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A Lattice-BGK Model for Miscible Fluids

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A previous lattice-kinetic model based on the Bhatnagar-Gross-Krook (BGK) approximation of the Boltzmann equation is extended to model a fluid consisting of an arbitrary number of miscible components. The extended model features Galilean invariant and noise-free dynamics as well as a velocity-independent pressure. The macrodynamical equations are derived using a Chapman-Enskog expansion and shown to be similar to the governing equations for a convective-diffusive mixture of fluids. Expressions for the transport coefficients, which are determined by free numerical parameters in the model, are obtained and numerically verified. The utility of the model is demonstrated by a simulation of 2-dimensional Rayleigh-Taylor instability.

1 Introduction

Since the pioneering work of Frisch et al[10], and of d'Humières et al[6], in which lattice gas cellular automata (LGA) in 2- and 3-dimensions respectively were introduced that captured the behavior of physical gases, these models have proven to be viable alternatives to conventional computational methods for simulating hydrodynamical phenomena[8]. Although the LGA has many advantages as numerical schemes, such as its intrinsic stability due to the boolean numerics, the ease with which boundary conditions can be incorporated, and high parallelizability, it suffers from several disadvantages. The severest one is the presence of a high level of statistical fluctuations in the microscopic dynamics, thus requiring the use of coarse-grain averages over space or time to obtain hydrodynamic variables. In addition, the dynamics of the LGA is not Galilean invariant, due to the presence of a density-dependent factor in the nonlinear advective term in the macrodynamical momentum equation. This factor also affects the pressure term, causing it to depend on the velocity. Also, spurious invariants may be present because of the oversimplified dynamics.

In this paper we show how to extend a model originally proposed in [16, 15], which is based on the Bhatnagar-Gross-Krook (BGK) approximation of the Boltzmann equation[2], to describe a fluid consisting of several miscible components. The models in [16, 15, 5] (henceforth refered to as LBGK models) are motivated by the restoring of Galilean invariance to the dynamics while at the same time retaining the advantages of the LGA and the lattice-Boltzmann equation[1] (LBE) models (in particular the absence of statistical noise in the latter). The LGA and LBE have been used to model miscible and immiscible mixtures before[3, 7, 12, 11]. In [12] for example, a low-diffusivity LBE model for a miscible two-phase fluid has been proposed that involves the use of non-local interactions. The procedure involves collision rules that require the maximization of the projection of the species flux on the species concentration gradient at each collision step. This procedure is computationally expensive and its extension to model a three-phase fluid appears to require substantially more computational resources than does the two-phase model[11]. The model we propose is simple, efficient, and can be extended trivially to an arbitrary number of components. The method is to define the appropriate local equilibrium population for a mixture of fluids and then employ discrete analogs of the BGK equations to compute the time evolution of the average population of each species. The generalization to a reacting mixture, in which particle sources and particle type exchanges are allowed, is straightforward[18].

The paper will be organized as follows: In Section 2, we briefly review the LBGK model proposed in [16], describe the extension of the model to miscible mixtures and derive the macrodynamical equations and the transport coefficients using a Chapman-Enskog analysis. In Section 3, we will numerically verify the theoretical predictions for the transport coefficients and also demonstrate the utility of the model with a 2-dimensional simulation of the growth of miscible fingers and bubbles on a Rayleigh-Taylor

unstable interface.

2 Miscible Fluids Model

2.1 The LBGK Model

In the spirit of the so-called LBE model with enhanced collisions[1], in which the elements of the collision matrix are considered as free parameters that are adjusted to obtain desired values of the transport coefficients, the LBGK model uses a similar evolution equation

$$N_{pi}(\mathbf{x}+\mathbf{c}_{pi}, t+1) = N_{pi}(\mathbf{x}, t) - \omega \left[N_{pi}(\mathbf{x}, t) - N^e_{pi}(\mathbf{x}, t)\right] \quad (1)$$

in which the collision matrix is replaced by a single parameter ω. Here N_{pi} is the average population of particles with velocity $\mathbf{c}_{pi}$ (the indices p and i are explained below), and $\mathbf{x}$ is the position vector of a node on the lattice. A generic choice for the equilibrium population, $N^e_{pi}(\mathbf{x}, t)$, is

$$N^e_{pi} = t_p \rho \left[1 + \frac{c_{pi\alpha} u_\alpha}{c_s^2} + \frac{u_\alpha u_\beta}{2c_s^2}\left(\frac{c_{pi\alpha} c_{pi\beta}}{c_s^2} - \delta_{\alpha\beta}\right)\right] \quad (2)$$

