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John D. Ramshaw
Portland State University, jdramshaw@yahoo.com

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Self-Consistent Effective Binary Interaction Approximation For Strongly Coupled Multifluid Dynamics[1)]

John D. Ramshaw
Lawrence Livermore National Laboratory, University of California, Livermore, CA, U. S. A.

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Abstract

An improved self-consistent effective binary diffusion approximation for multicomponent diffusion was recently described [1]. Here we develop an analogous self-consistent effective binary interaction (SCEBI) approximation for simplifying multifluid dynamical descriptions in which each fluid is strongly coupled to the other fluids by pairwise frictional forces. The net drag force on each fluid is the summation of the drag forces due to each of the other fluids. This summation is approximated by a single term proportional to the velocity of the fluid in question relative to an appropriately weighted average velocity. This approximation permits an explicit numerical solution for the fluid velocities even when the drag terms are evaluated at the advanced time level to avoid explicit stability restrictions on the time step.

Introduction and Summary

An improved self-consistent effective binary diffusion (SCEBD) approximation for multicomponent diffusion was recently described [1]. This approximation is used to obtain an explicit expression for the diffusion velocities without solving the full Stefan-Maxwell equations. Our purpose here is to develop an analogous approximation within the context of multifluid dynamical models in which each fluid satisfies its own momentum equation and is strongly coupled to the other fluids by pairwise frictional interaction forces. Such models are used, for example, in plasma physics [2] and multiphase flow [3]. In models of this type, the net drag force on each fluid is obtained by summing up the individual pairwise drag forces due to each of the other fluids, which are presumed to be proportional to the relative velocities of the fluid pairs. We shall approximate this summation by a single term proportional to the velocity of the fluid in question relative to an appropriately weighted average velocity. This approximation will be referred to as the self-consistent effective binary interaction (SCEBI) approximation. It is self-consistent in the sense that it introduces no net force into the total momentum of the multifluid mixture, which would of course be undesirable.

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The motivation for the SCEBI approximation is primarily computational. When the friction coefficients are large, the multifluid dynamical equations become stiff. If these equations were solved using an explicit numerical scheme, the stiffness would require the use of very small time steps to satisfy the explicit stability restriction. This restriction may be avoided by using an implicit numerical scheme in which the drag forces are evaluated at the advanced time level. This produces a linear system of equations for the advanced-time fluid velocities. These equations bear a strong formal resemblance to the Stefan-Maxwell equations, and are accordingly susceptible to an SCEBI approximation which is closely analogous to the SCEBD approximation. The SCEBI approximation permits an explicit solution for the advanced-time fluid velocities, thereby avoiding the solution of the original linear implicit system on each time step. Of course, this approximation is sensible only when there are at least three interacting fluids, and it is worthwhile only when the number of fluids is large enough that it becomes inconvenient or unpleasant to solve the linear implicit system directly.

The SCEBI approximation is only needed when the friction coefficients are large. However, if all of these coefficients are uniformly very large everywhere, then the multifluid description can be reduced to a diffusional description [4] to which the original SCEBD approximation could have been applied. The rationale for the SCEBI approximation is that it extends the previous SCEBD approximation to a wider class of multifluid flow problems in which large friction coefficients present unacceptable explicit stability restrictions but the diffusional limit cannot be invoked. Situations of this type include problems in which (a) some but not all of the friction coefficients are large, (b) the friction coefficients are large enough to impose unacceptable explicit stability conditions, but not large enough to reach the diffusional limit, and (c) some or all of the friction coefficients are large locally (or temporarily), but not everywhere.

2. The multifluid momentum equations

We consider multifluid momentum equations of the general form

$$\frac{\partial(\rho_i \mathbf{u}_i)}{\partial t} = \mathbf{S}_i + \sum_j \alpha_{ij}(\mathbf{u}_j - \mathbf{u}_i) \tag{1}$$

where $\mathbf{u}_i$ and ρ_i are respectively the velocity and partial mass density of fluid i, the α_{ij} are friction coefficients, and $\mathbf{S}_i$ represents convective, viscous, and source terms, the form of which is irrelevant for present purposes. Newton's third law implies that $\alpha_{ij} = \alpha_{ji}$. The term $j = i$ does not contribute to the sum in equation (1), so we are free to define $\alpha_{ii} = 0$ for later convenience. It is also convenient to define $\alpha_i = \Sigma_j \alpha_{ij}$. If equation (1) is summed over i, the friction terms cancel in pairs and we obtain $\partial(\rho\mathbf{u})/\partial t = \Sigma_i \mathbf{S}_i$, where $\rho = \Sigma_i \rho_i$ is the total mass density and $\rho\mathbf{u} = \Sigma_i \rho_i \mathbf{u}_i$ is the total momentum per unit volume. This cancellation occurs because the friction terms represent a conservative momentum exchange between the fluids with no net creation or destruction of total momentum.

