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CLOSURE OF DISPERSE-FLOW AVERAGED EQUATIONS MODELS BY DIRECT NUMERICAL SIMULATION

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Abstract

This paper presents a summary of some recent work on the systematic closure of disperse-flow averaged-equations models on the basis of direct numerical simulations. Since the average pressure is found by solving the equations rather than prescribed as a closure relation, it is important first to identify the pressure part of the average stress. This objective is achieved by examining the transformation properties of the average stress under the gauge transformation $p_C + p_C + \psi$, where $p_C$ is the continuous-phase pressure and $\psi$ the potential of the body forces. After this step, the stress is expressed in terms of computable quantities. A strategy to derive closure relations is then described. It is also shown that the rheological behavior of spatially non-uniform suspensions is described by a non-Newtonian constitutive equation.

1 Introduction

The day when the direct numerical simulation of multiphase flows of engineering significance will be possible is so far into the future that it appears quite safe to bet on the importance of averaged equations for many years to come. The difficulty with such approaches, however, is well known, and consists in the fact that the equations produced by averaging are not closed: some of the information lost in the averaging process needs to be restored for a solution to be possible. Unfortunately, in spite of many decades of efforts, this closure problem is still outstanding. All “simple” approaches seem to lead either to mathematical inconsistencies (e.g., ill-posedness of the equations) or insufficient physics (e.g., point-like particles). Attempts at using rigorous analytical tools seem to inevitably end up either in results that, in spite of the substantial effort required in the derivation, are rather limited (e.g., to second order in the volume fraction of the disperse phase), or in formal manipulations divorced from physics and practical relevance.

A potentially powerful tool that, it would seem, has not been sufficiently considered in tackling this problem is that of direct numerical simulations directed not to the solution of specific problems, but especially designed to aid in the formulation of accurate closure relations. This paper is devoted to a brief discussion of this approach and a description of some recent progress in this direction.

It is well known that convergence of volume averages is quite slow, in the sense that the size of the averaging volume must be much greater than the size of the inhomogeneities in order to calculate meaningful averages. As a consequence, volume averaging could at most be useful for spatially homogeneous systems which, however, are rather uninteresting as the chief difficulty of the problem lies in the correct formulation of terms containing derivatives. These considerations

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point to ensemble averaging as the method of choice, and this is the technique that we use after an adaptation that makes it much more convenient for computation.

2 Momentum balance

We consider a system in which the disperse phase (index $D$) consists of equal rigid spheres of radius $a$ suspended in an incompressible continuous phase (index $C$); we will refer to the $C$-phase and $D$-phase for brevity. The phase-ensemble average of the $C$-phase momentum equation is

$$ I_C = \beta_C \langle \nabla \cdot \sigma_C \rangle - \beta_C \nabla \psi_C, \quad (2.1) $$

where angle brackets denote the phase-ensemble average, $\rho_C$, $u_C$, and $\sigma_C$ are the density, velocity, and stress tensor of the $C$-phase, $\beta_C$ is the volume fraction, and $\psi_C$ the potential of the body force; the inertia terms in the left-hand side are denoted by $I_C$ for brevity:

$$ I_C = \rho_C \frac{\partial}{\partial t} (\beta_C \langle u_C \rangle) + \rho_C \nabla \cdot (\beta_C \langle u_C u_C \rangle). \quad (2.2) $$

