu_{\mathit{eff}_\varphi}(\nabla\widetilde{\mathbf{U}_\varphi}^T - \frac{2}{3}\mathbf{I}\nabla\bullet\widetilde{\mathbf{U}_\varphi}) + \frac{2}{3}\mathbf{I}\widetilde{k_\varphi}. \tag{53}$$

which, when substituted into Eqn. (50), gives

$$\begin{aligned}\frac{\partial\widetilde{\mathbf{U}_\varphi}}{\partial t} + \widetilde{\mathbf{U}_\varphi}\bullet\nabla\widetilde{\mathbf{U}_\varphi} - \nabla\bullet(\nu_{\mathit{eff}_\varphi}\nabla\widetilde{\mathbf{U}_\varphi}) + \nabla\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{\mathit{eff}_\varphi} - \nu_{\mathit{eff}_\varphi}\frac{\nabla(\alpha_\varphi\overline{\rho}_\varphi)}{\alpha_\varphi\overline{\rho}_\varphi}\bullet\nabla\widetilde{\mathbf{U}_\varphi} + \frac{\nabla(\alpha_\varphi\overline{\rho}_\varphi)}{\alpha_\varphi\overline{\rho}_\varphi}\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{\mathit{eff}_\varphi} \\ = -\frac{\nabla\overline{p}}{\overline{\rho}_\varphi} + \mathbf{g} + \frac{\mathbf{M}_\varphi}{\alpha_\varphi\overline{\rho}_\varphi}.\end{aligned} \tag{54}$$

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The two convection terms may be combined by defining a total phase velocity

$$\widetilde{\mathbf{U}}_\varphi^{\mathcal{T}} = \widetilde{\mathbf{U}}_\varphi - \nu_{eff_\varphi}\frac{\nabla(\alpha_\varphi\overline{\rho}_\varphi)}{\alpha_\varphi\overline{\rho}_\varphi} \tag{55}$$

which includes both in-phase and interface transport effects which, when substituted into Eqn. (54) together with Eqn. (42) gives

$$\begin{aligned}\frac{\partial\widetilde{\mathbf{U}}_a}{\partial t} + \widetilde{\mathbf{U}}_a^{\mathcal{T}}\bullet\nabla\widetilde{\mathbf{U}}_a - \nabla\bullet(\nu_{eff_a}\nabla\widetilde{\mathbf{U}}_a) + \nabla\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{eff_a} + \frac{\nabla\alpha_a\overline{\rho}_a}{\alpha_a\overline{\rho}_a}\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{eff_a}\\ = -\frac{\nabla\overline{p}}{\overline{\rho}_a} + \mathbf{g} + \frac{\alpha_b}{\overline{\rho}_a}\left(A_d(\widetilde{\mathbf{U}}_b - \widetilde{\mathbf{U}}_a) + A_l + A_{vm}\left(\frac{d_b\widetilde{\mathbf{U}}_b}{dt} - \frac{d_a\widetilde{\mathbf{U}}_a}{dt}\right)\right)\end{aligned} \tag{56}$$

and

$$\begin{aligned}\frac{\partial\widetilde{\mathbf{U}}_b}{\partial t} + \widetilde{\mathbf{U}}_b^{\mathcal{T}}\bullet\nabla\widetilde{\mathbf{U}}_b - \nabla\bullet(\nu_{eff_b}\nabla\widetilde{\mathbf{U}}_b) + \nabla\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{eff_b} + \frac{\nabla\alpha_b\overline{\rho}_b}{\alpha_b\overline{\rho}_b}\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{eff_b}\\ = -\frac{\nabla\overline{p}}{\overline{\rho}_b} + \mathbf{g} - \frac{\alpha_a}{\overline{\rho}_b}\left(A_d(\widetilde{\mathbf{U}}_b - \widetilde{\mathbf{U}}_a) + A_l + A_{vm}\left(\frac{d_b\widetilde{\mathbf{U}}_b}{dt} - \frac{d_a\widetilde{\mathbf{U}}_a}{dt}\right)\right)\end{aligned} \tag{57}$$

where

$$\begin{array}{lcll} A_d & = & \frac{3}{4}(\alpha_b\frac{C_{d_a}\rho_b}{d_a} + \alpha_a\frac{C_{d_b}\rho_a}{d_b})|\widetilde{\mathbf{U}}_r| & \text{drag} \\ A_l & = & (\alpha_b C_{l_a}\rho_b + \alpha_a C_{l_b}\rho_a)\widetilde{\mathbf{U}}_r\times\nabla\times\overline{\mathbf{U}} & \text{lift} \\ A_{vm} & = & \alpha_b C_{vm_a}\rho_b + \alpha_a C_{vm_b}\rho_a & \text{virtual mass.}\end{array} \tag{58}$$

5 Incompressible Two-Phase Flow Equations

Some simplification of the equations presented in the previous sections is possible if the two-phase system of interest may be assumed incompressible; in which case all density-weighted averaging may be replaced by the unweighted counterpart, the continuity equation Eqn. (33) becomes

$$\frac{\partial\alpha_\varphi}{\partial t} + \nabla\bullet(\overline{\mathbf{U}}_\varphi\alpha_\varphi) = 0 \tag{59}$$

and the phase intensive momentum equations become

$$\begin{aligned}\frac{\partial\overline{\mathbf{U}}_a}{\partial t} + \overline{\mathbf{U}}_a^{\mathcal{T}}\bullet\nabla\overline{\mathbf{U}}_a - \nabla\bullet(\nu_{eff_a}\nabla\overline{\mathbf{U}}_a) + \nabla\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{eff_a} + \frac{\nabla\alpha_a}{\alpha_a}\bullet\overline{\mathbf{R}}^{\mathcal{C}}_{eff_a}\\ = -\frac{\nabla\overline{p}}{\overline{\rho}_a} + \mathbf{g} + \frac{\alpha_b}{\overline{\rho}_a}\left(A_d(\overline{\mathbf{U}}_b - \overline{\mathbf{U}}_a) + A_l + A_{vm}\left(\frac{d_b\overline{\mathbf{U}}_b}{dt} - \frac{d_a\overline{\mathbf{U}}_a}{dt}\right)\right)\end{aligned} \tag{60}$$

