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On the mixture model for multiphase flow

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ABSTRACT

Numerical flow simulation utilising a full multiphase model is impractical for a suspension possessing wide distributions in the particle size or density. Various approximations are usually made to simplify the computational task. In the simplest approach, the suspension is represented by a homogeneous single-phase system and the influence of the particles is taken into account in the values of the physical properties. The multiphase nature of the flow cannot, however, be avoided when the concentration gradients are large and the dispersed phases alter the hydrodynamic behaviour of the mixture or when the distributions of the particles are studied. In many practical applications of multiphase flow, the mixture model is a sufficiently accurate approximation, with only a moderate increase in the computational effort compared to a single-phase simulation.

This study concentrates on the derivation and closing of the model equations. The validity of the mixture model is also carefully analysed. Starting from the continuity and momentum equations written for each phase in a multiphase system, the field equations for the mixture are derived. The mixture equations largely resemble those for a single-phase flow but are represented in terms of the mixture density and velocity. However, an additional term in the mixture momentum equation arises from the slip of the dispersed phases relative to the continuous phase. The volume fraction for each dispersed phase is solved from a phase continuity equation.

Various approaches applied in closing the mixture model equations are reviewed. An algebraic equation is derived for the velocity of a dispersed phase relative to the continuous phase. Simplifications made in calculating the relative velocity restrict the applicability of the mixture model to cases in which the particles reach the terminal velocity in a short time period compared to the characteristic time scale of the flow of the mixture. The terms for the viscous and turbulent stresses in the mixture momentum equation are usually combined to a generalised stress.

The mixture model applications reported in the literature are briefly summarised. The areas of application include gravity settling, rotational flows and turbulent flows. The multiphase models in three commercial codes, PHOENICS, FLUENT and CFX 4, are reviewed. The mixture model approach, in a simplified form, is implemented only in PHOENICS.

PREFACE

The interest of applying computational fluid dynamics in industrial multiphase processes has increased during the last few years. Fluidised beds, polymerisation processes, settling tanks, chemical reactors, gas dispersion in liquids and air-lift reactors are typical examples in process industry. Modelling of multiphase flows is, however, very complicated. Full multiphase modelling requires a large computing power, especially if several secondary phases need to be considered.

In this study, we investigate the mixture model, which is a simplification of the full models. This approach is a considerable alternative in simulating dilute suspensions of solid particles or small bubbles in liquids.

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CONTENTS

NOTATIONS

Latin letters

c	mass fraction [-]
$\mathbf{e}_r$	radial unit vector [-]
$\mathbf{g}$	gravitational acceleration [m/s^2]
$\mathbf{j}$	volumetric flux [m/s]
k	kinetic energy of turbulence [m^2/s^2]
m	mass [kg]
n	number of phases [-]
p	pressure [N/m^2]
r	radius [m]
t	time [s]
$u,\mathbf{u}$	velocity [m/s]
$\mathbf{u}_{Ik}$	local instant velocity of phase k [m/s]
$\mathbf{u}_{Fk}=\mathbf{u}_{Ik}-\mathbf{u}_k$	fluctuating component of the velocity of phase k [m/s]
$\mathbf{u}_{Ck}=\mathbf{u}_k-\mathbf{u}_c$	velocity of phase k relative to the continuous phase [m/s]
$\mathbf{u}_m$	velocity of the mixture mass centre
$\mathbf{u}_{Mk}=\mathbf{u}_k-\mathbf{u}_m$	diffusion velocity - velocity of phase k relative to the mixture mass centre [m/s]
$\mathbf{u}_{Vk}=\mathbf{u}_k-\mathbf{j}_m$	drift velocity - velocity of phase k relative to the mixture volume centre [m/s]
A	area [m^2]
C_D	drag coefficient [-]
D	diffusion coefficient [m^2/s]
$\mathbf{D}_{ki}$	interfacial extra deformation tensor
$\mathbf{F}$	drag force [N]
$\mathbf{M}$	momentum source [N/m^3]
Re	Reynolds number [-]
U_r	terminal velocity correction
V	volume [m^3]

Greek letters

α	volume fraction [-]
κ	curvature of the interface [m^{-1}]
μ	dynamic viscosity [kg/m·s]
ρ	material density [kg/m^3]
σ	surface tension [N/m]
τ, $\boldsymbol{\tau}$	stress tensor [N/m^2]
ω	angular frequency [s^{-1}]
λ	second (bulk) viscosity [kg/m·s]
Γ	rate of the mass transfer [kg/m^{3}s]

Subscripts

c	continuous phase
e	effective
i	coordinate index
k	phase index
m	mixture
p	dispersed phase, particle
r	radial
s	solid
t	terminal
x,y,z	rectangular coordinates
r,φ,z	cylindrical coordinates
C	relative to the continuous phase
D	diffusion
F	fluctuating component
I	local instant value
M	relative to the mass centre
T	turbulent
V	relative to the volume centre

Other symbols and operators

$\mathbf{ab}$	dyadic product of two vectors
$\bar{a}$	average of a
$\mathbf{A}^T$	transposed tensor
Δ	difference
∇	gradient operator

1 INTRODUCTION

A multiphase system is defined as a mixture of the phases of solid, liquid and gas. Common examples are water droplets falling in air, gas bubbles rising in a liquid and solid particles transported by a fluid. Multiphase flows are often classified according to the nature of the system (Ishii 1975): dispersed flows (particles or droplets in liquid or gas, bubbles in liquid), separated flows (annular flows in vertical pipes, stratified flows in horizontal pipes) and transitional flows, which are combinations of the other two classes. Free-surface flows can be described as stratified two-phase flows.

In many cases in which the flow phenomena are dominated by one phase and the amounts of the other, unimportant phases are small (like dusty gas flows, small gas bubbles in a liquid), multiphase flow is in practice described as single phase flow and all effects of the secondary phases are neglected. In this report we focus on multiphase flows where the secondary phases cannot be ignored due to their influence on the fluid dynamic behaviour of the mixture and partly also due to their importance for the process studied. Depending on the strength of the coupling between the phases, different modelling approaches are suggested. They can be classified into homogeneous flow models, mixture models and multiphase models. Combinations of these are possible, too. In most models, each phase is treated as an interpenetrating continuum with a volume fraction parameter, which is analogous to the porosity assigned to a fluid phase in flow through a porous medium.

The simplest, most common formulations of the hydrodynamics of a mixture refer to the motion of the centre of mass of the system. The motions of individual components are treated in terms of diffusion through the mixture. This homogeneous flow model is applicable in drag dominated flows in which the phases are strongly coupled and their velocities equalise over short spatial length scales. All phases are assumed to move at the same velocity. The velocity of the mixture is solved for from a single momentum equation. For each phase, an individual continuity equation is solved for to obtain its volume fraction.

In multiphase mixtures, gravity and centrifugal forces tend to cause velocity differences which have to be accounted for. A group of models has been developed on the basis of an assumption of a local equilibrium. Depending on the exact formulation of the equations used to determine the velocity differences (and on the personal preference of the author), this model is called the drift-flux model (Zuber & Findlay 1965), the mixture model (Ishii 1975), the algebraic-slip model (Pericleous & Drake 1986), the suspension model/approach (Verloop 1995), the diffusion model (Ungarish 1993, Ishii 1975) or the local-equilibrium model (Johansen et al. 1990). The model is given in the form of a continuity equation for each phase and one momentum equation, which contains an additional term representing the effect of velocity differences between the phases. A model based on a force balance for the dispersed phases is required for computation of the relative velocities.

The form of the constitutive equations for the relative velocities varies in the different mixture models. The basic assumption in this formulation is that a local equilibrium establishes over short spatial length scales. Due to the requirement of a strong coupling between the phases, the mixture model is more suited for liquid-particle mixtures than for gas-particle mixtures.

In processes, where the phases are weakly coupled and where there are regions of sudden acceleration, no local equilibrium is established. An example is the riser of a circulating gas fluidised bed. As the upward flow of gas causes the solid particles to accelerate from zero velocity at the bottom to an equilibrium velocity at the height of about five to ten meters, the full multiphase model is required to describe this process. The model consists of the continuity and momentum equations for each phase. The phase interactions are accounted for by interphase transfer terms.

In all multiphase models, the main difficulties are due to the interfaces between the phases and the discontinuities associated to them (Ishii & Mishima 1984). The formulation of the constitutive equations is the greatest difficulty when developing a multiphase model for a practical application (Drew & Lahey 1979). As a result, the constitutive equations applied still include considerable uncertainties. Empirical information thus forms an essential part of the model.

Although the full multiphase equations are theoretically more advanced, the uncertainties in the closure relations can make them less reliable than the simpler mixture model. This is another justification of using the simpler homogeneous flow models and the mixture models whenever possible. The most important advantage of the mixture model is the considerably smaller number of variables to be solved when compared to the full multiphase models.

This report is a review of the theory and applications of the mixture model in dispersed multiphase flows. Since we apply the approach in which the mixture model equations are derived from the multiphase model equations, a short review of the full multiphase models is given in Section 2. Section 3 introduces the mathematical formulations of the mixture model and Section 4 reviews some practical applications. In Section 5, a short discussion of the multiphase flow models of three commercial computer codes (PHOENICS, FLUENT and CFX 4) is given. Although the main interest of this work is in the mixture model, the multiphase models of the commercial codes are also described. The mixture model is implemented only in PHOENICS.

2 MODELLING OF MULTIPHASE FLOWS

2.1 MODELLING APPROACHES

A multiphase flow system consists of a number of single phase regions bounded by moving interfaces. The description here is limited to dispersed multiphase flows. A simplified theory can be used for stratified flows but this is outside the scope of this report.

In principle, a multiphase flow model could be formulated in terms of the local instant variables pertaining to each phase and matching boundary conditions at all phase interfaces. Obtaining a solution from this formulation is impossible in practice. However, it can be used as a starting point for derivation of macroscopic equations which replace the local instant description of each phase by a collective description of the phases. The first equation systems for multiphase flows were based on intuition and postulation of balance equations. Today the equations are based on mathematically formulated averaging methods.

Depending on the basic physical concepts used to formulate the multiphase flow, averaging procedures can be classified into three main groups (Ishii 1975), namely the Eulerian averaging, the Lagrangian averaging and the Boltzmann averaging. These groups can be further divided into sub-groups based on the variable with which a mathematical operator or averaging is defined, e.g., into spatial, time, statistical and ensemble averaging. Spatial averaging can be volume, area or line averaging and either local or macroscopic.

Like the kinetic gas theory, the kinetic theory of the gas-particle system can be treated on the basis of the Boltzmann equation of the distribution function for a single particle (Ahmadi & Ma 1990, Ding & Gidaspow 1990). A molecular distribution function for the gas and another distribution function for the particles are defined. The theory of gas-particle systems contains several complications, i.e., the size distribution, other physical properties of the solid particles, and the collision processes of the solid particles with each other and with the gas molecules are difficult to account for. From this approach, it is possible to derive the continuity equation, the momentum equation and the equation for the fluctuating kinetic energy of the solid phase. Constitutive equations for the stress term and the energy flux term are obtained in a straightforward way. The equation of the fluctuating kinetic energy is sometimes called pseudothermal energy balance and the fluctuating kinetic energy (multiplied by 2/3) the granular temperature.

The Lagrangian approach treats the fluid phase as a continuum and the time average is taken by following a certain solid particle and observing it at some time interval. Particle trajectories are calculated from the equation of particle motion. Lagrangian averages are popular especially in modelling the dynamics of a single particle or a dilute suspension. The method has been extended to more dense flows (Yonemura et al. 1993). Then each computational particle represents a group of real particles and the particles are allowed to collide by a Monte Carlo procedure.

In the Eulerian approach, the particle phase also is treated as a continuum. The Eulerian formulation consists of three essential parts: the derivation of field equations, constitutive equations and interfacial conditions. The field equations state the conservation principles for, e.g., the momentum and mass. The constitutive equations close the equation system by taking into account the structure of the flow field and material properties by experimental correlations. The Eulerian averaging uses spatial, statistical or time averages taken in the spatial coordinate system. The Eulerian approach has been, at least in the past, the most widely used group of averaging for multiphase flows, because of its close relation to measuring techniques.

An alternative method is applied in the classical mixture theory (Bowen 1976, Johnson et al. 1991, Joseph et al. 1990). In this approach the principles of continuum mechanics for a single phase are generalised to several interpenetrable continua. The basic assumption is that, at any instant of time, all phases are present at every material point. The equations of balance are postulated for mass and momentum conservation. Like other models, mixture theory requires constitutive relations to close the system of equations.

A large selection of software is available for multiphase flows. Models for multiphase flow have been implemented in the general purpose commercial codes for computational fluid dynamics. In addition, a number of computer codes for specific multiphase flows has been developed. Typical fields where multiphase models have been developed are the safety analysis of nuclear power plants and the fluidised bed technology. For some phenomena like clustering and bubble formation in fluidised beds, qualitatively reasonable behaviour has been obtained with both Eulerian (Tsuo & Gidaspow 1990), Lagrangian (Tsuji et al. 1993) and Boltzmannian methods (Ding & Gidaspow 1990). The results of full scale simulations have been less promising. By fitting the parameters in the closure relations to a specific process, quantitatively satisfying results have been obtained, however.

2.2 BASIC EQUATIONS

The averaged equations of multiphase flow can be written in numerous ways. Equations can be derived by time averaging, space averaging, ensemble averaging or by any combination of these. In all the methods, the resulting equations contain basically the same terms. Deviations from average velocities are described by pseudo-turbulent momentum transfer terms corresponding to the turbulent terms in the single phase momentum equations. Modelling of the turbulent terms is an essential part of the equation closure. In addition, a model for the collective momentum transfer between the phases has to be given.

The field equations are given below in a general form. These equations are used later in this report as the basis for deriving the mixture model equations. We restrict our analysis on the mechanics of the multiphase system. Therefore, we do not consider any thermodynamic relations.

Two different definitions of the average velocity are commonly used in deriving the equations for multiphase flow. If we denote the local instant velocity of phase k by $\mathbf{u}_{Ik}$, the average velocity can be defined as $\mathbf{u}_k = \overline{\mathbf{u}}_{Ik}$, where the overbar indicates an average inside some averaging domain (volume, time-step, a set of experiments, a group of particles). The alternative definition of the average velocity is based on weighting the velocity with the local density ρ_{Ik}

$$\mathbf{u}_k = \frac{\overline{\rho_{Ik}\mathbf{u}_{Ik}}}{\overline{\rho_{Ik}}} = \frac{\overline{\rho_{Ik}\mathbf{u}_{Ik}}}{\rho_k} \tag{1}$$

where ρ_k is the average material density. This mass-weighted averaging (Favre averaging, see Ishii 1975) yields a simple form for the continuity equation. Throughout this report, $\mathbf{u}_k$ denotes the Favre-averaged velocity.