At this point one faces the well-known problem that differentiation and averaging do not commute. However, in the bulk of the suspension, the macroscopic length scale $L$ is usually much greater than the particle radius $a$ and one has the approximate result (Zhang and Prosperetti 1994a; Zhang and Prosperetti 1997; Prosperetti 1998):

$$ \beta_C \langle \nabla \cdot \sigma_C \rangle = \nabla \cdot (\beta_C \langle \sigma_C \rangle) - n A[\sigma_C] + \nabla \cdot (\beta_D L[\sigma_C]), \quad (2.3) $$

where $n$ is the particle number density, $\beta_D$ the $D$-phase volume fraction, and

$$ \beta_D L[\sigma_C] = n T[\sigma_C] + \nabla \cdot \{n S[\sigma_C] + \nabla \cdot [n R[\sigma_C] + \ldots]\}, \quad (2.4) $$

with

$$ A[\sigma_C] = \int_{|r|=a} dS, \quad (2.5) $$

$$ T[\sigma_C] = a \int_{|r|=a} dS, \quad (2.6) $$

and $S$, $R$ given by similar expressions with one and two additional factors of $n$ in the integrand, respectively. In (2.5), (2.6) the integration is over the surface of the particle centered at $x$ and the overline denotes the particle average, i.e. the average over all the other particles. For a generic quantity $g^\alpha$ pertaining to particle $\alpha$ as a whole, such as the surface integrals in (2.5), (2.6), the precise definition of the particle average is as follows:

$$ n(x) \bar{g}(x) = \frac{1}{N!} \int dC^N P(N) \left[ \sum_{\alpha=1}^{N} \delta(x - y^\alpha) g^\alpha(N) \right]. \quad (2.7) $$

The number density $n$ is defined by the same equation (2.7) with $g^\alpha = 1$. It can be shown that the frequently adopted relation $\beta_D = n v$ is only strictly accurate for a uniform suspension; in the non-uniform case one finds

$$ \beta_D = \left[ 1 + \frac{a^2}{10} \nabla^2 + O \left( \frac{a}{L} \right)^4 \right] (n v). \quad (2.8) $$
The terms neglected in (2.4) are of higher order in \( a/L \). One recognizes that, in particular, \( \mathcal{A} \) is the average hydrodynamic force on the particle at \( x \).

The physical meaning of (2.3) can be made clear by integrating this expression over the unit volume. The term in the left-hand side is then evidently the average of the divergence of the \( C \)-phase stress over the volume occupied by the \( C \)-phase. The first term in the right-hand side is the resultant stress acting on the \( C \)-phase through the surface of the unit volume (only a fraction \( \beta_C \) of which is occupied by the \( C \)-phase). The second term is the total force exerted on the \( C \)-phase by the particles the center of which is in the unit volume. As made manifest by its divergence form, the last term also represents a surface stress, and since it contains the \( D \)-phase volume fraction it acts on the \( C \)-phase contained in the unit volume through the fraction of surface cutting through particles. Evidently it accounts for the stress communicated to the \( C \)-phase through the particles that are only partially contained in the unit volume. With (2.3) the \( C \)-phase momentum equations is thus

\[
\mathbf{I}_C = \nabla \cdot (\beta_C < \sigma_C > + \beta_D \mathbf{L}[\sigma_C]) - n\mathcal{A}[\sigma_C] - \beta_C \nabla \psi_C. \tag{2.9}
\]

Most averaging methods give an average equation of motion for the \( D \)-phase that involves the stress inside the particle. At a fundamental level it is trivially true that the particles influence the motion of the \( C \)-phase through their stress field. Yet it would be difficult to argue that a practically useful description of the flow on the basis of averaged equations should be able to distinguish, for example, between solid particles with and without residual stresses due to different manufacturing procedures. It would seem that, whenever it makes sense to approximate the particle behavior as rigid, useful averaged equations should not require further detailed information about the particle structure. On the basis of these considerations, in order to determine the average momentum equation for the \( D \)-phase, we average Newton's equation for the particles directly finding the result

\[
\mathbf{I}_w = n\mathcal{A} - n\mathbf{v} \nabla \psi_D, \tag{2.10}
\]

where \( \mathbf{v} = \frac{4}{3} \pi a^3 \) is the particle volume and, similarly to (2.2),

\[
\mathbf{I}_w = \rho_D \left[ \frac{\partial}{\partial t} (n\mathbf{v}\mathbf{w}) + \nabla \cdot (n\mathbf{v}\mathbf{w}\mathbf{w}) \right]. \tag{2.11}
\]

Here \( \mathbf{w} \) is the average center-of-mass velocity of the particles and \( \psi_D \) is the potential of the \( D \)-phase body force, e.g. \( \psi_D = -\rho_D g \cdot x \) in the case of gravity.