Here α and β are indices for the Cartesian components of the particle velocity (Greek letters shall henceforth denote the Cartesian components of a vector). The hydrodynamic velocity and density are denoted by u_α and ρ respectively. The additional index p is equal to the square of the modulus of the particle velocity $c_{pi\alpha}$ and has been used to distinguish between velocities having different moduli. The index i denotes the different velocities in the same speed class p. The constant c_s is proportional to a weighted average of the $c_{pi\alpha}$'s and is identified as the speed of sound in the model. Finally, t_p is a weighting factor, which depends on p and which is adjusted to obtain isotropic fourth-order tensor products of $c_{pi\alpha}$ and to ensure Galilean invariance of the dynamics. The choice (2) for the equilibrium population, when used together with (1), can be shown to lead to macrodynamical equations, which, when truncated after the second order in u_α, are similar to the Navier-Stokes equations[17].

Figure 1 shows an example of a lattice, together with its set of possible velocities, drawn from the class of square, cubic and hypercubic lattices to which the model may be applied[15]. We have followed the notation in [16] and denoted the lattices by DxQy, where x indicates the spatial dimension and y is the total number of different velocities. In this paper we will deal with the DxQy class of lattices only. However we emphasize that the idea that a weighting factor be used to insure the isotropy of the fourth-order tensor product of $c_{pi\alpha}$ can be applied to lattices not of the DxQy type as well[16].

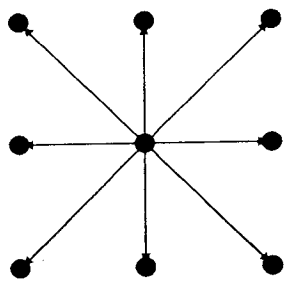

Figure 1: The D2Q9 lattice.

In the macrodynamical equations, we are always concerned with the moments of $\mathbf{c}_{pi}$. These involve the weighting factor t_p, which is determined by the requirement that $\sum_p t_p b_p = 1$ (where b_p denotes the number of different velocities in the same speed class) and that the fourth-order tensor product of velocities $\sum_{p,i} t_p c_{pi\alpha} c_{pi\beta} c_{pi\gamma} c_{pi\delta}$ is isotropic and also that the dynamics be Galilean invariant. The values of t_p for the DxQy lattices with various values of x and y may be found in [16]. For these lattices, the following relations hold

$$\sum_{i=1}^{b_p} c_{pi\alpha_1} c_{pi\alpha_2} \cdots c_{pi\alpha_m} = 0, \quad m = 1, 3, 5, \cdots \quad (3)$$

$$\sum_p t_p \sum_{i=1}^{b_p} c_{pi\alpha} c_{pi\beta} = c_s^2 \delta_{\alpha\beta} \quad (4)$$

$$\sum_p t_p \sum_{i=1}^{b_p} c_{pi\alpha} c_{pi\beta} c_{pi\gamma} c_{pi\delta} = c_s^4 \left(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\delta\beta}\delta_{\gamma\alpha} + \delta_{\gamma\beta}\delta_{\alpha\delta}\right) \quad (5)$$

where

$$c_s^2 = \frac{1}{3} \quad (6)$$

is a value that is independent of the spatial dimension but is correct for DxQy lattices only. Other values of c_s apply when the lattice is not of the DxQy type[16]. The relations (3)–(5) will be used in the derivation of the macrodynamical equations in Section 2.2.