Equations (1) are not closed by themselves, and must be solved simultaneously with the continuity, energy, and state equations for each fluid and/or the mixture as a whole. This can rarely be done analytically, so it is usually necessary to resort to numerical

methods; e.g., finite differences, finite elements, or spectral methods. These methods differ primarily in the way they approximate the spatial derivatives contained in $\mathbf{S}_i$, so these differences are irrelevant for present purposes. We may therefore focus attention on the time dependence, which is usually approximated by means of finite differences with respect to a sequence of discrete times t_n separated by time steps $\Delta t = t_{n+1} - t_n$. The numerical approximation to a quantity $Q(t)$ at time $t = t_n$ is denoted by Q^n. The simplest numerical approximation to equation (1) is the explicit scheme

$$\frac{\rho_i^{n+1}\mathbf{u}_i^{n+1} - \rho_i^n \mathbf{u}_i^n}{\Delta t} = \mathbf{S}_i^n + \sum_j \alpha_{ij}^n (\mathbf{u}_j^n - \mathbf{u}_i^n) \tag{2}$$

An alternative scheme with superior stability behaviour is the implicit (backward Euler) scheme

$$\frac{\rho_i^{n+1}\mathbf{u}_i^{n+1} - \rho_i^n \mathbf{u}_i^n}{\Delta t} = \mathbf{S}_i^n + \sum_j \alpha_{ij}^n (\mathbf{u}_j^{n+1} - \mathbf{u}_i^{n+1}) \tag{3}$$

We presume that ρ_i^{n+1} is known, having already been determined by prior solution of the continuity equations. (Alternatively, equation (1) could have been written in an equivalent "non-conservative" form with ρ_i outside the time derivative and $\mathbf{S}_i$ redefined accordingly, in which case ρ_i^{n+1} would be replaced by ρ_i^n in equations (2) and (3).) Equation (2) explicitly determines the $\mathbf{u}_i^{n+1}$ in terms of known quantities, whereas equation (3) constitutes a linear system of equations for the $\mathbf{u}_i^{n+1}$. Notice that both these schemes preserve the essential property that the friction terms cancel out when summed over i, so that there is no net frictional force or source of total momentum in the mixture as a whole. This property is not preserved by certain other obvious choices such as $\Sigma_j \alpha_{ij}^n (\mathbf{u}_j^n - \mathbf{u}_i^{n+1})$.

The stability properties of equations (1)–(3) are derived in the Appendix, which confirms one's intuitive expectation that (a) the original differential system (1) is inherently stable, (b) the explicit scheme (2) is conditionally stable but requires the use of very small Δt when any of the α_{ij} is large, and (c) the implicit scheme (3) is unconditionally stable for all Δt. We are concerned with situations in which the values of α_{ij} are large enough that the use of the explicit scheme (2) becomes undesirable or unacceptable. We therefore restrict attention to the implicit scheme (3), which allows the use of arbitrarily large values of Δt. The price that must be paid for this advantage is the need to generate an exact or approximate solution to the linear system of equation (3).

3. The SCEBI approximation

For simplicity we shall suppress the superscripts $n+1$ in equation (3), as well as the superscript n on α_{ij}. Equation (3) then becomes

$$\frac{\rho_i \mathbf{u}_i}{\Delta t} = \mathbf{T}_i + \sum_j \alpha_{ij}(\mathbf{u}_j - \mathbf{u}_i) = \mathbf{T}_i - \alpha_i \mathbf{u}_i + \sum_j \alpha_{ij}\mathbf{u}_j \tag{4}$$

where

$$\mathbf{T}_i = \frac{\rho_i^n \mathbf{u}_i^n}{\Delta t} + \mathbf{S}_i^n \tag{5}$$

Summing equation (4) over i, the friction terms cancel out as previously discussed and we obtain

$$\sum_i \rho_i \mathbf{u}_i = \rho \mathbf{u} = \Delta t \sum_i \mathbf{T}_i = \rho^n \mathbf{u}^n + \Delta t \sum_i \mathbf{S}_i^n \tag{6}$$

which explicitly expresses $\rho \mathbf{u} = \rho^{n+1} \mathbf{u}^{n+1}$ in terms of known quantities.