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and

$$\frac{\partial \overline{\mathbf{U}}_b}{\partial t} + \overline{\mathbf{U}}_b^{\mathcal{T}} \bullet \nabla \overline{\mathbf{U}}_b - \nabla \bullet (\nu_{eff_b} \nabla \overline{\mathbf{U}}_b) + \nabla \bullet \overline{\mathbf{R}}^{\mathcal{C}}_{eff_b} + \frac{\nabla \alpha_b}{\alpha_b} \bullet \overline{\mathbf{R}}^{\mathcal{C}}_{eff_b}$$
$$= -\frac{\nabla \overline{p}}{\overline{\rho}_b} + \mathbf{g} - \frac{\alpha_a}{\overline{\rho}_b} \left(A_d(\overline{\mathbf{U}}_b - \overline{\mathbf{U}}_a) + A_l + A_{vm} \left(\frac{d_b \overline{\mathbf{U}}_b}{dt} - \frac{d_a \overline{\mathbf{U}}_a}{dt} \right) \right) \quad (61)$$

Combining Eqn. (59) for both phases a and b demonstrates the incompressibility constraint

$$\nabla \bullet \overline{\mathbf{U}} = 0 \quad (62)$$

where $\overline{\mathbf{U}} = \alpha_a \overline{\mathbf{U}}_a + \alpha_b \overline{\mathbf{U}}_b$.

5.1 Phase-Fraction Boundedness

A key issue in the numerics of two-phase flow is the boundedness of the phase-fraction. If one attempts to solve Eqn. (59) in this form, applying an appropriate bounded discretisation scheme, then the constraint $\alpha_\varphi \geqslant 0$ will be obeyed but the constraint $\alpha_\varphi \leqslant 1$ may not be. However, if one solves both for $\alpha_a \geqslant 0$ and $\alpha_b \geqslant 0$ then it would be possible, by suitable blending, to obtain a value of α_φ which obeys both constraints; this value will of course not necessarily obey the equations and may not be conservative. This approach is therefore unacceptable as phase conservation is a critical issue in multi-phase flow with high density ratios because small volume-fraction errors may correspond to large mass-fraction errors. A better approach would be to rearrange Eqn. (59) such that a numerical approach may be applied which is bounded at both extremes of the phase-fraction range. One possibility is to decompose $\overline{\mathbf{U}}_a$ into the mean and relative parts

$$\overline{\mathbf{U}}_a = \overline{\mathbf{U}} + \alpha_b \overline{\mathbf{U}}_r \quad (63)$$

where

$$\overline{\mathbf{U}}_r = \overline{\mathbf{U}}_a - \overline{\mathbf{U}}_b \quad (64)$$

and

$$\overline{\mathbf{U}} = \alpha_a \overline{\mathbf{U}}_a + \alpha_b \overline{\mathbf{U}}_b. \quad (65)$$

Substituting Eqn. (63) into Eqn. (59) gives

$$\frac{\partial \alpha_a}{\partial t} + \nabla \bullet (\overline{\mathbf{U}} \alpha_a) + \nabla \bullet (\overline{\mathbf{U}}_r \alpha_a (1 - \alpha_a)) = 0. \quad (66)$$

The first convection term in Eqn. (66) is conservative and $0 \leqslant \alpha_a \leqslant 1$ because $\nabla \bullet \overline{\mathbf{U}} = 0$ (*cf.* Eqn. (62)) which means it is equivalent to $\overline{\mathbf{U}} \bullet \nabla \alpha_a$ which is an amplitude preserving

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wave transport term. The second convection term in Eqn. (66) is also conservative and $0 \leqslant \alpha_a \leqslant 1$ because the term becomes zero at both limits. An interesting and useful feature of this approach is that the α_a and α_b equations have the same form

$$\frac{\partial \alpha_b}{\partial t} + \nabla \bullet (\overline{\mathbf{U}} \alpha_b) - \nabla \bullet (\overline{\mathbf{U}}_r \alpha_b (1 - \alpha_b)) = 0. \tag{67}$$

The problem with this approach is that boundedness at both limits can only be guaranteed if the equation is solved fully implicitly, but the second convection term is non-linear in α_a so the use of a linear solver will require an iterative procedure to correct for the non-linearity. Such procedures are not guaranteed to be convergent, particularly if, in this case, slight unboundedness is generated during the iterations. Convergence of the iterative procedure may be accelerated by solving both Eqs. (66 and 67) and blending α_a and α_b to ensure $0 \leqslant \alpha_a \leqslant 1$, *e.g.*

$$\alpha_a^* = \frac{\alpha_a}{\alpha_a + \alpha_b}. \tag{68}$$

which only corrects the upper limit (the lower limit should not be violated because it is handled implicitly), or

$$\alpha_a^* = \frac{1}{2}(1 - (1 - \alpha_a)^2 + (1 - \alpha_b)^2) \tag{69}$$

which removes unboundedness at both limits. These methods should only be used during the iterations and not after the final iteration otherwise some small level of conservation error may result.