2.2 Extended Model

We first extend the definitions of the mass and momentum densities for a simple fluid to a mixture of fluids[4]. Let N_{rpi} denote the average population of particles of the rth species with velocity $c_{pi\alpha}$. The total mass density ρ is given by

$$\rho = \sum_{r,p,i} N_{rpi}(\mathbf{x}, t). \tag{7}$$

while the mass density ρ_r of the rth species is

$$\rho_r = \sum_{p,i} N_{rpi} \tag{8}$$

Note that the sum is not taken over r in (8). Also, the space and time dependence of N_{rpi} in (8) is implied, and will be implied henceforth in the analysis. The velocity u_α in a mixture of fluids is defined as the total momentum of unit mass of fluid. That is, it is defined via the relation

$$\rho u_\alpha = \sum_{r,p,i} N_{rpi} c_{pi\alpha}. \tag{9}$$

The additional hydrodynamical variables relevant to a mixture are those that describe the local composition of the fluid. These are the concentration c_r of the rth species and are defined as

$$c_r = \frac{\rho_r}{\rho} \tag{10}$$

In a mixture consisting of nonreacting species, the local concentration of each species changes through the mechanical mixing of the fluid and through mutual diffusion. From the definition (10), the c_r's satisfy

$$\sum_r c_r = 1. \tag{11}$$

Hence for a mixture having a total of R species, there will be $(R-1)$ independent equations of motion for the c_r's.

The generalization of (1) to a mixture of fluids is taken to be

$$N_{rpi}(x_\alpha + c_{pi\alpha}, t+1) = N_{rpi}(x_\alpha, t) - \omega_r \left[N_{rpi}(x_\alpha, t) - N^e_{rpi}(x_\alpha, t)\right] \tag{12}$$

where possibly different relaxation parameters ω_r may be assigned to each species. The local equilibrium population N^e_{rpi} can be inferred from a generalization of the H-theorem for a mixture of fluids and is given by

$$N^e_{rpi} = c_r N^e_{pi} \tag{13}$$

with N^e_{pi} given by (2). Equation (13) may be taken to imply that the dynamics are attracted to separate equilibrium states corresponding to each component but which are coupled via the velocity u_α.

The equations governing the large-scale dynamics of (12), in which the local equilibrium distribution N^e_{rpi} is taken to be given by (13), will now be derived using a Chapman-Enskog expansion. Since similar expansions for the LGA and LBE have been used before (see for example [8, 9]), we will only outline here the steps necessary to obtain expressions for the transport coefficients. We assume a weak disequilibrium expansion

$$N_{rpi} = N^e_{rpi} + \epsilon N^{(1)}_{rpi} + \epsilon^2 N^{(2)}_{rpi} + \cdots \tag{14}$$

where ϵ is the appropriate Knudsen number for the flow. The space and time derivatives are expressed in terms of multiple-scale variables as

$$\partial_\alpha = \epsilon \partial_\alpha \tag{15}$$

$$\partial_t = \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2}. \tag{16}$$

Since mass and momentum are conserved, it follows from (12) and (14) that

$$\sum_{r,p,i} \omega_r N^{(j)}_{rpi} = 0, \qquad j > 0 \tag{17}$$

$$\sum_{r,p,i} \omega_r N^{(j)}_{rpi} c_{pi\alpha} = 0, \qquad j > 0. \tag{18}$$

Also implicit in the lattice-BGK model is that the non-equilibrium populations $N^{(j)}_{rpi}$, $j > 0$, satisfy the constraints

$$\sum_{r,p,i} N^{(j)}_{rpi} = 0, \qquad j > 0 \tag{19}$$

$$\sum_{r,p,i} N^{(j)}_{rpi} c_{pi\alpha} = 0, \qquad j > 0 \tag{20}$$

$$\sum_{p,i} N^{(j)}_{rpi} = 0, \qquad j > 0 \tag{21}$$

where (21) expresses the conservation of the mass density of each species. However, $\sum_{p,i} N^{(j)}_{rpi} c_{pi\alpha}$ does not vanish in general, since there can be transfer of momentum from the particles of one species to particles of a different species.

By expanding N_{rpi} in a Taylor series about x_α and t, and using (15) and (16), we obtain first and second order equations in ϵ; we then take the zeroth and first moments of $\mathbf{c}_{pi}$ in these equations to obtain

$$\partial_{t_1} \rho + \partial_\alpha (\rho u_\alpha) = 0 \tag{22}$$

$$\partial_{t_1} (\rho u_\alpha) + \partial_\beta J_{\alpha\beta} = 0 \tag{23}$$

where it can be shown using (5) that

$$J_{\alpha\beta} = c_s^2 \rho \delta_{\alpha\beta} + \rho u_\alpha u_\beta \tag{24}$$

Using (17), (18), (22) and (23), we also obtain

$$\partial_{t_2} \rho = 0 \tag{25}$$

$$\partial_{t_2} \rho u_\alpha + \partial_\beta \sum_{r,p,i} (1 - \frac{\omega_r}{2}) N^{(1)}_{rpi} c_{pi\alpha} c_{pi\beta} = 0. \tag{26}$$

Equation (25) implies that there is no diffusion of the total mass density, while (26) accounts for the effect of viscous momentum fluxes.