The Favre-averaged balance equations have been presented by several authors (e.g., Ishii 1975, Ishii & Mishima 1984, Ahmadi & Ma 1990, Hwang 1989, Gidaspow 1994). We follow the notations of Ishii (1975) and write the continuity and momentum equations for each phase k as follows

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \mathit{\Gamma}_k \tag{2}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\alpha_k \rho_k \mathbf{u}_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k) = -\alpha_k \nabla p_k + \nabla \cdot \left[\alpha_k (\boldsymbol{\tau}_k + \boldsymbol{\tau}_{Tk})\right] \\ + \alpha_k \rho_k \mathbf{g} + \mathbf{M}_k\end{aligned} \tag{3}$$

where α_k is the volume fraction of phase k. The term $\mathit{\Gamma}_k$ represents the rate of mass generation of phase k at the interface and $\mathbf{M}_k$ is the average interfacial momentum source for phase k. In (3), $\boldsymbol{\tau}_k$ is the average viscous stress tensor. The turbulent stress tensor $\boldsymbol{\tau}_{Tk}$ is given by

$$\boldsymbol{\tau}_{Tk} = -\overline{\rho_{Ik}\mathbf{u}_{Fk}\mathbf{u}_{Fk}} \tag{4}$$

where $\mathbf{u}_{Fk}$ is the fluctuating component of the velocity, i.e. $\mathbf{u}_{Fk} = \mathbf{u}_{Ik} - \mathbf{u}_k$.

Equation (2) does not contain a term describing the turbulent diffusion due to concentration gradients. This is a consequence of the mass-weighted averaging, which removes all fluctuation correlations of the type $\overline{\rho_{Ik}\mathbf{u}_{Fk}}$. In this case, all turbulent terms appear in the momentum equations. In equations based on other averaging methods, corresponding terms are obtained also in the continuity equations. Soo (1990) employs volume averaging without mass-weighting. He obtains a fluctuating term in the dispersed phase continuity equation and writes it in the following form

$$\frac{\partial}{\partial t}\left(\alpha_k\rho_k\right) + \nabla\cdot\left(\alpha_k\rho_k\overline{\mathbf{u}}_{Ik}\right) = \Gamma_k + \nabla\cdot\left(D_{Tk}\rho_k\nabla\alpha_k\right) \tag{5}$$

Here D_{Tk} is a turbulent diffusion coefficient and the following constitutive equation is used

$$D_{Tk}\rho_k\nabla\alpha_k = \alpha_k\,\overline{\rho_{Ik}\mathbf{u}_{Fk}} \tag{6}$$

In Soo's (1990) formulation the turbulent stress term in the momentum equation becomes more complicated. We have

$$\tau_{Tk} = -\overline{\rho_{Ik}\mathbf{u}_{Fk}\mathbf{u}_{Fk}} - 2\overline{\rho_{Ik}\mathbf{u}_{Fk}}\;\overline{\mathbf{u}_{Ik}} \tag{7}$$

In addition, the diffusion term in the continuity equation appears also in the time rate of change term of the momentum equation. We will return to this matter in Section 3.2.2.

Equations (2) and (3) above look conveniently simple. Before they can be solved, constitutive equations for the average stress terms, turbulent stress and the interaction forces between phases have to be formulated, however. The type of the constitutive relations depends on the averaging approach used. The existence of several types of multiphase flows makes derivation of constitutive relations very complex. Various simplifications and assumptions are therefore made. In practice, multiphase modelling commonly employs single-phase closure relations extended to multiphase situations.

A common simplification in multiphase calculations is that the dispersed phase is assumed to consist of spherical particles of a single, average particle size. The interactions between different dispersed phases are frequently neglected. Moreover, simplified assumptions are used at the walls.

For turbulence, one-phase turbulence models are often employed, usually slightly modified and with specially chosen parameter values for each problem. Two-equation $k-\varepsilon$ turbulence models for two phase flows have been suggested (Elghobashi & Abou-Arab 1983, Mostafa & Mongia 1988, Adeniji-Fashola & Chen 1990, Tu & Fletcher 1994). However, these models are case-specific and the generalisation of the models requires more experimental data. The effect of particles on the continuous phase turbulence is not well known; it is non-isotropic and hence difficult to account for. In practice it is often neglected.

Some approaches yield Eq. (3) in a slightly different form for a dispersed solid phase. The solid stress is divided into a compressive normal stress, the so-called solid pressure and a shear stress. Hence, a solid pressure term is added to Eq. (3). The effect of the shear stress is commonly described by the effective viscosity, which can either be constant or vary as a function of time and position. Sometimes in dense suspensions, the shear stress term has been neglected and only the solid pressure is included. The kinetic theory of granular flow yields stress terms of a similar form in a more natural way: the forces in the solid phase caused by the fluctuating velocity components are divided in the normal forces expressed by means of a solid pressure and a bulk viscosity, and the tangential forces expressed by means of a shear viscosity.

For the interaction force between the phases, the three commonly used empirical correlations are based on the single particle drag force, the packed-bed pressure drop (Ergun 1952) and the bed expansion of a liquid-solid fluidised bed (Richardson & Zaki 1954).

No model generally valid for all possible multiphase situations exists. Due to the complexity of multiphase flows, there is little hope that very general models can ever be developed. Hence, a large portion of the work in the derivation of closure relations is based on empirical information. In many cases, little data are available to extend an existing data base to new situations. Prediction of new or hypothetical situations is therefore difficult (Ishii & Mishima 1984).

Often the limited computer resources restrict the possibilities of using fine computational meshes and full equation systems. Simplified forms of the interphase forces are often applied. In addition, the users of commercial codes have difficulties in implementing their own closure relations. In the models available in commercial codes, often severe limiting assumptions have been made. A typical assumption is that the particles are distributed in a fairly homogeneous way inside the local averaging domain corresponding to the control volumes of the calculations. Especially for gas-solid flows, this assumption is seldom valid in simulations of large industrial processes.

3 MATHEMATICAL FORMULATION OF THE MIXTURE MODEL

3.1 FIELD EQUATIONS

Consider a mixture with *n* phases. We assume that one of the phases is a continuous fluid (liquid or gas) indicated with a subscript of *c*. The dispersed phases can comprise of particles, bubbles or droplets. The dynamics of the system is thus comprehensively described with Eqs. (2) and (3) together with the appropriate constitutive equations.

The mixture model is an alternative formulation of the problem. In this approach both the continuity equation and the momentum equation are written for the mixture of the continuous and dispersed phases. In addition, particle concentrations are solved from continuity equations for each dispersed phase. The momentum equations for the dispersed phases are approximated by algebraic equations.

The mixture model equations are derived in the literature applying various approaches (Ishii 1975, Ungarish 1993, Gidaspow 1994). The form of the equations also varies depending on the application. In this section we derive the general equations of the mixture model starting from the equations for individual phases. Ishii (1975) derives the mixture equations from a general balance equation.

3.1.1 Continuity equation for the mixture

From the continuity equation (2) for phase *k*, we obtain by summing over all phases

$$\frac{\partial}{\partial t}\sum_{k=1}^{n}\left(\alpha_k\rho_k\right)+\nabla\cdot\sum_{k=1}^{n}\left(\alpha_k\rho_k\mathbf{u}_k\right)=\sum_{k=1}^{n}\mathit{\Gamma}_k \tag{8}$$

Because the total mass is conserved, the right hand side of Eq. (8) must vanish,

$$\sum_{k=1}^{n}\Gamma_k=0 \tag{9}$$

and we obtain the continuity equation of the mixture

$$\frac{\partial\rho_m}{\partial t}+\nabla\cdot\left(\rho_m\mathbf{u}_m\right)=0 \tag{10}$$

Here the mixture density and the mixture velocity are defined as

$$\rho_m = \sum_{k=1}^{n} \alpha_k \rho_k \tag{11}$$

$$\mathbf{u}_m = \frac{1}{\rho_m} \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k = \sum_{k=1}^{n} c_k \mathbf{u}_k \tag{12}$$

The mixture velocity $\mathbf{u}_m$ represents the velocity of the mass centre. Note that ρ_m varies although the component densities are constants. The mass fraction of phase k is defined as

$$c_k = \frac{\alpha_k \rho_k}{\rho_m} \tag{13}$$

Equation (10) has the same form as the continuity equation for single phase flow. If the density of each phase is a constant and the interphase mass transfer is excluded, the continuity equation for the mixture is

$$\nabla \cdot \sum_{k=1}^{n} \alpha_k \mathbf{u}_k = \nabla \cdot \sum_{k=1}^{n} \mathbf{j}_k = \nabla \cdot \mathbf{j}_m = 0 \tag{14}$$

Here we have defined the volumetric flux of phase k, $\mathbf{j}_k = \alpha_k \mathbf{u}_k$, and the volumetric flux of the mixture $\mathbf{j}_m = \Sigma\, \mathbf{j}_k$. The volumetric flux represents the velocity of the volume centre.

3.1.2 Momentum equation for the mixture

The momentum equation for the mixture follows from (3) by summing over the phases

$$\begin{aligned} &\frac{\partial}{\partial t} \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k + \nabla \cdot \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k \\ &= -\sum_{k=1}^{n} \alpha_k \nabla p_k + \nabla \cdot \sum_{k=1}^{n} \alpha_k \left(\boldsymbol{\tau}_k + \boldsymbol{\tau}_{Tk} \right) + \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{g} + \sum_{k=1}^{n} \mathbf{M}_k \end{aligned} \tag{15}$$

Using the definitions (11) and (12) of the mixture density ρ_m and the mixture velocity $\mathbf{u}_m$, the second term of (15) can be rewritten as

$$\nabla \cdot \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_k \mathbf{u}_k = \nabla \cdot \left(\rho_m \mathbf{u}_m \mathbf{u}_m \right) + \nabla \cdot \sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_{Mk} \mathbf{u}_{Mk} \tag{16}$$

where $\mathbf{u}_{Mk}$ is the diffusion velocity, i.e., the velocity of phase k relative to the centre of the mixture mass

$$\mathbf{u}_{Mk} = \mathbf{u}_k - \mathbf{u}_m \tag{17}$$

In terms of the mixture variables, the momentum equation takes the form

$$\begin{aligned} \frac{\partial}{\partial t}\rho_m \mathbf{u}_m + \nabla \cdot \left(\rho_m \mathbf{u}_m \mathbf{u}_m\right) = -\nabla p_m + \nabla \cdot \left(\boldsymbol{\tau}_m + \boldsymbol{\tau}_{Tm}\right) + \nabla \cdot \boldsymbol{\tau}_{Dm} \\ + \rho_m \mathbf{g} + \mathbf{M}_m \end{aligned} \tag{18}$$

The three stress tensors are defined as

$$\boldsymbol{\tau}_m = \sum_{k=1}^{n} \alpha_k \boldsymbol{\tau}_k \tag{19}$$

$$\boldsymbol{\tau}_{Tm} = -\sum_{k=1}^{n} \alpha_k \overline{\rho_{Ik} \mathbf{u}_{Fk} \mathbf{u}_{Fk}} \tag{20}$$

$$\boldsymbol{\tau}_{Dm} = -\sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_{Mk} \mathbf{u}_{Mk} \tag{21}$$

and represent the average viscous stress, turbulent stress and diffusion stress due to the phase slip, respectively. In Eq. (18), the pressure of the mixture is defined by the relation

$$\nabla p_m = \sum_{k=1}^{n} \alpha_k \nabla p_k \tag{22}$$

In practice, the phase pressures are often taken to be equal, i.e., $p_k = p_m$. This assumption is considered to be valid except in the case of expanding bubbles (Drew 1983).

The last term on the right hand side of (18) is the influence of the surface tension force on the mixture and is defined as

$$\mathbf{M}_m = \sum_{k=1}^{n} \mathbf{M}_k \tag{23}$$

The term $\mathbf{M}_m$ depends on the geometry of the interface. The other additional term in (18) compared to the one-phase equation (3) is the diffusion stress term $\nabla \cdot \boldsymbol{\tau}_{Dm}$ representing the momentum diffusion due to the relative motions.

Verloop (1995) has recently discussed the validity of the mixture model and derived the diffusion stress in Eq. (16) in a different way. Verloop argued that the mixture model is inaccurate if that term is missing. In the present derivation, the second term results from summing of the phase equations and is an essential part in the model.

3.1.3 Continuity equation for a phase

We return to consider an individual phase. Use of the definition of the diffusion velocity (17) to eliminate the phase velocity in the continuity equation (2) gives

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_m) = \mathit{\Gamma}_k - \nabla \cdot (\alpha_k \rho_k \mathbf{u}_{Mk}) \tag{24}$$

If the phase densities are constants and phase changes do not occur, the continuity equation reduces to

$$\frac{\partial}{\partial t}\alpha_k + \nabla \cdot (\alpha_k \mathbf{u}_m) = -\nabla \cdot (\alpha_k \mathbf{u}_{Mk}) \tag{25}$$

Some authors refer to (25) as the diffusion equation (e.g. Ungarish 1993). Accordingly, the mixture model is often called the diffusion model.

In practice, the diffusion velocity has to be determined through the relative (slip) velocity which is defined as the velocity of the dispersed phase relative to the velocity of the continuous phase, i.e.,

$$\mathbf{u}_{Ck} = \mathbf{u}_k - \mathbf{u}_c \tag{26}$$

The diffusion velocity of a dispersed phase *l*, $\mathbf{u}_{Ml} = \mathbf{u}_l - \mathbf{u}_m$, can be presented in terms of the relative velocities

$$\mathbf{u}_{Ml} = \mathbf{u}_{Cl} - \sum_{k=1}^{n} c_k \mathbf{u}_{Ck} \tag{27}$$

If only one dispersed phase *p* is present, its diffusion velocity is given by

$$\mathbf{u}_{Mp} = (1 - c_p)\mathbf{u}_{Cp} \tag{28}$$

An alternative formulation of the phase continuity equation

If the phase densities are constants and the interphase mass transfer can be neglected, the phase continuity equation (2) can be written by means of the volumetric flux $\mathbf{j}_k$

$$\frac{\partial \alpha_k}{\partial t} + \nabla \cdot \mathbf{j}_k = 0 \tag{29}$$

We will next introduce the drift velocity, $\mathbf{u}_{Vk}$, defined as the velocity of a dispersed phase relative to that of the volume centre of a mixture, namely,

$$\mathbf{u}_{Vk} = \mathbf{u}_k - \mathbf{j}_m \tag{30}$$

It follows from (30) and from the definition of $\mathbf{j}_m$ (14) that

$$\sum_{k=1}^{n} \alpha_k \mathbf{u}_{Vk} = 0 \tag{31}$$

Using the definition of the drift velocity, one obtains for the continuity of a phase

$$\frac{\partial}{\partial t}\alpha_k + \mathbf{j}_m \cdot \nabla \alpha_k = -\nabla \cdot \left(\alpha_k \mathbf{u}_{Vk} \right) \tag{32}$$

where the relation $\nabla \cdot \mathbf{j}_m = 0$ was applied. Often this formula of the phase continuity equation is employed in modelling and consequently the approach is called the drift-flux model.

As the diffusion velocity, the drift velocity can be determined from the relative velocity

$$\mathbf{u}_{Vl} = \mathbf{u}_{Cl} - \sum_{k=1}^{n} \alpha_k \mathbf{u}_{Ck} \tag{33}$$

If only one dispersed phase p is present, its drift velocity is

$$\mathbf{u}_{Vp} = \left(1 - \alpha_p \right) \mathbf{u}_{Cp} \tag{34}$$

In this case, the continuity equation (32) can be rewritten as

$$\frac{\partial}{\partial t}\alpha_p + \mathbf{j}_m \cdot \nabla\alpha_p = -\alpha_p\left(1-\alpha_p\right)\nabla\cdot\mathbf{u}_{Cp} - \left(1-2\alpha_p\right)\mathbf{u}_{Cp}\cdot\nabla\alpha_p \qquad (35)$$

This formulation shows that if α_p is equal to a constant, $\nabla\cdot\mathbf{u}_{Cp}=0$. Moreover, if α_p varies only as a function of time but not in space, $\nabla\cdot\mathbf{u}_{Cp}$ also depends only on time. The possibility of applying the same relative velocities throughout the modelling domain would simplify flow calculations (Ungarish 1993).