6 Two-Phase Flow Equation Solution

The system of equations for incompressible turbulent two-phase flow Eqs. (66, 60, 61 and 62) is complete, closed and susceptible to numerical solution. The need to obey the incompressibility constraint Eqn. (59) suggests that a pressure equation based solution algorithm would be most appropriate. For steady-state problems SIMPLE [7] or one of the variants could be used (as in the BRITE II project) or PISO [8] for transient runs; in either case a pressure equations is constructed from the discretised momentum equations Eqs. (66 and 60) and the incompressibility constraint Eqn. (59). Industrial two-phase flow typically occurs in complex geometries for which unstructured collocated computational meshes are most appropriate. However, difficulties arise in handling large density gradients, caused by *e.g.* complete phase separation, on such meshes (problems not encountered on staggered structured meshes) which require special interpolation practices. Implementation of these interpolation practices in traditional industrial CFD codes may cause some difficulty but may not be important for the flows of interest. Considering this, a fairly traditional algorithm is proposed here, capable of handling a wide range of two-phase flow including

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phase inversion and phase disappearance but not complete separation creating a free surface between the phases. An algorithm which can handle such extreme conditions has been developed and implemented in FOAM and will be described in detail in a subsequent report.

6.1 Discretisation

Equation discretisation is presented in the finite volume notation of Weller [1], a concise, code-independent form which should make it as easy as possible to understand the algorithm and to implement in the code of choice. Currently this notation is still under development and may require significant revision; if any of the terms are not clear or you have any suggestions please contact the author by Email at H.Weller@OpenCFD.co.uk.

6.1.1 Phase-Fraction Equations

Although only one of the phase fraction equations need be solved (the other phase fraction is obtained from $\alpha_b = 1 - \alpha_a$), maintaining boundedness may require the solution of both equations in conjunction with a recombination scheme described in Section 5.1. Discretisation requires the phase-relative fluxes

$$\phi_{r_a} = \alpha_{b f(-\phi_r,\Gamma,0.5)} \phi_r \tag{70}$$

and

$$\phi_{r_b} = -\alpha_{a f(\phi_r,\Gamma,0.5)} \phi_r \tag{71}$$

where

$$\phi_r = \phi_a - \phi_b \tag{72}$$

which are used in the second convection terms the phase-fraction equation pair

$$\left[\!\left[\frac{\partial[\alpha_a]}{\partial t}\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi [\alpha_a]_{f(\phi,\Gamma,0.5)}\right)\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi_{r_a} [\alpha_a]_{f(\phi_{r_a},\Gamma,0.5)}\right)\right]\!\right] = 0 \tag{73}$$

and

$$\left[\!\left[\frac{\partial[\alpha_b]}{\partial t}\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi [\alpha_b]_{f(\phi,\Gamma,0.5)}\right)\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi_{r_b} [\alpha_b]_{f(\phi_{r_b},\Gamma,0.5)}\right)\right]\!\right] = 0. \tag{74}$$

In order to ensure boundedness, an NVD or TVD scheme should be applied to all convection terms, the example here is the Γ scheme used in TVD mode. Upwind differencing could be applied if first-order accuracy is adequate. Note carefully the sign of the fluxes used to interpolate the phase fractions in the relative fluxes; this ensures the two equations are numerically equivalent *i.e.* $\alpha_b = 1 - \alpha_a$ even if both equations are solved, and the boundedness is guaranteed at both limits.

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6.1.2 Phase-Momentum Equations

The total convection fluxes of momentum, including in-phase convection and interface transport effects, are

$$\phi_a^{\mathcal{T}} = \phi_a - \nu_{eff_{af}} \frac{S_f \nabla_f^{\perp} \alpha_a}{\alpha_{af} + \delta} \tag{75}$$

and

$$\phi_b^{\mathcal{T}} = \phi_b - \nu_{eff_{bf}} \frac{S_f \nabla_f^{\perp} \alpha_b}{\alpha_{bf} + \delta}. \tag{76}$$

The momentum equations are discretised in the decoupled semi-implicit form

$$\begin{aligned}
&\left[\!\left[\frac{\partial[\overline{\mathbf{U}}_a]}{\partial t}\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi_a^{\mathcal{T}} [\overline{\mathbf{U}}_a]_{f(\phi_a^{\mathcal{T}},\mathrm{UD},)}\right)\right]\!\right] - \left[\!\left[\nabla \bullet \left(\phi_a^{\mathcal{T}}\right) [\overline{\mathbf{U}}_a]\right]\!\right] - \left[\!\left[\nabla \bullet \left(\nu_{eff_a} \nabla [\overline{\mathbf{U}}_a]\right)\right]\!\right] \\
&+ \nabla \bullet \overline{\mathbf{R}}_{eff_a}^{\mathcal{C}} + \frac{\nabla \alpha_a}{\langle \alpha_a \rangle_{\nabla} + \delta} \bullet \overline{\mathbf{R}}_{eff_a}^{\mathcal{C}} = -\frac{\nabla \overline{p}}{\overline{\rho}_a} + \mathbf{g} \\
&\qquad - \left[\!\left[\frac{\alpha_b}{\overline{\rho}_a} A_d [\overline{\mathbf{U}}_a]\right]\!\right] - \frac{\alpha_b}{\overline{\rho}_a} A_{vm} \left[\!\left[\frac{d_a[\overline{\mathbf{U}}_a]}{dt}\right]\!\right] + \frac{\alpha_b}{\overline{\rho}_a} \left(A_d \overline{\mathbf{U}}_b + A_l + A_{vm} \frac{d_b \overline{\mathbf{U}}_b}{dt}\right)
\end{aligned} \tag{77}$$

and

$$\begin{aligned}
&\left[\!\left[\frac{\partial[\overline{\mathbf{U}}_b]}{\partial t}\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi_b^{\mathcal{T}} [\overline{\mathbf{U}}_b]_{f(\phi_b^{\mathcal{T}},\mathrm{UD},)}\right)\right]\!\right] - \left[\!\left[\nabla \bullet \left(\phi_b^{\mathcal{T}}\right) [\overline{\mathbf{U}}_b]\right]\!\right] - \left[\!\left[\nabla \bullet \left(\nu_{eff_b} \nabla [\overline{\mathbf{U}}_b]\right)\right]\!\right] \\
&+ \nabla \bullet \overline{\mathbf{R}}_{eff_b}^{\mathcal{C}} + \frac{\nabla \alpha_b}{\langle \alpha_b \rangle_{\nabla} + \delta} \bullet \overline{\mathbf{R}}_{eff_b}^{\mathcal{C}} = -\frac{\nabla \overline{p}}{\overline{\rho}_b} + \mathbf{g} \\
&\qquad - \left[\!\left[\frac{\alpha_a}{\overline{\rho}_b} A_d [\overline{\mathbf{U}}_b]\right]\!\right] - \frac{\alpha_a}{\overline{\rho}_b} A_{vm} \left[\!\left[\frac{d_b[\overline{\mathbf{U}}_b]}{dt}\right]\!\right] + \frac{\alpha_a}{\overline{\rho}_b} \left(A_d \overline{\mathbf{U}}_a + A_l + A_{vm} \frac{d_a \overline{\mathbf{U}}_a}{dt}\right).
\end{aligned} \tag{78}$$