Following the development of the Chapman-Enskog expansion, $N^{(1)}_{rpi}$ will now be expressed in terms of derivatives of the macroscopic variables. Here we will also need equations corresponding to (22) and (23) in which the index r is not summed over. These are

$$\partial_{t_1} \rho_r + \partial_\alpha (\rho_r u_\alpha) = 0 \tag{27}$$

$$\partial_{t_1} (\rho_r u_\alpha) + c_s^2 \partial_\alpha \rho_r + \partial_\beta (\rho_r u_\alpha u_\beta) = -\omega_r \sum_{p,i} N^{(1)}_{rpi} c_{pi\alpha}. \tag{28}$$

Note that $\sum_{p,i} N^{(1)}_{rpi} c_{pi\alpha}$ corresponds to the non-equilibrium mass flux of species r and does not vanish in general. To $\mathcal{O}(u)$ this flux is given by

$$\sum_{p,i} N^{(1)}_{rpi} c_{pi\alpha} = -\frac{1}{\omega_r} \left[\partial_{t_1} (\rho_r u_\alpha) + c_s^2 \partial_\alpha \rho_r \right] + \mathcal{O}(u^2). \tag{29}$$

It is easy to show using (23), (24) and the relation $\rho_r = \rho c_r$ that $\partial_{t_1} (\rho c_r u_\alpha) = -c_s^2 c_r \partial_\alpha \rho + \mathcal{O}(u^2)$. Hence

$$\sum_{p,i} N^{(1)}_{rpi} c_{pi\alpha} = \frac{-c_s^2}{\omega_r} \rho \partial_\alpha c_r + \mathcal{O}(u^2). \tag{30}$$

Using (13), (27) and (28), we obtain finally,

$$N^{(1)}_{rpi} = -\frac{t_p}{\omega_r} \left[\left(\frac{c_{pi\alpha} c_{pi\beta}}{c_s^2} - \delta_{\alpha\beta} \right) \partial_\beta (\rho_r u_\alpha) + c_{pi\alpha} \rho \partial_\alpha c_r \right] \tag{31}$$

It is easy to check that the conditions (19)–(21) are satisfied by $N^{(1)}_{rpi}$. Substituting (31) into (26), we obtain finally

$$\partial_{t_2} (\rho u_\alpha) - \partial_\beta \left\{ \frac{c_s^2}{2} \left(\frac{2}{\omega} - 1 \right) \left[\partial_\alpha (\rho u_\beta) + \partial_\beta (\rho u_\alpha) \right] \right\} = 0 \tag{32}$$

where we have defined the "equivalent" relaxation parameter ω via the relation

$$\frac{1}{\omega} = \sum_r \frac{c_r}{\omega_r}. \tag{33}$$

Equations (22), (23), (25), and (32), i.e the dynamical equations from the two separated time scales $1/\epsilon$ and $1/\epsilon^2$, will now be reconstituted to obtain the macrodynamical equations for the model. The equation of continuity is obtained from (22) and (25) by multiplying the former by ϵ and the latter by ϵ^2 and then adding the two equations; and the Navier-Stokes equation is obtained from (23) and (32) in the same manner. We obtain

$$\partial_t \rho + \partial_\alpha (\rho u_\alpha) = 0 \tag{34}$$

$$\partial_t (\rho u_\alpha) + \partial_\beta (\rho u_\alpha u_\beta) = -c_s^2 \partial_\alpha \rho + \partial_\beta \left[\nu \partial_\beta (\rho u_\alpha) + \zeta \partial_\alpha (\rho u_\beta) \right] \tag{35}$$

where the coefficients of shear viscosity ν and bulk viscosity ζ are given by

$$\nu = \zeta = \frac{c_s^2}{2} \left(\frac{2}{\omega} - 1 \right). \tag{36}$$

We will now obtain the equation of motion for the concentration c_r. The equation corresponding to (25) in which indices p and i are not summed over is