## 3 The mixture pressure

Averaged equations are phrased in terms of primary variables such as mean mixture pressure, volume fractions, and mean velocities. All of these variables – except the first one – appear explicitly in the momentum equations. The average of the mean \( C \)-phase stress, \( < \sigma_C > \), will contain the mean \( C \)-phase pressure \( < p_C > \), but it is by no means obvious that this is the quantity to be identified with the mean mixture pressure \( p_m \). Yet, the correct identification of this quantity is essential for several reasons the most important of which is that all the terms appearing in the mean stress in Eq. (2.9) must be closed, except for \( p_m \), and therefore it is necessary to identify \( p_m \) correctly. In the literature one frequently encounters a relation like

\[
p_m = \beta_C < p_C > + \beta_D < p_D >
\]

which is problematic as, for example, the pressure inside a rigid particle is a physically ill-defined quantity.

The problem with the common Continuum Mechanics prescription to identify pressure with \(-\frac{1}{3}\) the trace of of the stress is that it can be shown that the stress tensor in (2.9) is defined up
to a divergenceless, but not traceless, tensor. Hence, a pressure defined in this way would not be unique.

For all these reasons we have taken a different approach to the identification of the mixture pressure. We start from the well-known fact that, in single-phase incompressible flow, a body force potential \( \psi \) can be absorbed into the pressure simply by making the gauge transformation \( \rho_C = p_C + \psi \). For this reason, it seems reasonable to identify as \( p_m \) the isotropic part of the stress in (2.9) that transforms in the same way, \( \rho_m = p_m + \psi \). This argument leads to a unique answer which is

\[
p_m = \beta_C < p_C > + \left( 1 + \frac{a^2}{10} \nabla^2 \right) (n_v \rho^p) + \frac{a^2}{5} \nabla \cdot \left( n \int_{|r|=a} dS_r (-p_C) \, n \right) + \ldots ,
\]

where

\[
p^p = \frac{1}{4 \pi a^2} \int_{|r|=a} dS_r p_C .
\]

In the case of a mixture in equilibrium at rest, \( p^p = p_C = < p_C > \), all derivatives vanish and \( p_m = < p_C > \) as expected. If the finite extent of the particles is negligible, \( a \approx 0, \, v \approx 0, \, \beta_C \approx 1 \) and (3.1) gives \( p_m = < p_C > \), which is also expected. For a flowing uniform mixture, while \( p^p \neq < p_C > \) in general, all derivatives vanish so that \( \beta_D = n_v \) and

\[
p_m = \beta_C < p_C > + \beta_D p^p .
\]

This expression gives a well-defined meaning to the particle contribution \( < p_D > \) in the formal expression quoted earlier. We can now write the total stress \( \beta_C < \sigma_C > + \beta_D \mathcal{L} \) as

\[
\beta_C < \sigma_C > + \beta_D \mathcal{L} - \frac{a^2}{10} (n \nabla \mathcal{A} - \mathcal{A} \nabla n) = - p_m I + \Sigma = -(p_m + q_m) I + S + A ,
\]

where the viscous part \( \Sigma \) has been decomposed into an isotropic part \( q_m \) (analogous to the volume, or second, viscosity of a Newtonian compressible fluid and here essentially related to the interphase slip velocity), traceless symmetric part \( S \), and an antisymmetric part \( A \). For the purpose of making the considerations that follow more concrete, it is useful to write down at least the first few terms of each one of these quantities for the case of a Newtonian fluid:

\[
S = 2 \mu_C E_m + \frac{n}{2} \left\{ \tau^0 \sigma_C + (\tau^0 \sigma_C)^T - \frac{a^2}{5} \left[ \nabla \mathcal{A} + (\nabla \mathcal{A})^T \right] \right\} + \ldots
\]

\[
A = \frac{n}{2} \left[ \tau^0 - (\tau^0)^T \right] + \ldots
\]

\[
q_m = \frac{a^2}{5} \nabla \cdot \left( n \int_{|r|=a} dS_r \, \tau_C \cdot n \right) + \frac{1}{15} a^2 n \nabla \cdot \mathcal{A} + \ldots
\]

In these equations the superscript \( T \) indicates the transpose, \( \tau_C = \sigma_C + p_C I \),

\[
E_m = \frac{1}{2} \left[ \nabla u_m + (\nabla u_m)^T \right] .
\]

is the rate of deformation tensor associated to the mean volumetric flux \( u_m \):

\[
u_m = \beta_C < u_C > + \beta_D < u_D > ,
\]

and

\[
\tau^0_{ij} \sigma_C = \int_{|r|=a} dS_r \left[ n (\sigma_C \cdot n) - \frac{1}{3} I (n \cdot \sigma_C \cdot n) \right] .
\]

The reason why it is necessary to subtract the last group of terms in the left-hand side containing derivatives of \( \mathcal{A} \) is explained in Marchioro et al. (1999c); space limitations prevent us from giving details here.
4 Averaged momentum equations

We now define an interphase force by

\[ f = \frac{1}{v} \mathcal{A} - \nabla \cdot (-p_m I + \Sigma) \]  

(4.1)

The C-phase momentum equation (2.9) then becomes

\[ I_C = \beta_C \nabla \cdot (-p_m I + \Sigma) - \beta_D f - \beta_C \nabla \psi_C + \frac{a^2}{10} [(\nabla n) \times (\nabla \times \mathcal{A}) + n \nabla (\nabla \cdot \mathcal{A})], \]  

(4.2)

while, for the D-phase,

\[ I_w = n v \nabla \cdot (-p_m + \Sigma) + n v f - n v \nabla \psi_D. \]  

(4.3)

Other than the last group of terms involving the derivatives of \( \mathcal{A} \) in (4.2) (which are a small correction due to the difference between the volume of the particles with center in the unit volume and the actual particle volume contained in the unit volume), these two momentum equation exhibit the expected symmetry between the two phases.

With the previous developments, the closure problem has been reduced to finding appropriate relations for \( S, \mathcal{A}, q_m \) introduced in (3.4), and \( f \). A procedure to accomplish this task in a systematic way with the help of direct numerical simulations is described in section 6.

5 Computational ensemble averaging

The plan that we follow is to parametrize the various particle averages appearing in the closure quantities in terms of the primary variables to be retained in the final equations, and to calculate the coefficients that arise in this step on the basis of the numerical results obtained by simulation.

Let us consider uniform systems first. In this case a powerful numerical technique consists in approximating an infinite suspension by the periodic repetition of a fundamental cell in which particles are randomly distributed. Numerically, this amounts to carrying out the simulation in a finite box with periodic boundary conditions (see e.g. Sangani and Yao 1988; Mo and Sangani 1994). In this case average quantities are spatially uniform and therefore they equal their volume average. On the basis of this remark, we may write, for example,

\[ n^0 w^0 = \frac{1}{V} \int d^3 x n^0 w^0, \]  

(5.1)

where the superscript 0 denotes spatially uniform quantities and the integration is over the fundamental cell with volume \( V \). Upon noting that in this uniform case \( n^0 = N/V \) and substituting here the definition (2.7) of particle average we have³

\[ \bar{w}^0 = \frac{1}{N!} \int d^N N P_0(N) \left( \frac{1}{N} \sum_{\alpha=1}^N w^\alpha \right), \]  

(5.2)

where we write \( P_0(N) \) rather than \( P(N) \) to emphasize the spatial uniformity of the ensemble.