The time derivative, convection and diffusion terms are handled implicitly, the Reynolds stress correction, pressure gradient, buoyancy and lift terms are handled explicitly and the drag and virtual mass terms handled semi-implicitly by making the part involving the velocity being solved for implicit and other part explicit. This discretisation approach has proved very stable in both transient and steady state modes; the complex partial-eliminations procedures of the BRITE II project [4] have not proved beneficial in the tests conducted in FOAM. For the construction of the pressure equation, the momentum matrices are stored without the pressure gradient term such that

$$[\![\boldsymbol{\mathcal{M}}_a [\mathbf{U}_a]]\!] = -\frac{\nabla \overline{p}}{\overline{\rho}_a} \tag{79}$$

and

$$[\![\boldsymbol{\mathcal{M}}_b [\mathbf{U}_b]]\!] = -\frac{\nabla \overline{p}}{\overline{\rho}_b}. \tag{80}$$

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6.1.3 Phase-Momentum Correction Equations

The phase-momentum correction equations are obtained by decomposing the matrixes in Eqs. (79 and 80) into diagonal and "H" parts and rearranging, giving

$$\overline{\mathbf{U}}_a = \frac{\mathbf{H}_a}{A_a} - \frac{\nabla \overline{p}}{\overline{\rho}_a A_a} \tag{81}$$

and

$$\overline{\mathbf{U}}_b = \frac{\mathbf{H}_b}{A_b} - \frac{\nabla \overline{p}}{\overline{\rho}_a A_b} \tag{82}$$

where

$$A_a = [\![\boldsymbol{\mathcal{M}}_a[\mathbf{U}_a]]\!]_D, \qquad \mathbf{H}_a = [\![\boldsymbol{\mathcal{M}}_a[\mathbf{U}_a]]\!]_H \tag{83}$$

and

$$A_b = [\![\boldsymbol{\mathcal{M}}_b[\mathbf{U}_b]]\!]_D, \qquad \mathbf{H}_b = [\![\boldsymbol{\mathcal{M}}_b[\mathbf{U}_b]]\!]_H \tag{84}$$

$$\tag{85}$$

6.1.4 Pressure Equation

Equations for the face volumetric fluxes are created by interpolating the momentum correction equations Eqs. (81 and 82) using central differencing giving

$$\phi_a = \phi_a^* - \left(\frac{1}{\overline{\rho}_a A_a}\right)_f S_f \nabla_f^\perp \overline{p} \tag{86}$$

and

$$\phi_b = \phi_b^* - \left(\frac{1}{\overline{\rho}_b A_b}\right)_f S_f \nabla_f^\perp \overline{p} \tag{87}$$

where the flux predictions are given by

$$\phi_a^* = \left(\frac{\mathbf{H}_a}{A_a}\right)_f \bullet \mathbf{S}_f \tag{88}$$

and

$$\phi_b^* = \left(\frac{\mathbf{H}_b}{A_b}\right)_f \bullet \mathbf{S}_f \tag{89}$$

Given that the total face volumetric flux is given by

$$\phi = \alpha_{af}\phi_a + \alpha_{bf}\phi_b \tag{90}$$

and the continuity constraint may be written

$$\nabla \bullet (\phi) = 0 \tag{91}$$

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the pressure equation is constructed by substituting Eqs. (88, 89 and 90) into Eqn. (91) giving

$$\left[\!\left[\nabla \bullet \left(\left(\alpha_{af}\left(\frac{1}{\overline{\rho}_a A_a}\right)_f + \alpha_{bf}\left(\frac{1}{\overline{\rho}_b A_b}\right)_f\right)\nabla[\overline{p}]\right)\right]\!\right] = \nabla \bullet (\alpha_{af}\phi_a^* + \alpha_{bf}\phi_b^*). \tag{92}$$

After the pressure solution the fluxes are corrected using Eqs. (86 and 87).

6.1.5 Substantive derivatives

After the PISO loop the substantive derivatives are corrected using

$$\frac{d_a \overline{\mathbf{U}}_a}{dt} = \frac{\partial \overline{\mathbf{U}}_a}{\partial t} + \nabla \bullet \left(\phi_a \overline{\mathbf{U}}_{a_{f(\phi_a,\Gamma,0.5)}}\right) - \nabla \bullet \left(\phi_a\right)\overline{\mathbf{U}}_a \tag{93}$$

$$\frac{d_b \overline{\mathbf{U}}_b}{dt} = \frac{\partial \overline{\mathbf{U}}_b}{\partial t} + \nabla \bullet \left(\phi_b \overline{\mathbf{U}}_{b_{f(\phi_b,\Gamma,0.5)}}\right) - \nabla \bullet \left(\phi_b\right)\overline{\mathbf{U}}_b \tag{94}$$

6.2 Solution Algorithm

The solution algorithm used PISO to handle the pressure-velocity coupling which requires a momentum predictor and a correction loop in which the pressure equation is solved and the momentum corrected based on the pressure change. The phase-fraction is solved only once per time step before the momentum predictor. For most cases solving only for the dispersed phase-fraction has proved adequate but for cases with strong phase-inversion in which there are significant regions where the nominally continuous phase has a very low phase fraction it may be advantageous to solve for both in an iterative sequence, correcting for unboundedness after each iteration.