Equation (4) is a linear system of equations for the unknown quantities $\mathbf{u}_i$. This system is formally identical to the Stefan-Maxwell equations of diffusion theory [1, 4] except for the additional diagonal term $\rho_i \mathbf{u}_i / \Delta t$. We therefore seek to approximate it in the same way that the Stefan-Maxwell equations may be approximated to obtain the SCEBD approximation [1]. In this approximation, the friction coefficients α_{ij} are approximated by $w_i w_j (1 - \delta_{ij})$, where δ_{ij} is the Kronecker delta and the w_i are yet to be determined. Equation (4) then becomes

$$\frac{\rho_i \mathbf{u}_i}{\Delta t} = \mathbf{T}_i - \alpha_i \mathbf{u}_i + w_i \sum_{j \neq i} w_j \mathbf{u}_j = \mathbf{T}_i - (\alpha_i + w_i^2) \mathbf{u}_i + w_i w \mathbf{a} \tag{7}$$

where $w = \Sigma_i w_i$ and $w\mathbf{a} = \Sigma_i w_i \mathbf{u}_i$. Summing equation (7) over i, we obtain

$$\rho \mathbf{u} = \Delta t \sum_i \mathbf{T}_i + \Delta t \sum_i [w_i (w - w_i) - \alpha_i] \mathbf{u}_i \tag{8}$$

In order to prevent our approximation from introducing an artificial net force into the total momentum equation, we must require our approximate $\mathbf{u}_i$ to satisfy equation (6). The second summation in equation (8) must therefore vanish identically, which may be ensured by setting

$$w_i (w - w_i) = \alpha_i \tag{9}$$

Equation (9) now defines the quantities w_i, and we observe that this is identical to the definition adopted on other grounds in the SCEBD approximation [1]. The present considerations provide a somewhat more compelling rationale for this definition, which is now seen to be essential for momentum conservation. Unfortunately, equation (9) cannot in general be solved for the w_i in closed form [1], so these quantities must be approximated as discussed below.

Combining equations (7) and (9), we obtain

$$\frac{\rho_i \mathbf{u}_i}{\Delta t} = \mathbf{T}_i + w_i w (\mathbf{a} - \mathbf{u}_i) \tag{10}$$

which manifestly satisfies equation (6). Comparison with equation (4) shows that the summation of drag forces over all the other fluids has now been approximated by a single drag term proportional to the velocity of fluid i relative to the w_i-weighted mean velocity $\mathbf{a}$. It follows from equation (9) that the coefficient $w_i w$ in equation (10) may be

written in the form

$$w_i w = \left(1 - \frac{w_i}{w}\right)^{-1} \alpha_i \tag{11}$$

so that only the normalized ratios w_i/w need to be approximated. Useful approximations for these quantities are given in [1].

Equation (10) may be rearranged into the form

$$\rho_i \mathbf{u}_i = \frac{\beta_i \mathbf{T}_i}{w_i w} + \beta_i \mathbf{a} \tag{12}$$

where

$$\beta_i = \left(\frac{1}{\rho_i} + \frac{1}{\Delta t w_i w}\right)^{-1} = \frac{\rho_i \Delta t w_i w}{\rho_i + \Delta t w_i w} \tag{13}$$