While powerful, the approach just described is evidently only applicable to spatially uniform systems and therefore, while it can still be applied to obtain terms that enter the averaged equations as the divergence of suitable fluxes (e.g., the part of the stress that has a Newtonian

³From now on \( N \) denotes the number of particles in the fundamental cell, rather than the total number of particles in the system.
structure with an effective viscosity), it cannot be used to determine other differential terms with a different structure. For such terms one needs a non-uniform ensemble that we construct in the following way. Start with the uniform ensemble with probability distribution \( P_0 \) and imagine subjecting each particle center \( y^\alpha \) to an infinitesimal displacement \( y^\alpha \rightarrow y^\alpha - \epsilon F(y^\alpha) \) where \( F \) is a given deterministic vector function and \( \epsilon \) a small parameter. It is easy to show that the ensemble thus constructed has a non-uniform probability distribution given by

\[
P(N) = P_0 [1 + \epsilon \Phi(N)], \quad \text{where} \quad \Phi(N) = \sum_{\alpha=1}^{N} \sin k \cdot y^\alpha,
\]

is found by taking \( \nabla \cdot F(y) = \sin k \cdot y \) with the direction of \( k \) is along one of the sides of the fundamental cell and \( k = 2\pi/L \) (\( L \) is the side of the cell). In this way \( P(N) \) acquires the same periodicity as the underlying cell structure and the machinery of the Fourier series is available to express the spatially non-uniform average quantities. This approach is particularly powerful as the coefficients of the Fourier representation are projections – i.e., volume integrals – over suitable basis functions.

The numerical simulations on which this work is based have been conducted according to the method described in Mo and Sangani (1994). Ensembles with about 2000 configurations were used and, for every volume fraction, it was necessary to vary the cell size so as to be able to extrapolate to \( k = 0 \).

6 A method for the numerical closure of the equations

We are now ready to describe how the method for the systematic closure of the equations that we propose is implemented. For simplicity we consider as an example the symmetric part of the stress defined in (3.5).

We consider three different physical situations: (a) a suspension settling under gravity; (b) a suspension subjected to a uniform shear; (c) a suspension with a couple acting on the particles. For each one of these situations we construct the possible symmetric traceless tensors linear in the forcing. Consider for example the case of a settling suspension. If the suspension is uniform, any vector must be proportional to

\[
W = \frac{2}{9} \alpha^2 \rho_D - \rho_C \mu_C g,
\]

which represents the settling velocity of an isolated particle under the action of the force \( g \) per unit mass; clearly no tensors can be constructed linear in the forcing. If the suspension is allowed to be non-uniform as described in the previous section, however, the vector \( m = k/k \) becomes available and one can construct two traceless symmetric tensors,

\[
G_S = W^\perp m + m W^\perp, \quad G_M = (W \cdot m) \left( mm^\perp - \frac{1}{3} I \right),
\]

where \( W^\perp = (W \cdot m) m, \ W^\perp = (I - mm) \cdot W \). We thus expect that \( S \) be expressible in the form

\[
S = \sum_{j=8,6} (s^j M_G + s^j S_G) \epsilon_j,
\]

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where we put $\epsilon_+ = \epsilon \sin k \cdot x$, $\epsilon_- = \epsilon \cos k \cdot x$ for brevity; the coefficients $s^j_{M,W}$ can be calculated because $S$ is expressed in terms of computable quantities in (3.5).\(^4\) On the basis of a similar argument, it must be possible to represent the vector $u_m$ in the form

$$u_m - U_{\infty} = (U^c \epsilon_+ + U^c \epsilon_-) W^\perp,$$

(6.4)

where $U_{\infty}$ is the arbitrary velocity of the frame of reference.\(^5\) Again, the dimensionless coefficients $U^c_{\epsilon,\epsilon}^\perp$ appearing in this equation can be obtained numerically from the simulations.