1. Optional α-Loop:
   (a) Solve the α_a-equation, Eqn. (73).
   (b) Solve the α_b-equation, Eqn. (74).
   (c) Bound α_a and α_b using Eqn. (68) or Eqn. (69).
2. Solve the α_a-equation, Eqn. (73).
3. Calculate coefficients A_d, A_l and A_{vm}, Eqn. (58).
4. Construct and solve the momentum equations, Eqs. (77 and 115).
5. PISO-Loop:
   (a) Predict fluxes using Eqs. (88 and 89).
   (b) Construct and solve the pressure equation Eqn. (92).

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(c) Correct fluxes using Eqs. (86, 87 and 90).

(d) Correct velocities using Eqs. (81 and 82).

6. Correct the convective derivatives using Eqs. (93 and 94)

7. Solve $k-\varepsilon$ equations (if required).

7 Compressible Two-Phase Flow Equations

Compressibility effects are important in many two-phase systems, in particular in bubble columns in which the pressure difference from top to bottom may be significant. However, the density variations within the phases is typically small compared with the density difference between the phases; this can cause numerical difficulties which must be handled carefully.

The momentum equations Eqs. (56 and 57) may be solved in this form without further manipulation or approximation but if the continuity equation Eqn. (33) were solved directly, obtaining the density field from the pressure and the phase equation of state, phase fraction boundedness would not be guaranteed. Another possibility is to cast Eqn. (33) i.t.o. the density-weighted phase fraction; in which case

$$\frac{\partial \widetilde{\alpha}_\varphi \overline{\rho}}{\partial t} + \nabla \bullet (\widetilde{\alpha}_\varphi \overline{\rho} \widetilde{\mathbf{U}_\varphi}) = 0. \tag{95}$$

This approach is common in turbulent combustion modelling where the density ratio is of the order of 8 but has proved very unstable for the large density ratios typical of two-phase flows. What is required is a method similar to that developed in Section 5.1 in which Eqn. (33) is manipulated into a form which guarantees boundedness of the phase-fraction even during extreme density changes. The starting point for this analysis is to separate the terms relating to the density variation from those relating to the transport of phase-fraction. This is achieved by decomposing the terms in Eqn. (33) thus

$$\overline{\rho}_\varphi \frac{\partial \alpha_\varphi}{\partial t} + \alpha_\varphi \frac{\partial \overline{\rho}_\varphi}{\partial t} + \overline{\rho}_\varphi \nabla \bullet (\alpha_\varphi \widetilde{\mathbf{U}_\varphi}) + \alpha_\varphi \widetilde{\mathbf{U}_\varphi} \bullet \nabla \overline{\rho}_\varphi = 0. \tag{96}$$

Dividing Eqn. (96) by $\overline{\rho}_\varphi$ and re-arranging using $\frac{d_\varphi \overline{\rho}_\varphi}{dt} = \frac{\partial \overline{\rho}_\varphi}{\partial t} + \widetilde{\mathbf{U}_\varphi} \bullet \nabla \overline{\rho}_\varphi$ gives

$$\frac{\partial \alpha_\varphi}{\partial t} + \nabla \bullet (\alpha_\varphi \widetilde{\mathbf{U}_\varphi}) + \frac{\alpha_\varphi}{\overline{\rho}_\varphi} \frac{d_\varphi \overline{\rho}_\varphi}{dt} = 0. \tag{97}$$

Decomposing the terms in Eqn. (97) for a two-phase system as described in Section 5.1 gives

$$\frac{\partial \alpha_a}{\partial t} + \nabla \bullet (\overline{\mathbf{U}} \alpha_a) + \nabla \bullet (\overline{\mathbf{U}}_r \alpha_a (1-\alpha_a)) + \frac{\alpha_a}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} = 0 \tag{98}$$

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and

$$\frac{\partial \alpha_b}{\partial t} + \nabla \bullet (\overline{\mathbf{U}} \alpha_b) - \nabla \bullet (\overline{\mathbf{U}}_r \alpha_b (1 - \alpha_b)) + \frac{\alpha_b}{\overline{\rho}_b} \frac{d_b \overline{\rho}_b}{dt} = 0. \tag{99}$$

However, unlike for the incompressible case, neither Eqn. (98) nor Eqn. (99) guarantees boundedness in the current form due to the presence of the additional compressibility terms which do not tend to zero when either phase-fraction approaches zero and the possibility that a divergent/convergent velocity field may induce unboundedness via the mean velocity conservative convection terms. The latter problem may be seen more clearly if the mean velocity convection term in Eqn. (98) is decomposed thus

$$\frac{\partial \alpha_a}{\partial t} + \overline{\mathbf{U}} \bullet \nabla \alpha_a + \nabla \bullet (\overline{\mathbf{U}}_r \alpha_a (1 - \alpha_a)) = -\alpha_a \nabla \bullet \overline{\mathbf{U}} - \frac{\alpha_a}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} \tag{100}$$