The momentum equation of the mixture (18) and the relations required to close the field equations can also be formulated by means of the drift velocity (or relative velocity). In fact, by using the drift velocity, some of the constitutive equations can be expressed in a simpler form (see Section 3.4). This is why relations for the drift velocity in various flow regimes have been examined carefully (e.g. Ishii & Zuber 1979). Those relations are nevertheless based on the determination of the relative velocity.

It is worthwhile to note that so far in formulating the mixture model equations from the full multiphase model we have not made any further assumptions. The field equations for the mixture (10) and (18) as well as the continuity equation for phase *k* in terms of the mixture velocity were obtained from the original phase equations (2) and (3) by using solely algebraic manipulations. However, the closure of the field equations requires some assumptions as in full multiphase models. The most critical approximation of the mixture model will be made in replacing the phase momentum equations with algebraic equations for the diffusion velocity $\mathbf{u}_{Mk}$.

3.2 THE RELATIVE VELOCITY

Before solving the continuity equation (24) for phase *k* and the momentum equation for the mixture (18), the diffusion velocity $\mathbf{u}_{Mk}$ has to be determined. The diffusion velocity of a phase is usually caused by the density differences, resulting in forces on the particles different from those on the fluid. The additional force is balanced by the drag force. The physical reasoning for the balance equation is illustrated by a simple example. Consider the one-dimensional equation of motion of a particle in a fluid under gravitational field *g*

$$m_p\frac{du_{Cp}}{dt} = V_p\Delta\rho g - \frac{1}{2}\rho_c A_p C_D u_{Cp}^2 \qquad (36)$$

where $\Delta\rho$ is the density difference, V_p and A_p are the volume and the cross-sectional area of the particle and C_D is the drag coefficient. It is assumed that the drag force is determined only by viscous forces. If the particle mass m_p is small, the particle is accelerated to a terminal velocity in a short distance.

The velocity of the particle with respect to the fluid is thus obtained by equating the right hand side of (36) to zero. In the present analysis, our task is to make the same ”local equilibrium” approximation in the momentum equations for the dispersed phases. In the following analysis, we will consider one dispersed phase, denoted by a subscript *p*.

As indicated by (36), it is the relative velocity $\mathbf{u}_{Cp}$, which is obtained from the force balance equation, rather than the diffusion velocity directly. The latter is calculated from the identity (28). Note that $\mathbf{u}_{Cp}$ is often called the slip velocity (Johansen et al. 1990, Kocaefe et al. 1994, Pericleous & Drake 1986). In most published applications of the mixture model, considerations have been restricted to gravitational or/and centrifugal forces. A more general approach has been implemented in PHOENICS (see Section 5.1).

We begin the analysis by examining the instantaneous drag force on a particle in the suspension. Next, the force balance equation is derived using the dispersed phase momentum equation as the starting point. The validity of the various assumptions made in deriving the balance equation is considered in Section 3.3.

3.2.1 Drag force

The drag force represents the additional forces on a particle due to the velocity relative to the fluid. For a single rigid spherical particle in a fluid, the drag force $\mathbf{F}_D$ can be written as follows (Clift et al. 1978)

$$\begin{aligned}\mathbf{F}_D = -\frac{1}{2}A_p\rho_c C_D\left|\mathbf{u}_{Cp}\right|\mathbf{u}_{Cp} - \frac{1}{2}V_p\rho_c\frac{d\mathbf{u}_{Cp}}{dt}\\ -6r_p^2\sqrt{\pi\rho_c\mu_c}\int_0^t\frac{\frac{d\mathbf{u}_{Cp}}{ds}}{\sqrt{t-s}}ds\end{aligned} \tag{37}$$

The first term on the right hand side is the viscous drag. The second term is the ”virtual mass” and it is needed because the acceleration of the particle also requires acceleration of the surrounding fluid. The last term is the Basset history term, which includes the effect of past acceleration. Other forces such as the forces due to the rotation of the particle, the concentration gradient and the pressure gradient have been omitted in (37). Within our mixture model, we will also neglect the virtual mass and Basset

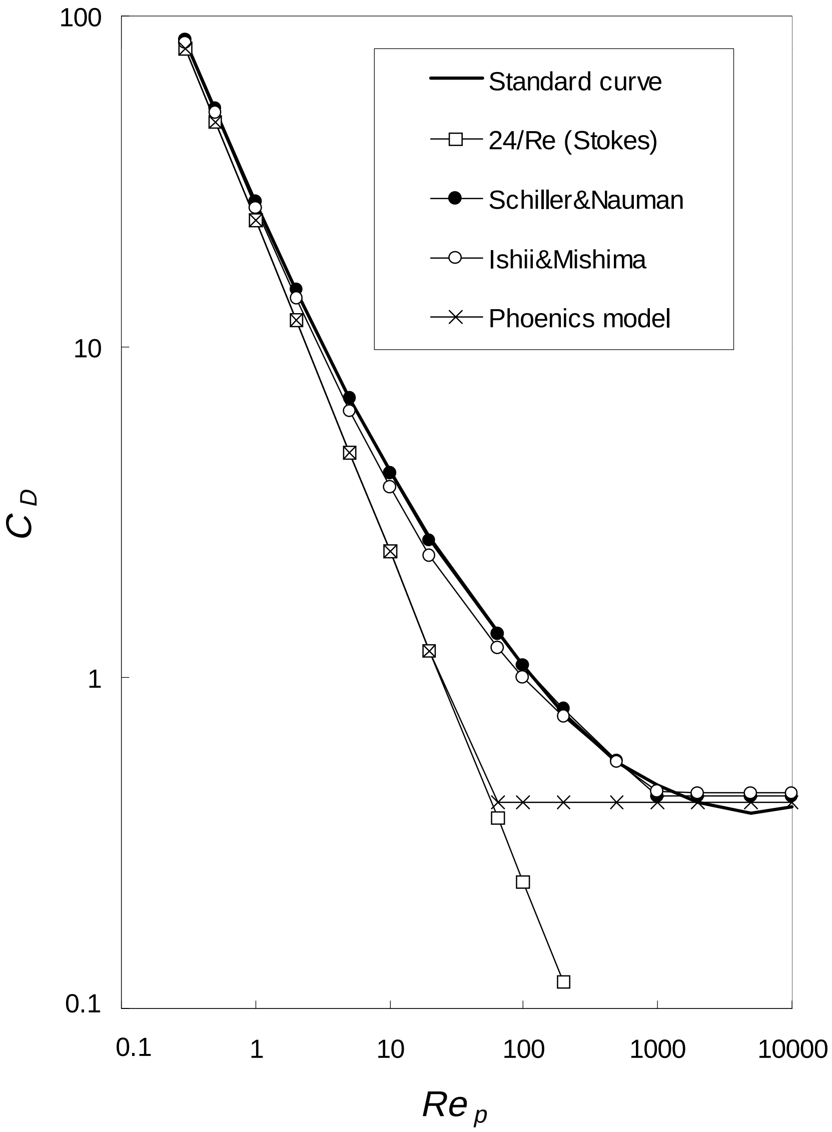

Fig. 1. The standard drag curve (Clift et al. 1978) and various simplified correlations in the low Reynolds number region (see text).

terms. This approximation is discussed further in Section 3.3. Above, $\mathbf{u}_{Cp}$ is the averaged relative velocity. In the averaging process, the fluctuating velocity components induce an additional term not shown in Eq. (37).

The drag coefficient C_D in (37) depends on various factors. At small particle Reynolds numbers, the total drag coefficient is given by Stokes's law (Clift et al. 1978)

$$C_{D,St} = \frac{24}{Re_p} \tag{38}$$

The particle Reynolds number, Re_p, is defined as follows

$$Re_p = \frac{d_p \rho_c \left| \mathbf{u}_{Cp} \right|}{\mu_c} \tag{39}$$

where d_p is the diameter of the particles. With an increasing particle Reynolds number, Stokes's law underestimates the drag. The standard drag curve in Fig. 1 shows the dependence of the drag on Re_p.

An often used expression for the drag coefficient is due to Schiller & Nauman (see Clift et al. 1978)

$$\begin{aligned} C_D &= \frac{24}{Re_p}\left(1 + 0.15 Re_p^{0.687}\right) && Re_p < 1000 \\ &= 0.44 && Re_p > 1000 \end{aligned} \tag{40}$$

The freestream turbulence modifies the flow field around a particle and thus has an influence on the drag. If the particle is small compared to the scale of the velocity variations and possesses a low particle Reynolds number, it follows the motion of the fluid. A rough but useful guide is given by Clift et al. (1978): A particle follows the fluid motion if its relaxation time t_p is small compared with the period of oscillation. In the Stokes regime, this condition can be written as

$$t_p = \frac{\rho_p d_p^2}{18 \mu_m} << \frac{1}{\omega} \tag{41}$$

where ω is the angular frequency of turbulence. Equation (41) applies unless ρ_p / ρ_c is close to unity. If the particle Reynolds number is well above the range for Stokes's flow, freestream turbulence may increase or decrease the mean drag. Clift et al. (1978) discuss this topic in more detail and give correlations for the effect of the freestream turbulence.

Above one particle in a fluid was considered. In a suspension, the influence of the distortion of the flow field caused by the presence of other particles has to be taken into account. With an increasing particle concentration, a particle feels an increase in the flow resistance which in turn leads to a higher drag coefficient. One way to take this into account is to modify the viscosity (Ishii & Zuber 1979, Hallanger et al. 1995). In this model the viscosity of the continuous phase in expressions for the drag coefficient should be replaced by the apparent viscosity of the mixture μ_m. According to Ishii & Mishima (1984), this concept is appropriate for low Reynolds numbers. Their formula for the drag coefficient of solid particles is

$$
\begin{aligned}
C_D &= \frac{24}{Re_p}\left(1+0.1Re_p^{0.75}\right) && Re_p < 1000 \\
&= 0.45\left\{\frac{1+17.67\left[f(\alpha_p)\right]^{6/7}}{18.67\,f(\alpha_p)}\right\} && Re_p > 1000 \\
f(\alpha_p) &= \sqrt{1-\alpha_p}\left(\frac{\mu_c}{\mu_m}\right) \\
Re_p &= \frac{d_p\left|\mathbf{u}_{Cp}\right|\rho_c}{\mu_m}
\end{aligned}
\tag{42}
$$

According to Ishii & Mishima (1984), a satisfactory agreement with the experimental data has been obtained at wide ranges of the concentration and Reynolds number. The data studied for solid-particle systems cover the concentration range of 0 - 0.55 but the authors do not show quantitative comparisons to experimental results.

The approach and results presented above also apply for fluid particles in the viscous regime $Re_p < 1000$. Other fluid regimes have to be considered differently. Ishii & Mishima (1984) also give the drag coefficient for the distorted particle, churn-turbulent and slug flow regimes.

In mixture model applications, the most often used correlation for the apparent viscosity of the mixture is that according to Ishii & Zuber (1979); see also Ishii & Mishima (1984) for a summary of the results. The general expression for the mixture viscosity, valid for solid particles as well as bubbles or drops, is given by

$$
\mu_m = \mu_c\left(1-\frac{\alpha_p}{\alpha_{pm}}\right)^{-2.5\alpha_{pm}\mu^*}
\tag{43}
$$

where α_{pm} is a concentration for maximum packing. For solid particles $\alpha_{pm} \approx 0.62$. In Eq. (43), $\mu^* = 1$ for solid particles and

$$
\mu^* = \frac{\mu_p + 0.4\mu_c}{\mu_p + \mu_c}
\tag{44}
$$

for bubbles or drops.

Numerous other correlations for the viscosity of solid suspensions are presented in the literature. Rutgers (1962a) compiled experimental data on the apparent viscosity of a suspension of spherical solid particles and

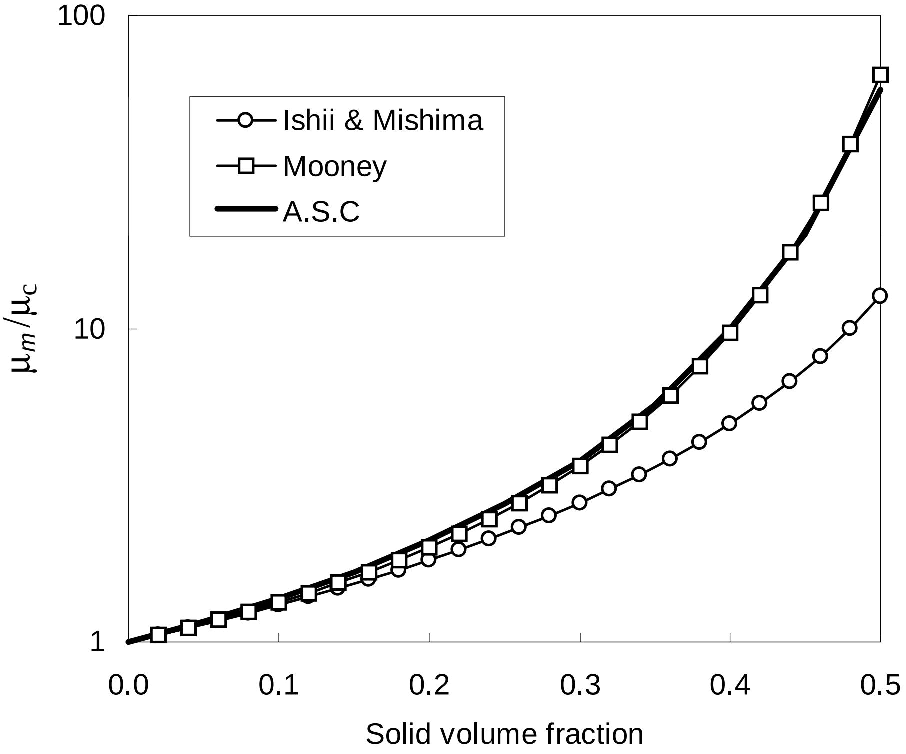

Fig. 2. Relative viscosity of a suspension of solid particles according to the "Average Sphere Curve" (Rutgers 1962a) and correlations due to Ishii & Mishima (1984) and Mooney (cf. Rutgers 1962b).

deduced, as a result, an "average sphere concentration curve". In a subsequent paper, Rutgers (1962b) presented a review of various empirical formulas for the relative viscosity. One of the correlations with a theoretical foundation is due to Mooney (cited in Rutgers 1962b)

$$\ln\left(\frac{\mu_m}{\mu_c}\right)=\frac{2.5\alpha_p}{1-1.4\alpha_p} \tag{45}$$

The correlations (43) and (45) together with the "average sphere curve" are shown in Fig. 2. It should be noted that the apparent viscosity of the suspension is not a well defined property of the mixture, but depends on many factors, including the method of measurement. However, it turns out that, at reasonably low concentrations, it can be correlated in a simple way to the concentration.