Now we observe that, in a theory constructed in terms of the vectors $W$, $u_m$ and of the scalar $\beta_D$\(^6\) the only possible traceless symmetric tensors are $E_m$ defined in (3.8) and

$$E_\Delta = \frac{1}{2} \left[ \nabla u_\Delta + (\nabla u_\Delta)^T \right] - \frac{1}{3} (\nabla \cdot u_\Delta) I,$$

(6.5)

$$E_\nabla = \frac{1}{2} \left[ u_\Delta \nabla \beta_D + (u_\Delta \nabla \beta_D)^T \right] - \frac{1}{3} (u_\Delta \cdot \nabla \beta_D) I,$$

(6.6)

where $u_\Delta = W - u_m$ is the slip velocity. Terms such as $\nabla^2 E_m$ are also traceless, but their inclusion in the averaged equations would raise the order and require new boundary conditions; for this reason they are omitted. From the representation (6.4) one can explicitly calculate that

$$E_m = -k (U^c \epsilon_+ - U^c \epsilon_-) G_S,$$

(6.7)

with similar expressions for $E_\Delta$ and $E_\nabla$. Upon writing the closure relation as

$$S = 2\mu_{\text{eff}} E_m + 2 \mu_\Delta E_\Delta + 2 \mu_\nabla E_\nabla,$$

(6.8)

and substituting (6.3) in the left-hand side and (6.7) and similar relations for $E_\Delta, E_\nabla$ in the right-hand side, it is possible to express the effective viscosity $\mu_{\text{eff}}$ and the generalized viscosities $\mu_\Delta, \mu_\nabla$ in terms of the computed coefficients in (6.3), (6.4), etc. A similar procedure is followed for the other two cases of imposed shear and imposed couple.

As an example of the results derived by this technique we show in the table the effective viscosity $\mu_{\text{eff}}$ calculated for the three different situations simulated. The first column shows the values found for a sheared uniform suspension (see Mo and Sangani 1994 and others). The last two columns show the values obtained for a slightly non-uniform suspension undergoing sedimentation or having particles subject to an external couple. It should be stressed that it would be impossible to calculate $\mu_{\text{eff}}$ for these other two cases if the suspension were uniform because $E_m$ would vanish identically.

It is also found that, for a uniform suspension, both the isotropic and the the antisymmetric part of the mixture stress vanish. As for the symmetric part, the only tensor that is needed is $G_S$ (and its analogues for the shear and applied couple cases). As a consequence the closure relation (6.8) only contains the first term and the suspension behaves like a Newtonian fluid with a rheology characterized by an effective viscosity. In the case of non-uniform suspensions, all three terms in the closure relation (6.8) are non-zero and, therefore, the suspension rheology does not satisfy a purely Newtonian constitutive relation.

One important limitation of the work described is that all the computations have been conducted assuming a random hard-sphere probability distribution for the particles. Thus, the effects

\(^4\) Note that this step has a built-in check in the sense that something is evidently wrong if the numerical results cannot be well represented as in (6.3).

\(^5\) Since $\nabla \cdot u_m = 0$ due the incompressibility of the phases, no term proportional to $W^\perp$ is possible in (6.4).

\(^6\) We do not consider $p_m$ as $S$, by construction, is gauge invariant and therefore independent of $p_m$. 

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Shear  Sedimentation  Couple
15%  1.51  1.49  1.50
25%  2.10  2.03  2.07
35%  3.02  2.91  3.01

Table 1: Effective viscosities calculated for the three different situations simulated.

of a flow-induced microstructure are disregarded. Additional efforts to include such effects are, of course, necessary.

The work presented here is a summary of an extensive investigation that is reported in much greater detail in Marchioro et al. (1999a, 1999b, 1999c).

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References