7.1 Phase-Fraction Boundedness in Compressible Flow

An expression for the divergence of the mean velocity may be obtained by adding Eqs. (98 and 99) giving

$$\nabla \bullet \overline{\mathbf{U}} = -\frac{\alpha_a}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} - \frac{\alpha_b}{\overline{\rho}_b} \frac{d_b \overline{\rho}_b}{dt}, \tag{101}$$

which when substituted into Eqn. (100) gives

$$\frac{\partial \alpha_a}{\partial t} + \overline{\mathbf{U}} \bullet \nabla \alpha_a + \nabla \bullet (\overline{\mathbf{U}}_r \alpha_a (1 - \alpha_a)) = \frac{\alpha_a^2}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} + \frac{\alpha_a \alpha_b}{\overline{\rho}_b} \frac{d_b \overline{\rho}_b}{dt} - \frac{\alpha_a}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} \tag{102}$$

which may be simplified, noting that $\alpha_a^2 - \alpha_a = -\alpha_a(1 - \alpha_a)$, resulting in

$$\frac{\partial \alpha_a}{\partial t} + \overline{\mathbf{U}} \bullet \nabla \alpha_a + \nabla \bullet (\overline{\mathbf{U}}_r \alpha_a (1 - \alpha_a)) = \alpha_a (1 - \alpha_a) \left(\frac{1}{\overline{\rho}_b} \frac{d_b \overline{\rho}_b}{dt} - \frac{1}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} \right). \tag{103}$$

The same procedure may be applied to the Eqn. (99) giving

$$\frac{\partial \alpha_b}{\partial t} + \overline{\mathbf{U}} \bullet \nabla \alpha_b - \nabla \bullet (\overline{\mathbf{U}}_r \alpha_a (1 - \alpha_b)) = \alpha_a (1 - \alpha_b) \left(\frac{1}{\overline{\rho}_a} \frac{d_a \overline{\rho}_a}{dt} - \frac{1}{\overline{\rho}_b} \frac{d_b \overline{\rho}_b}{dt} \right). \tag{104}$$

Equations (103 and 104) will ensure boundedness of the phase-fraction but are not in conservative form. This may not be an issue because in the incompressible limit Eqs. (103 and 104) recovers the bounded conservative form of Eqs. (66 and 67) and in compressible systems the phase-fraction is not a conserved property.

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8 Compressible Two-Phase Flow Equation Solution

The system of equations for compressible two-phase flow Eqs. (103, 56, 57 and 101) is complete and closed and susceptible to numerical solution. As in the incompressible case the need to obey the velocity divergence Eqn. (101) suggests that a pressure equation based solution algorithm would be most appropriate. The pressure equations is constructed from the discretised momentum equations Eqs. (56 and 57) and Eqn. (101).

8.1 Compressible Flow Equation Discretisation

Equations discretisation is presented in the finite volume notation of Weller [1]

8.1.1 Phase-Fraction Equations

Although only one of the phase fraction equations need be solved (the other phase fraction is obtained from $\alpha_b = 1-\alpha_a$), maintaining boundedness may require the solution of both equations in conjunction with a recombination scheme described in Section 5.1. Discretisation requires the phase-relative fluxes

$$\phi_{r_a} = \alpha_{b f(-\phi_r,\Gamma,0.5)}\phi_r \tag{105}$$

and

$$\phi_{r_b} = -\alpha_{a f(\phi_r,\Gamma,0.5)}\phi_r \tag{106}$$

where

$$\phi_r = \phi_a - \phi_b \tag{107}$$

which are used in the second convection terms the phase-fraction equation pair

$$\left[\!\left[\frac{\partial[\alpha_a]}{\partial t}\right]\!\right] + \left[\!\left[\nabla\bullet\left(\phi[\alpha_a]_{f(\phi,\Gamma,0.5)}\right)\right]\!\right] - \left[\!\left[\nabla\bullet\left(\phi\right)[\alpha_a]\right]\!\right] + \left[\!\left[\nabla\bullet\left(\phi_{r_a}[\alpha_a]_{f(\phi_{r_a},\Gamma,0.5)}\right)\right]\!\right] = \tag{108}$$

$$\left[\!\left[(1-\alpha_a)\left(\frac{1}{\overline{\rho}_b}\frac{D\overline{\rho}_b}{Dt} - \frac{1}{\overline{\rho}_a}\frac{D\overline{\rho}_a}{Dt}\right)[\alpha_a]\right]\!\right] \tag{109}$$

and

$$\left[\!\left[\frac{\partial[\alpha_b]}{\partial t}\right]\!\right] + \left[\!\left[\nabla\bullet\left(\phi[\alpha_b]_{f(\phi,\Gamma,0.5)}\right)\right]\!\right] - \left[\!\left[\nabla\bullet\left(\phi\right)[\alpha_b]\right]\!\right] + \left[\!\left[\nabla\bullet\left(\phi_{r_b}[\alpha_b]_{f(\phi_{r_b},\Gamma,0.5)}\right)\right]\!\right] = \tag{110}$$

$$\left[\!\left[(1-\alpha_b)\left(\frac{1}{\overline{\rho}_a}\frac{D\overline{\rho}_a}{Dt} - \frac{1}{\overline{\rho}_b}\frac{D\overline{\rho}_b}{Dt}\right)[\alpha_b]\right]\!\right] \tag{111}$$

In order to ensure boundedness, an NVD or TVD scheme should be applied to all convection terms, the example here is the Γ scheme used in TVD mode. Upwind differencing could be applied if first-order accuracy is adequate. Note carefully the sign of the fluxes used to interpolate the phase fractions in the relative fluxes; this ensures the two equations are numerically equivalent *i.e.* $\alpha_b = 1 - \alpha_a$ even if both equations are solved, and the

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boundedness is guaranteed at both limits. The source terms are handled semi-implicitly depending on the sign; implicit if negative otherwise explicit. This guarantees α_a and α_b remain separately positive and that the matrix remains well conditioned but does not prevent the solution from rising above 1, however the recombination scheme described in Section 5.1 may be used to ensure this.