The drag induced momentum transfer term can be written in the form

$$\mathbf{M}_p=-\beta\mathbf{u}_{Cp}+\mathbf{M}'_p \tag{46}$$

where $\mathbf{M}'_p$ is a term caused by the velocity fluctuations (Simonin 1990). The drag function β depends on the particle Reynolds number, solid concentration and particle size.

In the model of Ishii & Mishima (1984) discussed above, β has the form

$$\beta = \frac{3}{4} C_D \frac{\alpha_p \rho_c \left|\mathbf{u}_{Cp}\right|}{d_p} \tag{47}$$

where C_D is determined by Eqs. (42) and (43).

Syamlal & O'Brien (1988) used for β and C_D expressions derived from measurements in fluidised and settling beds. Their model can be expressed with the following equations

$$\begin{aligned}
\beta &= \frac{3}{4} C_D \frac{\alpha_p \left(1-\alpha_p\right) \rho_c \left|\mathbf{u}_{Cp}\right|}{d_p U_r^2} \\
C_D &= \left[0.63 + 4.8 \sqrt{\frac{U_r}{\mathrm{Re}_p}}\right]^2 \\
U_r &= \frac{1}{2}\left[A - 0.06 Re_p + \sqrt{\left(A - 0.06 Re_p\right)^2 + 0.24 B Re_p}\right] \\
A &= \alpha_c^{4.14} \\
B &= 0.8 \alpha_c^{1.28} \qquad \alpha_p \geq 0.15 \\
&= \alpha_c^{2.65} \qquad \alpha_p < 0.15
\end{aligned} \tag{48}$$

Here U_r represents the ratio of the terminal velocity of a group of particles to that of a single particle (Garside & Al Dibouni 1977). The form of the drag coefficient in (48) is due to Dalla Valle (1948).

Ding & Gidaspow (1990) employ Ergun's equation (originally derived for packed beds) for dense suspensions and another expression for β (derived from measurements of liquid-solid flows) for dilute suspensions:

$$
\begin{aligned}
\beta &= 150\frac{\alpha_p^2\mu_c}{\alpha_c d_p^2} + 1.75\frac{\alpha_p\rho_c\left|\mathbf{u}_{Cp}\right|}{d_p} && \alpha_p > 0.2 \\
&= \frac{3}{4}C_D\alpha_c^{-2.65}\frac{\alpha_c\alpha_p\rho_c\left|\mathbf{u}_{Cp}\right|}{d_p} && \alpha_p \le 0.2 \\
C_D &= \frac{24}{\alpha_c Re_p}\left[1+0.15\left(\alpha_c \mathrm{Re}_p\right)^{0.687}\right] && \alpha_c Re_p < 1000 \\
&= 0.44 && \alpha_c Re_p \ge 1000
\end{aligned}
\tag{49}
$$

In (48) and (49) the apparent relative velocity $\alpha_c|\mathbf{u}_{Cp}|$ is used in the expression of β and for the model of Ding & Gidaspow also in the expression for C_D. The drag function for the three models is plotted in Fig. 3 as a function of α_p for two particle diameters and slip velocities, normalised with the single-particle drag function calculated using Eq. (40).

These drag correlations are mostly based on measurements in homogeneous liquid-solid suspensions. In dense gas-solid suspensions, particles tend to form clusters, which strongly affect the average drag forces (O'Brien & Syamlal 1993).

3.2.2 Force balance equation

The balance equation for calculating the relative velocity can be rigorously derived by combining the momentum equations for the dispersed phase and the mixture. Using the continuity equation (2), the momentum equation (3) of the dispersed phase *p* can be rewritten as follows

$$
\begin{aligned}
&\alpha_p\rho_p\frac{\partial \mathbf{u}_p}{\partial t} + \alpha_p\rho_p\left(\mathbf{u}_p\cdot\nabla\right)\mathbf{u}_p = \\
&-\alpha_p\nabla p_p + \nabla\cdot\left[\alpha_p\left(\boldsymbol{\tau}_p + \boldsymbol{\tau}_{Tp}\right)\right] + \alpha_p\rho_p\mathbf{g} + \mathbf{M}_p
\end{aligned}
\tag{50}
$$

The corresponding equation for the mixture is

$$
\rho_m\frac{\partial \mathbf{u}_m}{\partial t} + \rho_m\left(\mathbf{u}_m\cdot\nabla\right)\mathbf{u}_m = -\nabla p_m + \nabla\cdot\left(\boldsymbol{\tau}_m + \boldsymbol{\tau}_{Tm} + \boldsymbol{\tau}_{Dm}\right) + \rho_m\mathbf{g} \tag{51}
$$

Here we have assumed that the surface tension forces are negligible and consequently $\mathbf{M}_m = 0$.

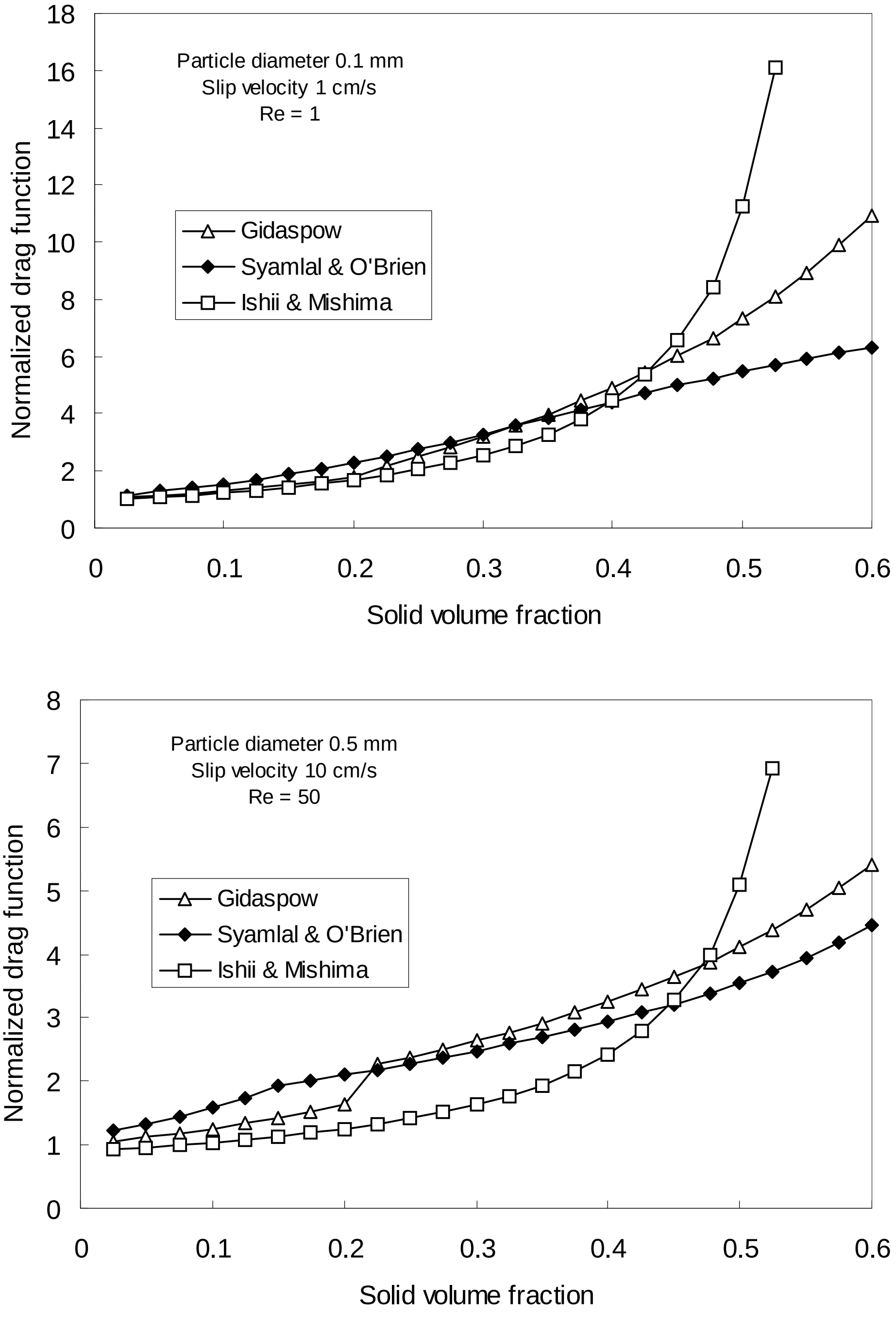

Fig. 3. Comparison of the drag models given in Eqs. (49) (Gidaspow), (48) (Syamlal & O'Brien), and (42), (43) and (47) (Ishii & Mishima). The drag function is normalised with the single-particle drag function calculated from Eqs. (40) and (47).

We make the assumption that the phase pressures are equal, i.e.,

$$p_p = p_m = p \tag{52}$$

and eliminate the pressure gradient from (50) and (51). As a result we obtain an equation for $\mathbf{M}_p$

$$\begin{aligned}\mathbf{M}_p = {} & \alpha_p\left[\rho_p \frac{\partial \mathbf{u}_{Mp}}{\partial t} + \left(\rho_p - \rho_m\right)\frac{\partial \mathbf{u}_m}{\partial t}\right] \\ & + \alpha_p\left[\rho_p\left(\mathbf{u}_p \cdot \nabla\right)\mathbf{u}_p - \rho_m\left(\mathbf{u}_m \cdot \nabla\right)\mathbf{u}_m\right] \\ & - \nabla \cdot \left[\alpha_p\left(\boldsymbol{\tau}_p + \boldsymbol{\tau}_{Tp}\right)\right] + \alpha_p \nabla \cdot \left(\boldsymbol{\tau}_m + \boldsymbol{\tau}_{Tm} + \boldsymbol{\tau}_{Dm}\right) - \alpha_p\left(\rho_p - \rho_m\right)\mathbf{g}\end{aligned} \tag{53}$$

In (53) we have utilised the definition (17) of the diffusion velocity $\mathbf{u}_{Mp}$.

Next we will make several approximations to simplify Eq. (53). Using the local equilibrium approximation, we drop from the first term the time derivative of $\mathbf{u}_{Mp}$. In the second term, we approximate

$$\left(\mathbf{u}_p \cdot \nabla\right)\mathbf{u}_p \approx (\mathbf{u}_m \cdot \nabla)\mathbf{u}_m \tag{54}$$

The viscous and diffusion stresses are omitted as small compared to the leading terms. The turbulent stress cannot be neglected if we wish to keep the turbulent diffusion of the dispersed phase in the model. In the Favre averaged equations, all turbulent effects are included in the stress terms of the momentum equation, as discussed in Section 2.2. Combining the terms involving $\boldsymbol{\tau}_{Tm}$ and $\boldsymbol{\tau}_{Tp}$ on the right hand side of (53), we obtain

$$-\nabla \cdot \left(\alpha_p \boldsymbol{\tau}_{Tp}\right) + \alpha_p \nabla \cdot \boldsymbol{\tau}_{Tm} = \alpha_p \nabla \cdot \left(\alpha_c \boldsymbol{\tau}_{Tc}\right) - \alpha_c \nabla \cdot \left(\alpha_p \boldsymbol{\tau}_{Tp}\right) \tag{55}$$

In a dilute suspension of small particles that follow the turbulent fluctuations of the fluid, the sum above becomes roughly equal to $\nabla \cdot \left(\alpha_c \boldsymbol{\tau}_{Tc}\right)$.

Neglecting in $\mathbf{F}_D$ all other effects except the viscous drag and using Eqs. (46) and (47) for $\mathbf{M}_p$ and β, we obtain the final simplified equilibrium equation for the relative velocity

$$\begin{aligned}\frac{1}{2}\rho_c A_p C_D \left|\mathbf{u}_{Cp}\right| \mathbf{u}_{Cp} = {} & V_p(\rho_p - \rho_m)\left[\mathbf{g} - \left(\mathbf{u}_m \cdot \nabla\right)\mathbf{u}_m - \frac{\partial \mathbf{u}_m}{\partial t}\right] \\ & - \frac{V_p}{\alpha_p}\left[\alpha_p \nabla \cdot \left(\alpha_c \boldsymbol{\tau}_{Tc}\right) - \alpha_c \nabla \cdot \left(\alpha_p \boldsymbol{\tau}_{Tp}\right)\right] + \mathbf{M}'_p\end{aligned} \tag{56}$$

where the drag coefficient C_D is a function of $\left|\mathbf{u}_{Cp}\right|$. In practice, a constitutive equation is required for the fluctuation terms. To accomplish this, we postulate the following solution for Eq. (56) (cf. Ishii 1975, Simonin 1990)

$$\mathbf{u}_{Cp} = \mathbf{u}_{Cp0} + \frac{D_{Cp}}{\alpha_p}\nabla\alpha_p \tag{57}$$

Here $\mathbf{u}_{Cp0}$ is a solution of (56) without the fluctuation terms, i.e.,

$$\frac{1}{2}\rho_c A_p C_D \left|\mathbf{u}_{Cp0}\right| \mathbf{u}_{Cp0} = V_p\left(\rho_p - \rho_m\right)\left[\mathbf{g} - \left(\mathbf{u}_m \cdot \nabla\right)\mathbf{u}_m - \frac{\partial \mathbf{u}_m}{\partial t}\right] \tag{58}$$

Note that the appearance of the diffusion term due to turbulent fluctuations in (57) can be traced back to the averaging process. In the equations derived without mass-averaging, the diffusion term appears in the continuity equation (5). In a sense, the velocity $\mathbf{u}_{Cp0}$ can be interpreted as the velocity obtained with an averaging without mass-weighting.

Equations (57) and (58) are our final relations for determining the relative velocity. In rotational motion, $(\mathbf{u}_m \cdot \nabla)\mathbf{u}_m$ is equal to the centrifugal acceleration. An alternative form of Eq. (58) can be derived by making the approximation (54) at the outset and eliminating $(\mathbf{u}_m \cdot \nabla)\mathbf{u}_m$ instead of the pressure gradient:

$$\frac{1}{2}\rho_c A_p C_D \left|\mathbf{u}_{Cp0}\right| \mathbf{u}_{Cp0} = V_p \frac{\left(\rho_m - \rho_p\right)}{\rho_m}\nabla p \tag{59}$$

Note that p in (59) is the total pressure including the hydrostatic component determined by the mixture density.

The simplest case to apply the above results is the Stokesian flow of spherical particles in dilute suspension under gravitational and centrifugal force field. The Stokes formula for the drag force is

$$\mathbf{F}_D = 3\pi d_p \mu_c \mathbf{u}_{Cp0} \tag{60}$$

The relative velocity is given by

$$\mathbf{u}_{Cp0} = \frac{d_p^2\left(\rho_p - \rho_m\right)}{18\mu_c}\left[\mathbf{g} - \frac{u_{m\varphi}^2}{r}\mathbf{e}_r\right] \tag{61}$$

where $u_{m\varphi}$ is the tangential component of the mixture velocity and $\mathbf{e}_r$ is the radial unit vector.