However, equation (12) is not yet an explicit expression for $\mathbf{u}_i$ because $\mathbf{a}$ has not yet been determined. This may be done by summing equation (12) over i to obtain

$$\rho \mathbf{u} = \beta \mathbf{a} + \sum_i \frac{\beta_i \mathbf{T}_i}{w_i w} \tag{14}$$

where $\beta = \Sigma_i \beta_i$. Combining equations (12) and (14), we obtain

$$\begin{aligned} \rho_i \mathbf{u}_i &= \frac{\beta_i}{\beta} \rho \mathbf{u} + \frac{\beta_i \mathbf{T}_i}{w_i w} - \frac{\beta_i}{\beta} \sum_j \frac{\beta_j \mathbf{T}_j}{w_j w} \\ &= \frac{\beta_i}{\beta} \rho \mathbf{u} + \frac{\beta_i}{\alpha_i}\left(1 - \frac{w_i}{w}\right)\mathbf{T}_i - \frac{\beta_i}{\beta} \sum_j \frac{\beta_j}{\alpha_j}\left(1 - \frac{w_j}{w}\right)\mathbf{T}_j \end{aligned} \tag{15}$$

where $\rho \mathbf{u}$ is of course given by equation (6), and use has been made of equation (11).

Equation (15) is our final expression for $\mathbf{u}_i$ in the SCEBI approximation. In the limit of large Δt, $\beta_i \to \rho_i$, $\beta \to \rho$, $\mathbf{T}_i \to \mathbf{S}_i$, equation (4) becomes formally identical to the Stefan-Maxwell equations, and equation (15) becomes formally identical to the expression for the diffusion velocities in the SCEBD approximation [1]. The overall accuracy of the SCEBI approximation would be expected to be similar to that of the SCEBD approximation, which has previously been studied [1]. If this level of accuracy is not sufficient, it might be possible to improve upon it by using the SCEBI approximation as the predictor step in a predictor-corrector approximation, in which a corrected value of $\mathbf{u}_i$ is obtained by using equation (15) to evaluate the term $\Sigma_j \alpha_{ij}(\mathbf{u}_j - \mathbf{u}_i)$ in equation (4). The SCEBI approximation could also be used as an initialization procedure for the solution of equation (4) by iterative methods.

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Appendix

Stability properties of the multifluid momentum equations

For stability purposes we may restrict attention to the case in which the ρ_i and $\mathbf{S}_i$ are constant in time. Linearization removes the source terms $\mathbf{S}_i$ in the usual way, whereupon equation (1) reduces to

$$\frac{\partial \mathbf{u}_i}{\partial t} = -\sum_j M_{ij}\mathbf{u}_j \tag{A1}$$

where $M_{ij} = (1/\rho_i)(\alpha_i\delta_{ij} - \alpha_{ij})$, and δ_{ij} is the Kronecker delta. Equation (A1) is stable if $\mathrm{Re}\,\lambda_i \geq 0$ for all i, where the λ_i are the eigenvalues of the matrix M_{ij}. In spite of the asymmetry of M_{ij}, the λ_i are in fact all real, since it is easy to show that the real symmetric matrix $N_{ij} = (1/\sqrt{\rho_i\rho_j})(\alpha_i\delta_{ij} - \alpha_{ij})$ has the same eigenvalues as M_{ij}. The diagonal elements of N_{ij} are all positive, and one readily verifies that $\Sigma_j \alpha_{ij}/\sqrt{\rho_i\rho_j} = \alpha_i/\rho_i$, so that N_{ij} is diagonally semidominant. Its eigenvalues are therefore all nonnegative, a conclusion which may easily be directly confirmed by means of the Gershgorin circle theorem. Thus $\lambda_i \geq 0$ and equation (A1) is stable.

The amplification matrix for the explicit scheme of equation (2) is $\delta_{ij} - \Delta t M_{ij}$, the eigenvalues of which are $\xi_i = 1 - \lambda_i\Delta t$. The stability condition for this scheme is that $|\xi_i| \leq 1$ for all i, or $\lambda_{\max}\Delta t \leq 2$, where $\lambda_{\max} = \max_i \lambda_i$. The λ_i will generally scale linearly with the α_i, so this condition requires unacceptably small Δt when the friction coefficients are large.

The amplification matrix for the implicit scheme of equation (3) is the inverse of the matrix $\delta_{ij} + \Delta t M_{ij}$, the eigenvalues of which are $\mu_i = 1 + \lambda_i\Delta t$. The stability condition for this scheme is that $|\mu_i| \geq 1$ for all i. This condition is always satisfied, so the implicit scheme of equation (3) is unconditionally stable for all Δt.

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Dr. John D. Ramshaw
Lawrence Livermore National Laboratory
University of California
P. O. Box 808, L-018
Livermore, CA 94551
U. S. A.