8.1.2 Phase-Momentum Equations

The total convection fluxes of momentum, including in-phase convection and interface transport effects, are

$$\phi_a^{\mathcal{T}} = \phi_a - \nu_{eff_{af}} \frac{S_f \nabla_f^{\perp} \alpha_a}{\alpha_{af} + \delta} \tag{112}$$

and

$$\phi_b^{\mathcal{T}} = \phi_b - \nu_{eff_{bf}} \frac{S_f \nabla_f^{\perp} \alpha_b}{\alpha_{bf} + \delta}. \tag{113}$$

The momentum equations are discretised in the decoupled semi-implicit form

$$\begin{aligned}
&\left[\!\left[\frac{\partial[\widetilde{\mathbf{U}_a}]}{\partial t}\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi_a^{\mathcal{T}} [\widetilde{\mathbf{U}_a}]_{f(\phi_a^{\mathcal{T}},\mathrm{UD},)}\right)\right]\!\right] - \left[\!\left[\nabla \bullet \left(\phi_a^{\mathcal{T}}\right) [\widetilde{\mathbf{U}_a}]\right]\!\right] - \left[\!\left[\nabla \bullet \left(\nu_{eff_a} \nabla [\widetilde{\mathbf{U}_a}]\right)\right]\!\right] \\
&+ \nabla \bullet \overline{\mathbf{R}}_{eff_a}^{\mathcal{C}} + \frac{\nabla \alpha_a \overline{\rho}_a}{\langle \alpha_a \overline{\rho}_a \rangle_{\nabla} + \delta} \bullet \overline{\mathbf{R}}_{eff_a}^{\mathcal{C}} = -\frac{\nabla \overline{p}}{\overline{\rho}_a} + \mathbf{g} \\
&\qquad - \left[\!\left[\frac{\alpha_b}{\overline{\rho}_a} A_d [\widetilde{\mathbf{U}_a}]\right]\!\right] - \frac{\alpha_b}{\overline{\rho}_a} A_{vm} \left[\!\left[\frac{d_a[\widetilde{\mathbf{U}_a}]}{dt}\right]\!\right] + \frac{\alpha_b}{\overline{\rho}_a} \left(A_d \widetilde{\mathbf{U}_b} + A_l + A_{vm} \frac{d_b \widetilde{\mathbf{U}_b}}{dt}\right)
\end{aligned} \tag{114}$$

and

$$\begin{aligned}
&\left[\!\left[\frac{\partial[\widetilde{\mathbf{U}_b}]}{\partial t}\right]\!\right] + \left[\!\left[\nabla \bullet \left(\phi_b^{\mathcal{T}} [\widetilde{\mathbf{U}_b}]_{f(\phi_b^{\mathcal{T}},\mathrm{UD},)}\right)\right]\!\right] - \left[\!\left[\nabla \bullet \left(\phi_b^{\mathcal{T}}\right) [\widetilde{\mathbf{U}_b}]\right]\!\right] - \left[\!\left[\nabla \bullet \left(\nu_{eff_b} \nabla [\widetilde{\mathbf{U}_b}]\right)\right]\!\right] \\
&+ \nabla \bullet \overline{\mathbf{R}}_{eff_b}^{\mathcal{C}} + \frac{\nabla \alpha_b \overline{\rho}_b}{\langle \alpha_b \overline{\rho}_b \rangle_{\nabla} + \delta} \bullet \overline{\mathbf{R}}_{eff_b}^{\mathcal{C}} = -\frac{\nabla \overline{p}}{\overline{\rho}_b} + \mathbf{g} \\
&\qquad - \left[\!\left[\frac{\alpha_a}{\overline{\rho}_b} A_d [\widetilde{\mathbf{U}_b}]\right]\!\right] - \frac{\alpha_a}{\overline{\rho}_b} A_{vm} \left[\!\left[\frac{d_b[\widetilde{\mathbf{U}_b}]}{dt}\right]\!\right] + \frac{\alpha_a}{\overline{\rho}_b} \left(A_d \widetilde{\mathbf{U}_a} + A_l + A_{vm} \frac{d_a \widetilde{\mathbf{U}_a}}{dt}\right).
\end{aligned} \tag{115}$$

The time derivative, convection and diffusion terms are handled implicitly, the Reynolds stress correction, pressure gradient, buoyancy and lift terms are handled explicitly and the drag and virtual mass terms handled semi-implicitly by making the part involving the velocity being solved for implicit and other part explicit. This discretisation approach has proved very stable in both transient and steady state modes; the complex partial-eliminations procedures of the BRITE II project [4] have not proved beneficial in the tests

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conducted in FOAM. For the construction of the pressure equation, the momentum matrices are stored without the pressure gradient term such that

$$[\![\boldsymbol{\mathcal{M}}_a[\mathbf{U}_a]]\!] = -\frac{\nabla \overline{p}}{\overline{\rho}_a} \tag{116}$$

and

$$[\![\boldsymbol{\mathcal{M}}_b[\mathbf{U}_b]]\!] = -\frac{\nabla \overline{p}}{\overline{\rho}_b}. \tag{117}$$

8.1.3 Phase-Momentum Correction Equations

The phase-momentum correction equations are obtained by decomposing the matrixes in Eqs. (116 and 117) into diagonal and "H" parts and rearranging, giving

$$\widetilde{\mathbf{U}_a} = \frac{\mathbf{H}_a}{A_a} - \frac{\nabla \overline{p}}{\overline{\rho}_a A_a} \tag{118}$$

and

$$\widetilde{\mathbf{U}_b} = \frac{\mathbf{H}_b}{A_b} - \frac{\nabla \overline{p}}{\overline{\rho}_a A_b} \tag{119}$$

where

$$A_a = [\![\boldsymbol{\mathcal{M}}_a[\mathbf{U}_a]]\!]_D, \qquad \mathbf{H}_a = [\![\boldsymbol{\mathcal{M}}_a[\mathbf{U}_a]]\!]_H \tag{120}$$

and

$$A_b = [\![\boldsymbol{\mathcal{M}}_b[\mathbf{U}_b]]\!]_D, \qquad \mathbf{H}_b = [\![\boldsymbol{\mathcal{M}}_b[\mathbf{U}_b]]\!]_H \tag{121}$$

$$\tag{122}$$

8.1.4 Pressure Equation

Equations for the face volumetric fluxes are created by interpolating the momentum correction equations Eqs. (118 and 119) using central differencing giving

$$\phi_a = \phi_a^* - \left(\frac{1}{\overline{\rho}_a A_a}\right)_f S_f \nabla_f^{\perp} \overline{p} \tag{123}$$

and

$$\phi_b = \phi_b^* - \left(\frac{1}{\overline{\rho}_b A_b}\right)_f S_f \nabla_f^{\perp} \overline{p} \tag{124}$$

where the flux predictions are given by

$$\phi_a^* = \left(\frac{\mathbf{H}_a}{A_a}\right)_f \bullet \mathbf{S}_f \tag{125}$$

and

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$$\phi_b^* = \left(\frac{\mathbf{H}_b}{A_b}\right)_f \bullet \mathbf{S}_f \tag{126}$$