3.3 VALIDITY OF THE MIXTURE MODEL

In arriving to Eqs. (56) and (59), we made a number of approximations, which will be analysed in detail in the following. The terms omitted in Eq. (53) can be rewritten in the following form

$$
\begin{aligned}
&\alpha_p\rho_p\left[\frac{\partial \mathbf{u}_{Mp}}{\partial t}+\left(\mathbf{u}_{Mp}\cdot\nabla\right)\mathbf{u}_{Mp}\right]\\
&+\alpha_p\rho_p\left[\left(\mathbf{u}_m\cdot\nabla\right)\mathbf{u}_{Mp}+\left(\mathbf{u}_{Mp}\cdot\nabla\right)\mathbf{u}_m\right]\\
&+\alpha_p\nabla\cdot\left(\tau_m+\tau_{Dm}\right)-\nabla\cdot\left(\alpha_p\tau_p\right)
\end{aligned}
\tag{62}
$$

The local equilibrium approximation requires that the particles are rapidly accelerated to the terminal velocity. This corresponds to setting the first term in (62) equal to zero. Consider first a constant body force, like gravitation. A criterion for neglecting the acceleration is related to the relaxation time of a particle, t_p, defined through the simplified equation (36). In the Stokes regime t_p is given by

$$t_p=\frac{\rho_p d_p^2}{18\mu_m},\qquad Re_p<1 \tag{63}$$

and in the Newton regime (constant C_D) by

$$t_p=\frac{2\rho_p d_p}{3\rho_c C_D u_t},\qquad Re_p>1000 \tag{64}$$

where u_t is the terminal velocity. Within the time t_p, a particle travels the distance $\ell_p=t_p u_t/e$, which characterises the length scale of the acceleration.

If the density ratio ρ_p/ρ_c is small the virtual mass and Basset terms in the equation of motion cannot be neglected. The Basset term in particular effectively increases the relaxation time. The length scale ℓ'_p is defined as the distance travelled by the particle, until its velocity is $u_t(1-e^{-1})\approx 0.63u_t$. The length scale ℓ'_p and the corresponding characteristic time t'_p are plotted in Fig. 4 as a function of ρ_p/ρ_c for the Stokes flow. A suitable requirement for the local equilibrium is thus $\ell'_p << L$, where L is a typical dimension of the system. Figure 5 shows ℓ'_p for two particle sizes in water.

The form of the Basset term is strictly valid only in the Stokes regime. Results for ℓ'_p / ℓ_p are shown in Clift et al. (1978) for higher Reynolds numbers.

If the mixture is in accelerating motion, the above condition is not sufficient. In that case the particle relaxation time has to be compared to a characteristic time scale of the flow field of the mixture, t_F (Johansen et al. 1990, Ungarish 1993). This time scale can be estimated from

$$t_F = \left| \frac{\mathbf{u}_m}{\partial \mathbf{u}_m / \partial t + (\mathbf{u}_m \cdot \nabla)\mathbf{u}_m} \right| \tag{65}$$

In pure rotational flow, the condition for the local equilibrium can be analysed in more detail. The radial equation of motion of the particles is, neglecting the virtual mass and Basset terms,

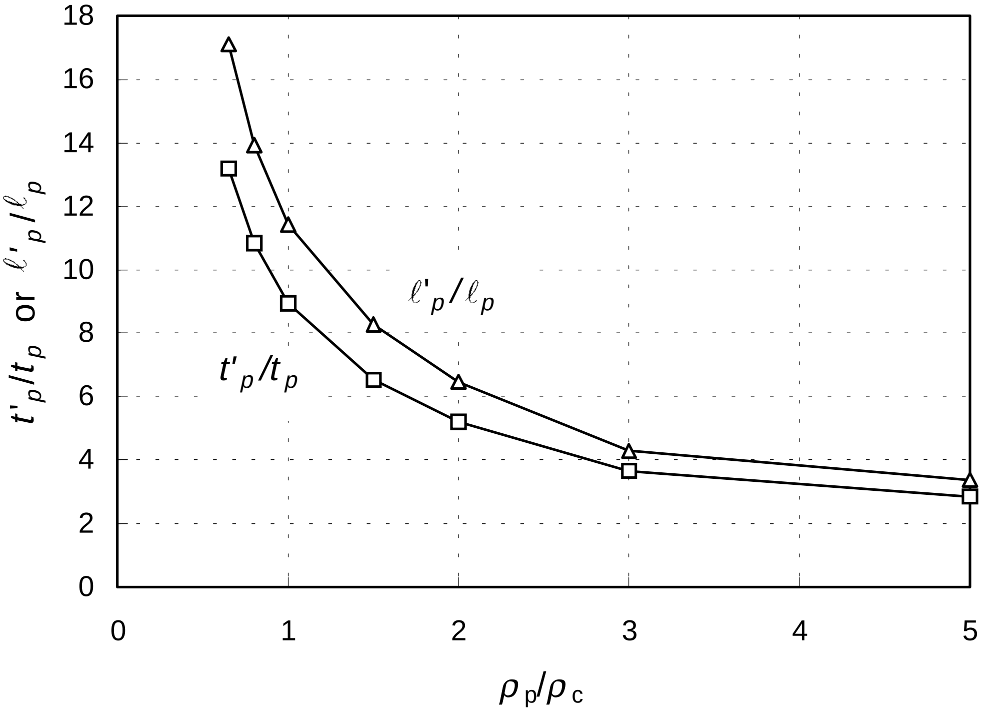

Fig. 4. The normalised characteristic time and length associated with the acceleration of a spherical particle as a function of the density ratio.

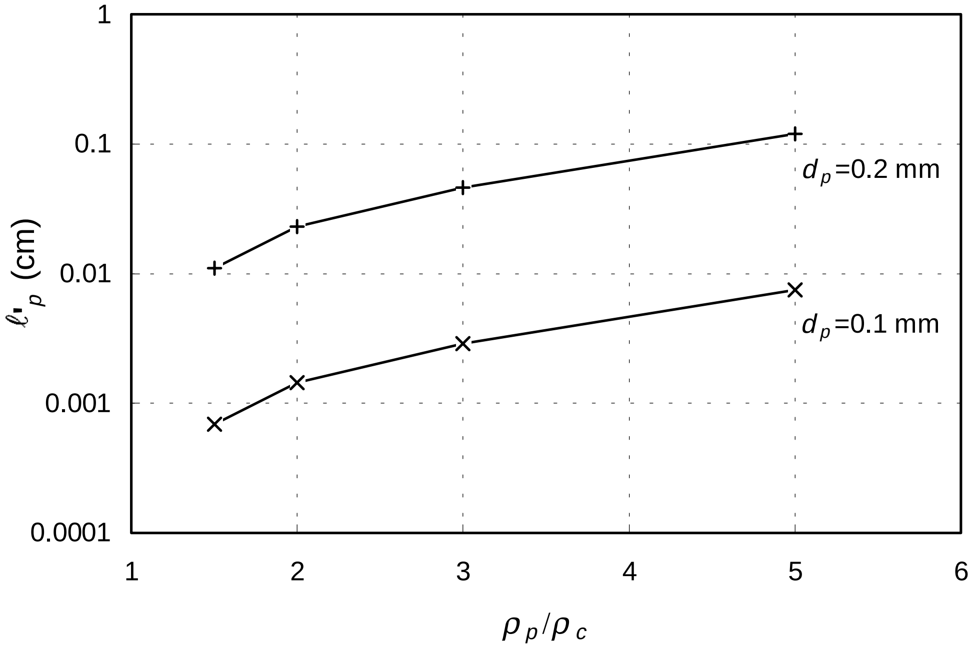

Fig. 5. The characteristic length scale of acceleration in water for two particles with different diameters as a function of the density ratio.

$$m_p u_{Cp} \frac{du_{Cp}}{dr} = \left(\rho_p - \rho_c\right) V_p \omega^2 r - \frac{1}{2} C_D A_p \rho_c u_{Cp}^2 \tag{66}$$

where ω is the angular velocity. Eq. (66) can be integrated if C_D is a constant. The solution for a spherical particle is

$$u_{Cp}^2 = Ce^{-r/\ell_p} + 2\frac{\left(\rho_p - \rho_c\right)}{\rho_p} \omega^2 \ell_p^2 \left(\frac{r}{\ell_p} - 1 \right) \tag{67}$$

where *C* is a constant and the length scale ℓ_p is given by

$$\ell_p = \frac{2 d_p \rho_p}{3 C_D \rho_c} \tag{68}$$

Consequently, u_{Cp} can be approximated by the local equilibrium solution if $r >> \ell_p$, i.e.,

$$d_p << \frac{3 C_D \rho_c r}{2 \rho_p} \tag{69}$$

This result is the same as for a constant body force, cf. Eq (64). The effect of the Basset term, estimated from the analysis in Clift et al. (1978), reduces the right hand side of (69) by a factor of 5, at most. For solid particles in liquid, the requirement in (69) does not restrict the application of the mixture model.

The second term in (62) corresponds, in rotational motion, the Coriolis force. The radial particle velocity caused by the centrifugal acceleration causes in turn a tangential acceleration. To the first order, the second term in (62) is equal to $u_{m\varphi} u_{Cp} / r$, which has to be compared to the leading term $u_{m\varphi}^2 / r$. Neglecting the second term thus requires simply

$$\frac{u_{Cp}}{u_{m\varphi}} << 1 \qquad (70)$$

In the Stokes regime, this condition can be expressed as

$$d_p << \sqrt{\frac{18\mu_c}{\omega(\rho_p - \rho_c)}} \qquad (71)$$

In a typical stirred tank reactor with solid particles in water, Eq. (71) gives $d_p << 1\ \mathrm{mm}$.

In the last term of Eq. (62), the viscous stress can obviously be regarded as small compared to the leading terms, except possibly inside a boundary layer. The diffusion stress can be neglected within the approximation of local equilibrium.

In the above analysis, we assumed that the suspension is homogeneous in small spatial scales. If this is not the case and dense clusters of particles are formed, the mixture model is usually not applicable. Clustering in a scale comparable to the length scale of turbulent fluctuations is typical for small particles (d_p < 200 μm) in gases. The clustering can lead to a substantial decrease in the effective drag coefficient. Consequently, the particle relaxation time becomes large and the local equilibrium approximation is not valid. Although the mixture model is in principle valid for small particles (d_p < 50 μm) in gases, it can be used only for dilute suspensions with solids to gas mass ratio below 1.

3.4 CONSTITUTIVE EQUATIONS

In order to have the field equations (10), (18) and (24) for the mixture model in a form suitable for applications, they have to be closed, i.e., constitutive models for the various terms are required. This closure problem is often very difficult. Some of the closure equations are obvious consequences from the approach used in developing the field equations, such as the definition of the velocity and density of a mixture. Other constitutive laws like those for the turbulence stress are considerably less understood.

The basic principles for formulating constitutive equations have been available for three decades (Drew & Lahey 1979). However, the development of the most general form of constitutive equations by starting from the basic principles is not practical because of the large number of possible terms. In practice, constitutive relations are postulated and their agreement with the basic principles are tested afterwards (Drew & Lahey 1979, Drew 1983, Hwang 1989, Ahmadi & Ma 1990). If possible, the developed constitutive model should be validated against experimental data, which would significantly reduce the possibility of a missing important term.

Constitutive equations of mixture models are not theoretically studied as extensively as those for full multiphase modelling. The task of deriving generally applicable constitutive equations of the mixture model starting from those for the full multiphase model is not trivial. In addition, the closure relations for the full multiphase models include uncertainties (Drew & Lahey 1979, Drew 1983). On the other hand, that approach is unnecessarily complex because it ignores the fact that, for the mixture model, the constitutive equations are simpler. Some of the terms for various phases cancel each other, for instance. The approach of writing the closure laws directly in terms of the mixture model parameters is more straightforward and consistent with derivation of the field equations. The study of Ishii (1975) is likely the most comprehensive treatment of the closure problem of the mixture model from a theoretical point of view. In their practical applications, most researchers (Johansen et al. 1990, Ungarish 1993, Hallanger et al. 1995) utilise a more pragmatic approach, especially in the constitutive relations for the stress terms.

Saturation condition

When the mixture is fully saturated

$$\sum_{k=1}^{n} \alpha_k = 1 \tag{72}$$

This was already utilised when deriving the relations between various velocities in Section 3.1. Eq. (72) indicates that computation of the volume fraction from the phase continuity equation can be omitted for one phase. In most cases, the volume fraction of the continuous phase is determined with (72) from the fractions of the other phases.

Mixture properties

The mixture density was defined in (11) as follows

$$\rho_m = \sum_{k=1}^{n} \alpha_k \rho_k \tag{73}$$

The viscosity of the mixture was discussed in Section 3.2.1. In practical applications, an empirical correlation for the viscosity has to be employed.

Kinematic closure relations

The determination of the relative velocity was discussed in Section 3.2.2. The relationships between the diffusion and relative velocities and, on the other hand, between the drift and relative velocities were given in (27) and (33). For the diffusion velocity we have

$$\sum_{k=1}^{n} \alpha_k \rho_k \mathbf{u}_{Mk} = 0 \tag{74}$$

Equations equivalent to (74) can also be written for the relative and drift velocities.

More kinematic relations were given in Section 3.1. Employing these results, the diffusion stress (21) can be expressed as a function of $\mathbf{u}_{Ck}$ as follows

$$\tau_{Dm} = -\rho_m \sum_{k=1}^{n} c_k \mathbf{u}_{Ck} \mathbf{u}_{Ck} + \rho_m \sum_{k,l=1}^{n} c_k c_l \mathbf{u}_{Ck} \mathbf{u}_{Cl} \tag{75}$$

If only one dispersed phase is present, this equation simplifies to

$$\tau_{Dm} = -\rho_m c_p \left(1 - c_p\right) \mathbf{u}_{Cp} \mathbf{u}_{Cp} \tag{76}$$

Pressure differences

The jump condition for the pressure over the interface between the phases *k* and *l* is (Drew 1983)

$$p_k - p_l = \kappa_{kl} \sigma \tag{77}$$

where κ_{kl} is the average mean curvature of the interface and σ is the surface tension. The properties of the interface determine the pressure difference. Without any surface tension, $p_k = p_l$. This assumption is customarily made except in the case of expanding bubbles (Ahmadi & Ma 1990, Drew & Lahey 1979, Drew 1983).

When deriving the mixture momentum equation, we assumed in (18) for the pressure of the mixture that

$$\nabla p_m = \sum_{k=1}^{n} \alpha_k \nabla p_k \tag{78}$$

If the surface tension is ignored, the pressure p_k is phase-independent and we have $p_m = p_k$.

Interfacial momentum conservation

The term $\mathbf{M}_m$ in the mixture momentum equation (18) denotes the mixture momentum source due to the surface tension and depends on the geometry of the interface. In the case of two-phase flow, the mixture momentum source is given by (Ishii 1975)

$$\mathbf{M}_m = \nabla\left(\kappa_{pc}\sigma\alpha_p\right) \tag{79}$$

Ishii continues by writing

$$\mathbf{M}_m = \kappa_{pc}\sigma\nabla\alpha_p + \mathbf{M}_{Hm} \tag{80}$$

The first term on the right hand side is zero if the surface tension is neglected. The last term $\mathbf{M}_{Hm}$ represents the effect of the changes in the mean curvature. Drew and Lahey (1979) assume that $\mathbf{M}_{Hm}$= 0. Commonly and especially in practical applications, the mixture momentum source $\mathbf{M}_m$ is ignored (Ungarish 1993, Johansen et al. 1990, Hallanger et al. 1995).