Given that the total face volumetric flux is given by

$$\phi = \alpha_{af}\phi_a + \alpha_{bf}\phi_b \tag{127}$$

and the continuity constraint may be written

$$\nabla \bullet (\phi) = -\frac{\alpha_a}{\overline{\rho}_a}\frac{d_a\overline{\rho}_a}{dt} - \frac{\alpha_b}{\overline{\rho}_b}\frac{d_b\overline{\rho}_b}{dt}, \tag{128}$$

the pressure equation is constructed by substituting Eqs. (125, 126 and 127) into Eqn. (128) giving

$$\left[\!\left[\nabla \bullet \left(\left(\alpha_{af}\left(\frac{1}{\overline{\rho}_a A_a}\right)_f + \alpha_{bf}\left(\frac{1}{\overline{\rho}_b A_b}\right)_f\right)\nabla[\overline{p}]\right)\right]\!\right] = \nabla \bullet (\alpha_{af}\phi_a^* + \alpha_{bf}\phi_b^*) \tag{129}$$

$$+ \frac{\alpha_a}{\overline{\rho}_a}\left(\left[\!\left[\frac{\partial[\overline{\psi}_a]}{\partial t}\right]\!\right]p + \nabla \bullet \left(\phi_a \overline{\rho}_{a_{f(\phi_a,\Gamma,0.5)}}\right) - \nabla \bullet (\phi_a)\,\overline{\rho}_a\right) \tag{130}$$

$$+ \frac{\alpha_b}{\overline{\rho}_b}\left(\left[\!\left[\frac{\partial[\overline{\psi}_b]}{\partial t}\right]\!\right]p + \nabla \bullet \left(\phi_b \overline{\rho}_{b_{f(\phi_b,\Gamma,0.5)}}\right) - \nabla \bullet (\phi_b)\,\overline{\rho}_b\right). \tag{131}$$

After the pressure solution the fluxes are corrected using Eqs. (123 and 124).

8.1.5 Substantive derivatives

After the PISO loop the phase velocity substantive derivatives are corrected using

$$\frac{d_a\widetilde{\mathbf{U}}_a}{dt} = \frac{\partial\widetilde{\mathbf{U}}_a}{\partial t} + \nabla \bullet \left(\phi_a \widetilde{\mathbf{U}}_{a_{f(\phi_a,\Gamma,0.5)}}\right) - \nabla \bullet (\phi_a)\,\widetilde{\mathbf{U}}_a \tag{132}$$

$$\frac{d_b\widetilde{\mathbf{U}}_b}{dt} = \frac{\partial\widetilde{\mathbf{U}}_b}{\partial t} + \nabla \bullet \left(\phi_b \widetilde{\mathbf{U}}_{b_{f(\phi_b,\Gamma,0.5)}}\right) - \nabla \bullet (\phi_b)\,\widetilde{\mathbf{U}}_b \tag{133}$$

8.2 Solution Algorithm

The solution algorithm used PISO to handle the pressure-velocity coupling which requires a momentum predictor and a correction loop in which the pressure equation is solved and the momentum corrected based on the pressure change. The phase-fraction is solved only once per time step before the momentum predictor. For most cases solving only for the dispersed phase-fraction has proved adequate but for cases with strong phase-inversion in which there are significant regions where the nominally continuous phase has a very low phase fraction it may be advantageous to solve for both in an iterative sequence, correcting for unboundedness after each iteration.

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1. Optional α-Loop:
   (a) Solve the α_a-equation, Eqn. (109).
   (b) Solve the α_b-equation, Eqn. (111).
   (c) Bound α_a and α_b using Eqn. (68) or Eqn. (69).
2. Solve the α_a-equation, Eqn. (109).
3. Calculate coefficients A_d, A_l and A_{vm}, Eqn. (58).
4. Construct and solve the momentum equations, Eqs. (114 and 115).
5. PISO-Loop:
   (a) Predict fluxes using Eqs. (125 and 126).
   (b) Construct and solve the pressure equation Eqn. (131).
   (c) Correct fluxes using Eqs. (123, 124 and 127).
   (d) Correct velocities using Eqs. (118 and 119).
6. Correct the convective derivatives using Eqs. (132 and 133)
7. Solve $k - \varepsilon$ equations (if required).

9 Conclusion

The two-phase flow algorithm presented in this report is the result of an intensive research effort using FOAM. Careful consideration of the failings of the BRITE II algorithm has lead to a new set of practices designed to create a more general and robust approach. In particular, the problems in solving for the phase velocities in the limit of the phase-fractions going to zero is remedied by creating a phase-intensive form of the equations by decomposing terms and dividing by the phase fractions. This approach requires that the phase-fractions be bounded and conservative which is achieved by a novel splitting of the convection term in the phase-fraction equation and the application of appropriate discretisation practices. This new algorithm is capable of handling the full range of phase-fraction, phase-inversion and local phase-separation but only for modest density ratios. If phase separation at large density ratios occurs, *e.g.* the free surface in a bubble-column, then a more complex pressure interpolation practice is required; this is the subject of a subsequent report. A FOAM code containing this algorithm will be supplied with pre-run test cases and documentation.

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