Interfacial mass conservation

The balance equation for interfacial mass transfer is given by (9)

$$\sum_{k=1}^{n} \Gamma_k = 0 \tag{81}$$

If phase changes do not occur at the interfaces between the phases, Γ_k=0.

Viscous shear stress

Before discussing the stress terms in the mixture momentum equation (18), the closure laws for a single-fluid system is briefly reviewed. The general form for the viscous shear stress tensor in a Newtonian (linear) viscous fluid is (Hirsch 1992)

$$\boldsymbol{\tau} = \mu\left[\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right] + \lambda(\nabla\cdot\mathbf{u})\mathbf{I} \tag{82}$$

where λ is the second viscosity coefficient and $\mathbf{I}$ is the unit tensor. The Stokes relation,

$$\lambda = -\frac{2}{3}\mu \tag{83}$$

is generally assumed to be valid. Experimental evidence against the Stokes relation exists only in very high temperatures or pressures, or in the case of sound-wave absorption and attenuation (Hirsch 1992, White 1974). The term involving the shear stress tensor in the Navier-Stokes equation would thus be

$$\nabla\cdot\boldsymbol{\tau} = \mu\left[\nabla^2\mathbf{u} + \frac{1}{3}\nabla(\nabla\cdot\mathbf{u})\right] \tag{84}$$

where a constant viscosity coefficient μ is assumed. For a single incompressible fluid,

$$\nabla\cdot\mathbf{u} = 0 \tag{85}$$

Accordingly, the last terms in (82) and (84) can be neglected. Furthermore, the term $\lambda(\nabla\cdot\mathbf{u})$ is argued to be almost always very small and it can therefore usually be ignored altogether (White 1974).

In multiphase flow Eq. (85) is not necessary valid for an individual phase. The divergence of the mixture velocity is neither generally equal to zero, cf. Eq. (12).

In his theoretical study for two-phase flow, Ishii (1975) applied time-averaging on Eq. (82) and obtained the following closure law for the viscous stress tensor of a phase (the velocity in (82) was interpreted as an instantaneous velocity)

$$\boldsymbol{\tau}_k = \mu_k \left[\nabla \mathbf{u}_k + \left(\nabla \mathbf{u}_k \right)^T \right] + 2\mu_k \mathbf{D}_{ki} \tag{86}$$

Here $\mathbf{D}_{ki}$ is the interfacial extra deformation tensor and arises from the fluctuating component of the fluid velocity. The deformation tensor $\mathbf{D}_{ki}$ takes into account the influence of the interfacial motions and mass transfer on the average deformation. The total viscous shear stress for a multiphase mixture can be represented as a sum of the contributions of the individual phases present in the mixture (the deformation tensor $\mathbf{D}_{ki}$ is taken once per interface).

Representing the phase velocity in terms of the mixture and diffusion velocities, the viscous shear stress tensor for the mixture can be written as follows

$$\boldsymbol{\tau}_m = \sum_{k=1}^{n} \alpha_k \mu_k \left[\nabla \mathbf{u}_m + \left(\nabla \mathbf{u}_m \right)^T \right] + \sum_{k=1}^{n} \alpha_k \mu_k \left\{ \left[\nabla \mathbf{u}_{Mk} + \left(\nabla \mathbf{u}_{Mk} \right)^T \right] + 2\mathbf{D}_{ki} \right\} \tag{87}$$

Specifying the deformation tensor is in general quite complex (Ishii 1975, Drew & Lahey 1979, Drew 1983), but under special conditions, $\mathbf{D}_{ki}$ can be simplified. If in two-phase dispersed flow, for instance, the motions of the interfaces are quite regular with little effects from the phase changes, the deformation tensor for the continuous phase can be written according to Ishii (1975) as

$$\mathbf{D}_{ci} = -\frac{1}{2\alpha_c} \left[\nabla \alpha_c \left(\mathbf{u}_p - \mathbf{u}_c \right) + \left(\mathbf{u}_p - \mathbf{u}_c \right) \nabla \alpha_c \right] \tag{88}$$

For the dispersed phase, $D_{pi} = 0$ (Ishii 1975, Drew & Lahey 1979). Unfortunately, Eq. (88) is a postulation without any experimental evidence (Drew 1983).

Utilising the approximation (88) for $\mathbf{D}_{ci}$, Eq. (87) can be rewritten for two-phase flow in terms of the volumetric flux $\mathbf{j}_m$ and the drift velocity $\mathbf{u}_{Vk}$ as follows (Ishii 1975)

$$\boldsymbol{\tau}_m = \sum_{k=1}^{2} \alpha_k \mu_k \left[\nabla \mathbf{j}_m + \left(\nabla \mathbf{j}_m \right)^T \right] + \alpha_p \left(\mu_p - \mu_c \right) \left[\nabla \mathbf{u}_{Vp} + \left(\nabla \mathbf{u}_{Vp} \right)^T \right] \tag{89}$$

Equation (89) shows interestingly that the mixture viscous stress is mainly determined by the velocity of the volume centre, $\mathbf{j}_m$, rather than that of the mass centre. This is one of the reasons why the mixture model is often formulated by means of the volumetric flux and called the drift-flux model. Compared to the formula (82) for a single-phase flow, the viscous stress in a mixture has an additional term caused by the relative motion. This term is often small and, when the drift velocity is constant, it can even be ignored.

Equation (87) suggests that when the effects of the relative motion and the interfacial deformation are not important, the viscosity of the mixture is

$$\mu_m = \sum_{k=1}^{n} \alpha_k \mu_k \tag{90}$$

Equation (90) should not be taken as a general definition of the mixture viscosity (see Section 3.2.1), however. When the dispersed phase consists of solid particles, Eq. (90) obviously has no relevance.

If a disperse phase *k* consists of solid particles, it is commonly assumed that $\tau_k = 0$ (Drew 1983, Joseph et al. 1990). This means that the viscous shear stress in a solid-fluid suspension reduces to that of the continuous phase in the mixture.

Ahmadi & Ma (1988) considered the total (viscous + turbulent) stress tensor of the solid phase differently. The total stress was divided to the collision, fluctuation and remaining stresses. The collision part of the total stress tensor was combined with the fluctuation (kinetic) stress tensor. For the remaining part of the total solid stress tensor and for the viscous stress tensor of the fluid phase, they propose formulas equivalent to (82) with the Stokes relation. In that case, the viscosities are, however, functions of the volume fractions of the dispersed phases.

When the mixture theory (Johnson et al. 1991) is applied in deriving the governing equations, the viscous stress tensor for the mixture is obtained as a sum of the stress tensors of various phases multiplied by the volume fractions. The constitutive equation for the viscous stress tensor of the fluid phase greatly resembles to that in (82). The closure equation for the viscous stress tensor of a dispersed phase shows the dependence on the dispersed phase fraction.

In practical applications, more straightforward approaches to determine the viscous stress tensor are usually employed (Ungarish 1993). Considering the contribution of one phase to the viscous stress term of the mixture momentum equation, we obtain from (87) by neglecting the last term

$$\nabla \cdot \left(\alpha_k \boldsymbol{\tau}_k\right) = \alpha_k \mu_k \left[\nabla^2 \mathbf{u}_k + \nabla\left(\nabla \cdot \mathbf{u}_k\right)\right] + \nabla\left(\alpha_k \mu_k\right) \cdot \left[\nabla \mathbf{u}_k + \left(\nabla \mathbf{u}_k\right)^T\right] \tag{91}$$

Eq. (91) can be simplified further assuming that $\nabla \cdot \mathbf{u}_k = 0$ (Cook & Harlow 1986). Sometimes the last term in (91) is omitted.

Alternatively, the closure law for the viscous stress can be formulated by considering the mixture as a single-phase fluid and determining the viscous stress tensor analogously to single-fluid flow in terms of the mixture parameters. Accordingly, one gets

$$\tau_m = \mu_m \left[\nabla \mathbf{u}_m + \left(\nabla \mathbf{u}_m \right)^T - \frac{2}{3} (\nabla \cdot \mathbf{u}_m) \mathbf{I} \right] \tag{92}$$

where μ_m is the dynamic viscosity for the mixture. Determination of the mixture viscosity is discussed more in section 3.2.1. It is often assumed that $\nabla \cdot \mathbf{u}_m = 0$. The need of this approximation could be avoided by rewriting Eq. (92) in terms of the volumetric flux $\mathbf{j}_m$ and utilising the relation $\nabla \cdot \mathbf{j}_m = 0$ Although other new terms would be created in a general case, they would be less significant and in many cases equal to zero.

Turbulent stress

The turbulent (Reynolds) stresses are caused by the fluctuations of the velocity relative to the mean velocity. The turbulent term is in general more important in multiphase flow than in single-phase flow. Even if the freestream turbulence is negligible, the flow around individual particles can generate velocity fluctuations (Gore & Crowe 1989). These fluctuations appear in the model in the turbulent stresses. Therefore, the turbulent stresses usually dominate over the viscous term. On the other hand, a dispersed phase may decrease the velocity fluctuations compared to single-fluid flow. Consequently, the traditional approach of dividing the total stress to viscous and turbulent stresses is sometimes discarded in multiphase flow (Hwang & Shen 1991).

Consider the term for the turbulence stress tensor in the mixture momentum equation (18). As the viscous stress above, the turbulent stress in a mixture could be presented as a sum of the contributions of the phases present in the mixture. Unfortunately, relations for the turbulent stress of a phase in multiphase flow are not well established.

Attempts have been made to develop theoretically a general formulation for the closure relation of the turbulent stresses in full multiphase modelling (Ishii 1975, Drew & Lahey 1979, Drew 1983, Nigmatulin 1979, Hwang & Shen 1989). The results are mostly questionable postulations with uncertain case-specific coefficients, however. The lack of experimental data hinders the use of the postulations suggested. Accordingly, utilisation of them when applying the mixture model may not be sensible.

Boussinesq’s assumption for the Reynolds stresses is usually extended to multiphase systems. Consequently, for an individual phase (Ahmadi & Ma 1990)

$$\boldsymbol{\tau}_{Tk} = \mu_{Tk}\left[\nabla\mathbf{u}_k + (\nabla\mathbf{u}_k)^T - \frac{2}{3}(\nabla\cdot\mathbf{u}_k)\mathbf{I}\right] - \gamma_k\rho_k k_k\mathbf{I} \tag{93}$$

where μ_{Tk} is a coefficient of the turbulent eddy viscosity and k_k is the turbulent kinetic energy density for phase k. The parameter γ_k is equal to 2/3 for the continuous phase. For dispersed phases its value depends on the volume fractions of the dispersed phases (Ahmadi & Ma 1990). A closed expression of γ_k is given by Ahmadi & Ma for a case of spherical particles. Sometimes the last term in (93) is considered insignificant and ignored (Picart et al. 1986, Cook & Harlow 1986).

In their study for solid-fluid mixtures, Ahmadi & Ma (1990) lumped the fluctuating and collision components of the stress tensor for a solid phase. For the sum a constitutive equation equivalent to (93) was proposed. Following the Kolmogorov-Prandtl hypothesis, they assumed that the coefficient of the turbulent viscosity is

$$\mu_{Tp} = C_{\mu p}\rho_p l_p\sqrt{k_p} \tag{94}$$

for the solid phase and

$$\mu_{Tc} = \frac{C_{\mu c}\rho_c {k_c}^2}{\varepsilon_c} \tag{95}$$

for the fluid phase. Here parameters $C_{\mu p}$ and $C_{\mu c}$ depend on the volume fractions, l_k is an appropriate length scale for phase k and ε_c is the dissipation rate for the fluid phase. The length scale of a solid phase varies. In dense mixtures, collisions are frequent and the particle diameter is an appropriate choice. For dilute suspensions, the fluid turbulence dominates and the fluid length scale can be used for the solid phase, too.

An alternative formulation for the solid phase stress was given by Hwang & Shen (1989). They divided the total stress tensor of the solid phase to the collision/contact, kinetic and particle-presence stresses. The collision stress arises from the momentum transfer in particle collisions. The kinetic stress is caused by the momentum transfer from the random motion of the particles and it is equivalent to the Reynolds stress in fluid turbulence. The particle-presence stress is the hydrodynamic contribution of the solid phase and it results from the hydrodynamic stress on the particle’s surface. The total stress tensor for the liquid phase comprise the viscous and turbulent stress tensors as usually.

When applying the mixture model on practical application cases, utilisation of the closure relations for the turbulent stress of individual phases is not worthwhile. The contributions of individual phases include uncertainties and, on the other hand, the result would not be presented in terms of the mixture parameters.

Often when applying the mixture model on turbulent multiphase flow, the viscous and turbulent stresses in a mixture arising from complex mechanisms are lumped to one quantity sometimes called the generalised (shear) stress (Ungarish 1993, Johansen et al. 1990, Hallanger et al. 1995). There are two slightly different alternatives to determine the generalised stress tensor. We can either take the generalised stress of the mixture as a sum of the contributions of various phases or, alternatively, we could determine the total stress for the mixture directly as for single-phase flow. Following the former approach, we thus assume that

$$\boldsymbol{\tau}_{Gm} = \boldsymbol{\tau}_m + \boldsymbol{\tau}_{Tm} = \sum_{k=1}^{n} \alpha_k \boldsymbol{\tau}_{Gk} = \sum_{k=1}^{n} \alpha_k \left(\boldsymbol{\tau}_k + \boldsymbol{\tau}_{Tk} \right) \tag{96}$$

where $\boldsymbol{\tau}_{Gm}$ is the generalised stress tensor in the mixture and $\boldsymbol{\tau}_{Gk}$ is the generalised stress tensor for phase *k*. For an individual phase *k*, Eq. (93) can be employed to determine the generalised stress tensor. The turbulent eddy viscosity in (93) is, however, replaced by the effective dynamic viscosity, which is a sum of the dynamic and turbulent eddy viscosities, i.e.,

$$\mu_{ek} = \mu_k + \mu_{Tk} \tag{97}$$

The effective viscosity can depend on the concentrations of the dispersed phases.

Substituting the relation $\mathbf{u}_k = \mathbf{u}_{Mk} + \mathbf{u}_m$ into (93), the generalised stresses could be represented in terms of the mixture model parameters. The viscous and turbulent stress term in the mixture momentum equation (18) would thus be a sum of the phase contributions.

It should be noted that stresses caused by the interfaces are not explicitly included in (96). In case of turbulent flow, they are not important. Actually, the viscous stress tensors can often be ignored because the turbulence viscosity of the continuous fluid is in many cases much larger than the dynamic viscosity.

The approach in Eq. (96) was followed by Johansen et al. (1990) in their study of simulating air classification of powders. Johansen et al. made additional simplifications based on the small differences in the velocity and turbulent viscosity and, on the other hand, on a large density difference between the phases. They include only the turbulent dispersion. The turbulent viscosity of the gas phase was computed with a modified *k*-*ε* model. The turbulent viscosity (dispersion coefficient) of a particle phase was close to that of the gas with an additional term depending on the relative velocity (cf. Eq. (104)).

A similar approach was also employed by Hallanger et al. (1995) in their study for a gas-oil-water mixture in a separator. The turbulent viscosity was taken as a constant. They obtained reasonable velocity profiles compared with the experimental data.

The other approach to handle turbulent flows is to determine the generalised stress equivalent to that for single-fluid flow directly to the mixture. Then we would obtain

$$\boldsymbol{\tau}_{Gm} = \mu_{em}\left[\nabla \mathbf{u}_m + \left(\nabla \mathbf{u}_m\right)^T - \frac{2}{3}\left(\nabla \cdot \mathbf{u}_m\right)\mathbf{I}\right] - \frac{2}{3}\rho_m k_m \mathbf{I} \tag{98}$$

where μ_{em} is the effective viscosity of the mixture. As in one phase flow, the effective viscosity of a mixture is also commonly represented as a sum of the dynamic and turbulent eddy viscosities for the mixture. Note that the effective viscosity is a function of the volume fractions which in general vary in space. The effective viscosity depends on the volume fractions as discussed previously in Section 3.2.1. The turbulent viscosity is calculated from the turbulence model applied, e.g. the k-ε model.

This approach was employed by Ungarish (1993) in his studies for liquid-solid suspensions (the turbulent kinetic energy term was excluded, however). He postulated that the term arising from the dependence of the effective dynamic viscosity on the volume fractions can be ignored. This approach was also applied for mixtures by Passman et al. (1984).

The discussion about the closure models for the viscous and turbulent stresses in the mixture momentum equation (18) can be summarised as follows. For viscous flow, the approach of Ishii (1975) can in simple cases be applicable but it is in a general case complex due to the interfacial extra deformation tensor $\mathbf{D}_{ki}$. In a solid-liquid suspension, the viscous stress of the solid phase is commonly assumed to be zero. Application of the generalised stress is most straightforward, especially in turbulent flows. Uncertainties in the influence of turbulence are naturally significant because of our limited capability of modelling turbulent flows in general. The influence of the dispersed phases on the turbulence behaviour of the mixture is small for moderate concentrations. If the concentrations change significantly, one should consider incorporation of the terms depending on the volume fractions.

3.5 MODEL CONSIDERATIONS

3.5.1 Mixture model equations

In the following, a summary of the mixture model equations is presented. We take here a practical point of view and write the equations in a form suitable for numerical solution.

The mixture model equations derived in Section 3.1 consist of the continuity and momentum equations for the mixture, (10) and (18), the continuity equations for the dispersed phases (24) and the algebraic equations for the relative velocities (58). According to Eq. (56), the relative velocity comprise the terminal velocity and the diffusion term. We substitute this result in Eq. (24) so that the diffusion term appears explicitly in the dispersed phase continuity equation.

The balance equations of the mixture model are summarised below for the case of one dispersed phase *p*

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot (\rho_m \mathbf{u}_m) = 0 \tag{99}$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho_m \mathbf{u}_m + \nabla \cdot (\rho_m \mathbf{u}_m \mathbf{u}_m) &= -\nabla p_m - \nabla \cdot \left[\rho_m c_p \left(1 - c_p\right) \mathbf{u}_{Cp0} \mathbf{u}_{Cp0}\right] \\ &\quad + \nabla \cdot \boldsymbol{\tau}_{Gm} + \rho_m \mathbf{g} \end{aligned} \tag{100}$$

$$\frac{\partial \alpha_p}{\partial t} + \nabla \cdot \left(\alpha_p \mathbf{u}_m - D_{Mp} \nabla \alpha_p\right) = -\nabla \cdot \left[\alpha_p \left(1 - c_p\right) \mathbf{u}_{Cp0}\right] \tag{101}$$

$$\boldsymbol{\tau}_{Gm} = (\mu_m + \mu_{Tm})\left[\nabla \mathbf{u}_m + (\nabla \mathbf{u}_m)^T\right] - \frac{2}{3}\rho_m k_m \mathbf{I} \tag{102}$$

In Eqs. (100) and (101), the phase slip terms are expressed explicitly as functions of the relative velocity, rather than the diffusion velocity. The former is obtained from the constitutive equation

$$\left|\mathbf{u}_{Cp0}\right| \mathbf{u}_{Cp0} = \frac{4 d_p}{3 C_D} \frac{\left(\rho_p - \rho_m\right)}{\rho_c} \left[\mathbf{g} - (\mathbf{u}_m \cdot \nabla)\mathbf{u}_m - \frac{\partial \mathbf{u}_m}{\partial t}\right] \tag{103}$$

where the particles are assumed to be spherical. The diffusion constant in the continuity equation of the dispersed phase is defined as $D_{Mp} = \left(1 - c_p\right) D_{Cp}$. In dilute suspensions, Eq. (101) is only weakly coupled to the mixture equations, through the variations of the mixture density and viscosity, and through the diffusion stress term. In (100), we made a further approximation by writing the diffusion stress in terms of $\mathbf{u}_{Cp0}$ instead of $\mathbf{u}_{Cp}$. The diffusion component of $\mathbf{u}_{Cp}$ can be dropped from the momentum equation as a second order term. The principal contributions of turbulence are in the turbulent stress term in the momentum equation and in the diffusion term in the dispersed phase continuity equation.

For the viscous and turbulent stresses, we adopted the generalised stress approach simplified by dropping the term involving $\nabla \cdot \mathbf{u}_m$. For laminar flow the set of equations is now complete. Empirical correlations have to be used for the quantities C_D and μ_m.

In turbulent flow, μ_{Tm} has to be computed from a suitable turbulence model. The k-ε model can also be applied in dispersed multiphase flows, if the solid concentration is not high. Corrections due to the dispersed phase to the standard single-fluid model have been developed (Elghobashi & Abou-Arab 1983, Mostafa & Mongia 1988, Adeniji-Fashola & Chen 1990, Tu & Fletcher 1994). In addition to Eqs. (99) - (103), the equations for the turbulent kinetic energy and turbulent dissipation have to be solved.

A correlation for D_{Mp} is required in a turbulent case. Based on the study of Csanady (1963), Picart et al. (1986) suggested a simplified theoretical model for the diffusion of solid particles in turbulent pipe flow. The analysis is based on the $k-\varepsilon$ model. Their result for the diffusion coefficient is given by

$$D_{Mp} = \nu_T \left(1 + 0.85 \frac{u_{Cp}^2}{2k/3} \right)^{-1/2} \tag{104}$$

where ν_T is the turbulent kinematic viscosity of the fluid and k the kinetic energy of turbulence. Thus D_{Mp} equals ν_T if the relative velocity is small compared to $\sqrt{k}$, i.e., if the particles are small and follow the fluid motion. This approach is commonly applied in numerical simulations for turbulent multiphase flows (Simonin 1990).

Bakker et al. (1994) use a different form for the diffusion coefficient. Their expression is modelled in analogy to the kinetic gas theory:

$$D_{Mp} = \frac{d_p \sqrt{k}}{18 \alpha_p} \tag{105}$$

If multiple dispersed phases are present, the mixture model equations are not as simple. The continuity equation is solved for each dispersed phase. According to Eq. (27), the relative velocities of all dispersed phases are coupled to the continuity equation of a single phase. Similarly, the diffusion stress in the momentum equation involves all relative velocity components, according to Eq. (75).

Determining the relative velocity becomes more complicated, because the hindrance effects of the particles of the other phases need to be taken into account in (103) in addition to the particles of the phase in question (Ungarish 1995).

Mixtures including several particle phases with different material densities can be considered as presented above. The formulation applies also if the density of the material of the dispersed phases is constant but the particle size varies. Particles are classified according to their size and each group is considered as a separate phase.

3.5.2 Implementation

The implementation of the above model in an existing cfd solver is fairly straightforward. The starting point is a solver for single phase flow with $\mathbf{u}_m$ and p_m as the solved for variables. The continuity equation is identical to that of single phase flow. In the momentum equation, the diffusion stress has to be added. The simplest way to implement this in an existing cfd code is to introduce it as a source term.

The particle concentration has to be solved as a scalar equation. The term involving $\mathbf{u}_{Cd}$ can be treated as additional convection, cf. Eq. (101). Thus, the convection flux has to be modified owing to the phase slip.

Finally, the relative velocity must be solved from (103). The solution is iterative, because C_D depends on $|\mathbf{u}_{Cd}|$. The iterative procedure can be avoided by approximating C_D piecewise by simpler expressions.

4 MIXTURE MODEL APPLICATIONS

As concluded in the previous section, the mixture model is applicable when the motions of various phases are closely related. It depends on constitutive models applied how comprehensively the influence of the dispersed phases on the motion of the mixture is taken into account. When the particle relaxation time is short, cases with large density differences and high dispersed-phase fractions can be modelled successfully with the mixture model formulation.

The mixture model has a wide range of applications. We will start with the most common application area, namely one-dimensional vertical flows of gas-liquid mixtures and continue the discussion with horizontal flows and particle suspensions. Next we will consider more complicated flow patterns and, finally, the applications of the mixture model on turbulent flows.

4.1 ONE-DIMENSIONAL FLOWS

For about 30 years, the concept of the mixture model has frequently been applied to predict the gas void fraction in upward gas-liquid flows (Wallis 1969). In these applications, the formulation has often been based on the volumetric fluxes of gas and liquid. The model is therefore called the drift-flux model, formulated comprehensively first by Zuber and Findlay (1965). The uneven distribution of the gas across the pipe cross-section is important and was included in the model by employing a distribution parameter. The approach was extended by Kataoka & Ishii (1987). Modelling in one-dimensional cases is straightforward. The conditions in a vertical flow pipe depend on the velocity and pipe size as well as the gas void fraction and its distribution (Clark et al. 1990). These parameters should thus be known, as well as the dependence of the distribution parameter on them. In vertical pipes, the flow velocity is usually high and the diameter of the pipes is small. The drift-flux model is applied on, for instance, boiling flows in nuclear reactors (Bottoni & Lyczkowski 1994, Kim & Doster 1991) and on flows in vertical air-lift pumps. In nuclear reactors, the drift-flux formulation is often applied in simulators and control systems. The mixture model approach is attractive in these applications because simulations which are faster than the real time are needed. Brockmeier et al. (1995) extended the application of the drift-flux approach to horizontal pipes. They also performed verification and validation studies.

Mixtures of two fluids have also been modelled with the drift-flux formulation. Franca & Lahey (1992) applied the drift-flux approach for horizontal flow of air-water mixtures.

The mixture model approach is also often applied on particle-fluid mixtures. Soria & de Lasa (1992) utilised the mixture model in their study for liquid fluidised beds. They developed kinematic equations for a liquid fluidised bed in terms of a set of measurable macroscopic parameters. The local instantaneous kinematic formulation was averaged over a three-dimensional volume which was larger than the microscopic scale but smaller than the macroscopic scale.

The mixture model has also applications with more than two phases involved. The motion of the mixture of gas, liquid and solid particles in vertical pipes was studied by Sakaguchi et al. (1987) with a modified drift-flux model. The approach was validated quite successfully by comparing the results with experimental data for aluminium particles with a mean diameter of 3 mm in water and in a water-air mixture.

4.2 APPLICATIONS WITH GRAVITATIONAL AND CENTRIFUGAL FORCE

The mixture model has been applied on gas-liquid mixtures in more complex flow geometries, too. Bakker et al. (1993) simulated multiple air-lift loop reactors. Chemical reactors loaded with vapour-liquid mixtures were analysed with the mixture model formulation by Wehmeier et al. (1994). Singhal et al. (1980) applied the concept of the mixture model implemented in PHOENICS (see the next section) to simulate steady three-dimensional two-phase flow and heat transfer in a recirculating-type steam reactor. In the gas-liquid applications, the bubbles are commonly assumed to behave like solid spheres. However, the virtual mass, arrangement of the bubbles in a swarm and most importantly the presence of surfactants should be taken into consideration (Zhou & Egiebor 1993).

The separation of solid particles in a liquid due to gravitation and centrifugal forces is extensively studied using the mixture model (Ungarish 1993, Ungarish 1995, Dahlkild & Amberg 1994, Amberg & Ungarish 1993, Ungarish 1990). Ungarish (1993) reviews the basic equations and physical models involved in the analysis and presents the results of the analysis of several geometries. The emphasis in Ungarish’s work is in developing asymptotic analytical solutions to the equations in sufficiently simple geometries. Numerical solutions for both mixture model and two-phase model equations are also presented. The practical cases include one-dimensional gravity settling, centrifugal settling in cylinders, spin-up from rest in rotating cylinders, and containers with inclined walls. Turbulent effects were not considered in these investigations.

The solid particle distribution in a stirred tank was simulated by Bakker et al. (1994) using FLUENT combined with a separate computer code for computing the particle concentration according to a mixture model. Effects of the solid particles on the average liquid flow were neglected and the diffusion velocity of the particles was assumed to be in the axial direction. Turbulent diffusion of particles was included in the model using the diffusion coefficient (105). Similar computation of gas dispersion was made by Myers et al. (1994) using the same computational tools. Comparison with experimental data indicated that the mixture-model simulations provided reliable prediction of the agitated gas-liquid dispersions.

Kocaefe et al. (1994) applied the mixture model of PHOENICS in simulating the stirring of a solid-liquid mixture in a tank. They stated that only the influence of the gravity was taken into account when determining the relative velocity. The case was highly three-dimensional: the tank was rectangular with rounded corners and equipped with three flat blade impellers. The model was validated by comparing the simulation results against the limited experimental data available.

Pericleous & Drake (1986) implemented the earlier version of the mixture model in PHOENICS and modelled the flow of the mixture of air, liquid and particles in a complicated hydrocyclone classifier. The classifier was modelled with a two-dimensional axisymmetric grid. The vertical and radial components of the relative velocity were calculated from the gravitational and centripetal accelerations, respectively. In their validation study, Pericleous & Drake noted that the limitations do not lie so much in the mixture model itself but in the modelling of uncertain quantities like turbulence and of the behaviour of particles near solid boundaries. They also studied the behaviour of a particle-fluid suspension in a simple two-dimensional duct.

Pericleous & Patel (1987) used the mixture model in PHOENICS in simulating a stirred biochemical reactor with a number of baffles and heating coils and equipped with three impellers. They investigated the distribution of gas bubbles in liquid. The simulation results were quantitatively correct; large bubbles rose directly to the surface and small bubbles followed closely the motion of the liquid and dispersed more uniformly throughout the reactor.

Polydispersions in the gravity field have been investigated closely (Greenspan & Ungarish 1982, Ungarish 1993). The developed theory is applicable in vertical flow for suspensions of particles which differ considerably in size or density as long as the total volume fraction of particles is less than 0.16. However, if the total volume fraction is more than 0.16, strong instabilities occur producing fingering and lateral segregation.

Studies on rotating polydispersions are more infrequent. The works of Ungarish & Greenspan (1984), Johansen et al. (1990) and Ungarish (1995) are among the few. The results of the studies for polydispersions in the gravity field cannot necessarily be generalised to rotating motion. The theory indicates that in centrifugal separation large particles may settle slower than the smaller ones (Ungarish 1995). In determining the relative velocities Ungarish uses a hindrance function, which depends on the density of the particle population in question.

4.3 TURBULENT FLOWS

The mixture model has been applied only in a few cases on turbulent flows. Often, the influence of turbulence is considered insignificant or turbulence is not included in a model (Pericleous & Drake 1986).

Hallanger et al. (1995) employed the mixture model formulation when they simulated the flow of the mixture of gas, oil and water in a gravity separator. The oil formed the continuous phase. The size of the fluid particles was found to be an important parameter. Therefore, the particles were classified according to their size and each group was considered as a separate phase. The turbulent stress tensor was modelled by means of the turbulent viscosity. Despite the complexity of the system and the simplicity of the approach, a good correspondence of calculated and measured results was obtained. The approach gave reasonable velocity profiles in comparison with the experimental data for air-water separators.

Johansen et al. (1990) studied air classification of fine powders. They analysed the turbulent flow pattern and predicted the grade efficiency for a classifier. Johansen et al. developed a stationary model which is close to the mixture model presented in the previous section. Since the volume fraction of the particle phase was small, the mixture continuity equation was approximated with the one-phase continuity equation for an incompressible gas. In modelling turbulence, they applied an extended k-ε model. The turbulent viscosity for the phases was calculated separately because they wrote the constitutive equation for the turbulent stress term as a sum of contributions from various phases. The turbulent viscosity of the gas was obtained from the k-ε model. Turbulent diffusivity of the particle phase was calculated from (104). The viscous stress was omitted. The particles were classified into groups according to their size (1.5 - 5.5 μm). The model was implemented to the commercial computer code FLUENT (see next section). The modelling results indicated a possibility of unwanted flow patterns for certain power feed rates. Increased particle fraction damps turbulence reducing the turbulent viscosity and consequently improves the efficiency of the classifier. The results are in agreement with the experience of using the classifier. Although air was the carrier fluid, the mixture-model approach was applicable because the particles were small. Johansen et al. believed that the model can be employed in studies of improving the design and the ways of introducing gas and particles into the classifier.

5 MULTIPHASE MODELS IN COMMERCIAL COMPUTER CODES

First versions of the commercial codes for computational fluid dynamics were written for single phase flows. A natural development was to add particle tracking methods to the one-phase codes. Still today, this type of Lagrangian simulation of two-phase flows dominates the multiphase field and it can be found in most general purpose codes. The Lagrangian description is best fitted for simulation of dilute mixtures. In later versions of the codes, an Eulerian description of dense multiphase flows has been included. In addition to the Lagrangian and Eulerian descriptions, many codes contain simplified equation systems for simulation of special cases of two-phase flows. In the following, we give a short description of the Eulerian multiphase models of PHOENICS, FLUENT and CFX 4 (former FLOW3D).

5.1 PHOENICS

Two-fluid model

The true Eulerian multi-fluid model in PHOENICS (CHAM 1991) is restricted to two phases. For turbulent flows PHOENICS solves equations that are time-averaged without mass weighting. This implies that a diffusion term is included in the phase continuity equations by default. Inter-Phase Slip Algorithm (IPSA) is used in solving the two fluid equations.

The interphase transfer models included in the code are limited. For example the drag force can be directly given only as the Stokes formula or as proportional to a given power of the relative velocity. In practice the user has to add the appropriate formulas through Fortran coding, which however is made simple by the structure of the code. Interphase mass-transfer models are similarly very simple.

Algebraic slip model

In PHOENICS, the mixture model is called the Algebraic Slip Model (ASM), which emphasises the fact that the relative velocity is calculated from an algebraic relation rather than solving the phase velocities from differential equations as in the genuine multiphase model. Details of the ASM model are not given in PHOENICS user manuals. The source code for the model implementation is, however, available, because it has been written as a separate subroutine.

The ASM model assumes incompressibility of both the continuous phase and the dispersed phases. Therefore, the volumetric continuity equation (14) for the mixture has been utilised. The diffusion stress term in the mixture momentum equation (18) has been omitted in the model, i.e. the momentum equation is in the same form as for single fluid flow.

The drag coefficient is modelled in a simplified way as follows:

$$\begin{aligned} C_D &= \frac{24}{Re} \qquad Re < 64 \\ C_D &= 0.42 \qquad Re > 64 \end{aligned} \tag{106}$$

This is a crude approximation of the more accurate formulas presented in section 3.2.1 and underestimates the drag force more than 50% around Re = 64, as illustrated in Fig. 1. The Reynolds number is based in PHOENICS on the fluid viscosity of the continuous phase rather than on the viscosity of the mixture.

No empirical correlations for the mixture viscosity have been included in the ASM model. Instead, it is calculated from the phase viscosities using the expression (90). In practice, however, an empirical model for the mixture viscosity is necessary.

The implementation of the ASM model has been realised in a separate subroutine called on every slab during the sweep iteration. The body force per unit mass is computed from the pressure gradient divided by the mixture density. The slip velocity components for each cell face are calculated from Eq. (59) using the drag coefficient (106). The solution of the dispersed phase continuity equation based on the volumetric flow is then solved iteratively within the subroutine for the current slab, allowing for time dependence, inlets and outlets.

The ASM model seems to be the only mixture model implemented in commercial CFD codes. The simplifications made in computing the mixture viscosity and the drag force have to be corrected, however, before the model can be used in practice. In order to make the model applicable in turbulent flow one has to add the corresponding diffusion term in accordance with Eq. (101). In addition, a diffusion term due to the phase slip should be included in the momentum equation. All these modifications are fairly easily made, because the source code for the model implementation is available.

5.2 CFX 4

The following summary of CFX 4 is based on the CFDS-FLOW3D release 3.3 user manual (AEA Technology 1994) and on material received from CFDS (Lo 1994). In addition to the Lagrangian and Eulerian multiphase models, this code contains a simplified, homogeneous flow model for two-phase flows that can be used for free surface flows and drag-dominated multiphase flows.

In the Eulerian multiphase model of CFX 4, the phases can be any combinations of incompressible and weakly compressible phases and laminar or turbulent phases. For each of the turbulent phases, the same turbulence model, i.e. one of the versions of the k-ε model, the Reynolds stress model or the Reynolds flux model, must be used. Each of the phases can consist of a number of species which undergo mass transfer by diffusion within each phase and which can be transferred across the phase boundaries. A dispersed phase with a wide range of particle sizes should be split into a number of phases, each with mean diameter averaged over a fixed range of particle sizes. In the code, it is assumed that all the phases share the same pressure field.

The inter-phase transfer models can be modified by the user via special subroutines. Only a limited range very basic correlations are available in the code. These are based on fairly dilute disperse two-phase flow of particles or droplets in a gas or liquid. For the drag force, well known correlations for the flow of a single particle in infinite fluid, including the correlation of Ihme et al. (1972) applicable for all sub-critical Reynolds numbers and special models for the Stokes, Allen and Newton regimes, are available. Mass transfer is described by means of a simple mass transfer coefficient. More complicated models can be added by the user.

A special feature of CFX 4 is the possibility of including turbulent diffusion terms in the transport equation of mass. A turbulent Prandtl number for turbulent dispersion of volume fraction can be set by the user. It should be noted that including this type of terms in the continuity equation should be only done with special care since it distorts the definition of the average velocities. With the extra diffusion terms, the velocities are not the mass averaged velocities most users are used to. Hence, before giving the Prandtl number finite values, the user should first carefully derive a set of equations where this type of terms occur by a proper averaging method and then determine the turbulent Prandtl number from experimental data.

The equations system of the multiphase model is solved using the IPSA algorithm. Alternatively, a modified algorithm, called IPSA-C, could be used for drag-dominated flows where the velocity differences are small.

There are several limitations to the use of the multiphase model CFX 4. No radiation heat transfer is described in multiphase flows. Conduction in solids is not allowed. Another limitation is that the model assumes a fixed grid. No model for the interaction between two dispersed phases is implemented in the code; the user can write models for the interaction processes in special subroutines.

No mixture model is available in the code. It can be implemented in the form of a scalar transport equation written for the volume fractions. The suspension can then be described as laminar Newtonian or non-Newtonian single phase fluid. Several models of non-Newtonian fluids have been included into the program: the Bingham model, Bird-Carreau model, Cross model, Herschel-Bulkley model and power-law model. In these models the viscosity is a function of the shear rate of the fluid. Each of the models contain a set of parameters that must be given by the user.

5.3 FLUENT

The following summary is based on the user manual for FLUENT V4.3 (Fluent Inc. 1995) and on experience in using the code. Similarly with CFX 4, FLUENT contains both the Lagrangian and the Eulerian description of multiphase flow. In addition, a special simplified two-phase model is available for stratified and free-surface flows.

The Eulerian multiphase model applies different closure relations to fluid-solid and fluid-fluid flows. In the former case the flow properties are derived from equations based on kinetic theory. The gas law can be used in both cases for the primary, continuous phase. One turbulence field is shared by all phases. Same simple drag laws are available for both fluid-fluid and fluid-solid flows.

In fluid-fluid flows, a single pressure is shared by all phases. All secondary phases are assumed to form droplets or bubbles the size of which has to be specified. Temperature-dependent properties are available for all phases. The inter-phase momentum exchange coefficients between primary and secondary phases are based on the properties of the primary continuous fluid. The exchange coefficients for two secondary phases is determined by the density and viscosity of the mixture of the two phases and on an averaged particle diameter. The drag coefficient is calculated following the models given for a single spherical particle.

The development of models for granular flows was based on a cooperation between Fluent Inc. and Morgantown Energy Technology Center. In the granular (fluid-solid) flow model it is assumed that all secondary, dispersed phases are solids. The fluid pressure field is shared by all phases and a solids pressure field is calculated for each solid phase. Granular temperature (solids fluctuating energy) is calculated for each solid phase. Solid phase shear and bulk viscosities are obtained from application of kinetic theory for granular flows.

In granular flows, the fluid-solid exchange coefficient is calculated from the model of Syamlal and O’Brien (1988), Eq. (48), which is based on measurements of terminal velocities of particles settling in liquid-solid fluidised beds (Richardson & Zaki 1954). Drag coefficient is then a function of the volume fraction and the relative Reynolds number. For dense gas-solid flows, this model overestimates the drag force.

Several limitations restrict the applicability of other models along with the multiphase model. Multiple species can be specified only for the primary phase and multi-component diffusion is not allowed. Sliding or deforming meshes cannot be used for multiphase calculations. Phase change and compressible flow are forbidden. Pressure boundary conditions and specified periodic mass flows are not allowed. Lagrangian particle tracking can be used but it interacts only with the primary phase.

The Reynolds stress model for turbulence cannot be used. All turbulent quantities are based on the primary phase flow using the k-ε or RNG (renormalisation group) k-ε model. The effective viscosity of the secondary phase is obtained from the primary phase turbulent viscosity. Turbulence generation in the secondary phases is not accounted for, nor is the turbulence of the primary phase directly affected by the presence of secondary phases (only effects come through reduced volume fractions).

Mass transfer between phases can be defined in user-defined subroutines. Heat transfer is based on the primary phase only. User-defined subroutines should be used to account for heat transfer in the other phases. Radiative heat transfer and combustion are not allowed. All phases are assumed to be in thermal equilibrium at all times.

Mixture modelling in Fluent has been made by Johansen et al. (1990). The models developed by him are not available in the commercial code. The scalar transport equations can be used to implement the mixture model. Similarly with CFX 4, models for non-Newtonian fluids are available which allows modelling of multiphase flows as laminar non-Newtonian flows.

6 SUMMARY AND DISCUSSION

The concept of the mixture model is intuitively simple. Considering a mixture of continuous and dispersed phases, one could write down the continuity and momentum equations for the mixture analogously to the homogeneous model. The slip of a dispersed phase relative to the continuous phase is calculated by balancing the drag and body forces resulting from density differences. The underlying assumption is a local equilibrium, in which the dispersed particles always move with their terminal velocity relative to the continuous phase. The concentrations of the dispersed phases are solved from scalar equations taking into account the correction due to the phase slip in the convective terms.

The essential character of the mixture model is that only one set of velocity components is solved from the differential equation for momentum conservation. The velocities of the dispersed phases are inferred from the algebraic balance equations. This reduces the computational effort considerably, especially if several dispersed phases need to be considered due to the varying density or size of the particles.

The mixture model equations were, however, derived in this study starting from the full multiphase flow equations. This approach is transparent and the simplifications additional to the full multiphase models are clearly shown. It also introduces in a natural way the diffusion stress due to the phase slip in the momentum equation. The balance equation for the relative velocity was carefully developed from the original equations by first retaining all terms and then making the necessary approximations. In this way, the validity of the model in comparison to a full multi-fluid model can be explicitly analysed. For each neglected term, a condition was derived to justify the approximation.

The constitutive equations required to close the set of conservation equations are generally complicated in multiphase problems. In particular, the viscous and turbulent stress terms are troublesome. Theoretical models are presented in the literature, but they are difficult to apply in practice. In the concept of the mixture model, a simpler approach generalised from single-phase models is appropriate. The viscous and turbulent stress terms are assumed to have the same form and they are lumped to the generalised stress term. The k-ε or equivalent model, modified to account for the presence of the dispersed phases, is then applied to calculate the effective turbulent viscosity for the mixture.

The mixture model can be applied in flows for wide ranges of the velocity difference, particle size and density ratios as long as the force equilibrium is achieved, i.e., particles reach the terminal velocity in a short time compared to the time scale characterising the flow. The mixture model has had numerous applications in one-dimensional flows during the last 30 years. In three-dimensional flows, the model has not been employed as frequently.

The suitability of the mixture model approach and evaluation of it are more difficult in the case of turbulent flows because of the complexity of the turbulent multiphase flow. The applications made indicate that in engineering studies the mixture model approach can be satisfactory. The reasons for the deviations from experimental data arise from the approach itself but also from other assumptions like omitted interaction forces or the incompleteness of turbulence modelling. These problems are equally well present in the full multiphase models.

The mixture model is best suited for small particles or bubbles in liquids. In gas-particle flows, the length scales related to particle acceleration are often long, which prevents the application of the model. In addition, clustering effects increase the effective drag force, indicating that the single-particle formulation cannot be used in estimating the usability of the model.

The most important advantage of the mixture model approach is the reduction in the need for computing resources. It is a considerable alternative when the speed of the simulation is a decisive factor. When several dispersed phases are present, simulations with the mixture model can be significantly faster than with the full multiphase model. Moreover, simulations with the mixture model require less computer memory and disk space, which usually also affects the computing time.

The mathematical framework of the mixture model was established in detail in this report. Nevertheless, several aspects still need further refinement. Modelling of turbulence is one of the main difficulties in multiphase flows in general. The practical questions with regard to the mixture model involves the modifications of the appropriate single-phase turbulence model to account for the presence of the particles, and the determination of the form of the diffusion coefficient appearing in the continuity equation for the dispersed phase.

For the viscosity of the mixture, an appropriate empirical expression has to be used. For dilute suspensions of spherical particles in a liquid, correlations of the viscosity as a function of the concentration are well established. If different size particles are present, the modelling is more complicated. In this case the effect of particles of varying size on each other has to be accounted for. In practice, the expression for the relative velocity has to be modified to include this effect.

In dense suspensions, the mixture becomes non-Newtonian, i.e., the effective viscosity depends on the shear rate. If the flow is laminar, this causes no additional problems in the mixture model formulation, as long as the dependence of the viscosity on the shear rate and solids concentration is known. Models for turbulent flow of non-Newtonian fluids are not available even for single-fluid cases, however.

Implementation of the mixture model in an existing cfd solver is, in principle, straightforward. It involves the addition of the diffusion stress in the mixture momentum equation, solving for the relative velocity from the algebraic balance equation and the implementation of a scalar equation for the concentration of each dispersed phase. Furthermore, one needs empirical expressions for the mixture viscosity and the turbulent diffusion coefficient for the particles.

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