$$\partial_{t_2} \rho_r - \left(\frac{\omega_r}{2} - 1 \right) \partial_\alpha \left(\sum_{p,i} N^{(1)}_{rpi} c_{pi\alpha} \right) = 0 \tag{37}$$

which shows that there in general the species mass densities changes on the diffusive time scale. Substituting (30) into (37), we obtain, correct to $\mathcal{O}(u)$, the convective-diffusive equations for mass density of each species

$$\partial_t (\rho c_r) + \partial_\alpha (\rho c_r u_\alpha) = \partial_\alpha (D_r \rho \partial_\alpha c_r) \tag{38}$$

where the diffusivity is given by

$$D_r = \frac{c_s^2}{2} \left(\frac{2}{\omega_r} - 1 \right). \tag{39}$$

For a mixture of two species with $\rho_1 = \rho_2$ and $\omega_1 = \omega_2$, we find that $D_1 = D_2 = \nu$. This is not surprising, since the concentration variable is analogous to the temperature in the BGK approximation and the Prandtl number (ratio of viscosity to temperature diffusivity) of a gas that satisfies the BGK equation is unity. Also, notice that since $\sum_{p,i} N^{(1)}_{rpi} c_{pi\alpha}$ does not vanish in general, (18) implies all but one of the

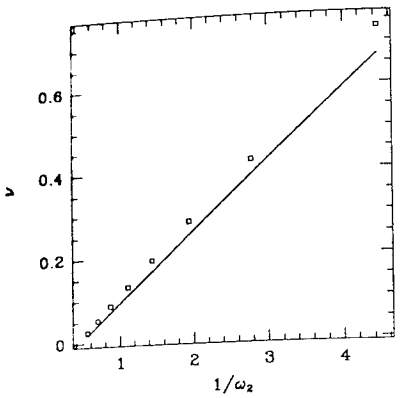

Figure 2: The shear viscosity ν for a two-species fluid as a function of $1/\omega_2$ for a fixed value of $\omega_1 = 1.8$. The solid line through the experimental points corresponds to the prediction of the Chapman-Enskog analysis, and the measurements are made on a 32×32 D2Q9 lattice.

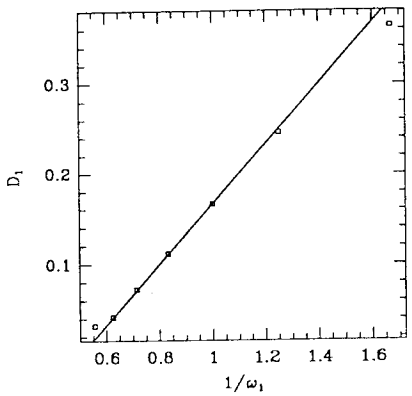

Figure 3: The diffusivity D_1 for a two-species fluid as a function of $1/\omega_1$ for a fixed value of $\omega_2 = 1.8$. The solid line through the experimental points corresponds to the prediction of the Chapman-Enskog analysis, and the measurements are made on a 32×32 D2Q9 lattice.

ω_r's are freely adjustable. Thus in practice one prescribes values for the equivalent relaxation parameter ω and ω_r, $r = 1, 2, \cdots, R-1$ (where R is the total number of species) and uses the equations (12) for $N_{rpi}, r = 1, 2, \cdots, R-1$, together with an additional equation for the total population $N_{pi} \equiv \sum_{r,p,i} N_{rpi}$ (which is exactly similar in form to (1) with the corresponding N^e_{pi} given by (2)) to compute the evolution of the dynamics.

3 Numerical Experiments

Here we present measurements of the diffusivity and shear viscosity for a two-species fluid modeled on a D2Q9 lattice with 1 rest and 8 moving particles. Figure 2 shows ν as a function of ω_1 for a fixed value of $\omega_2 = 1.8$. Here the density is the same for both species and ν is obtained by measuring the relaxation of a sinusoidal shear fluctuation. Figure 3 shows the diffusivity D_1 as a function of ω_1 for fixed $\omega_2 = 1.8$. It is obtained by measuring the decay of a sinusoidal perturbation in the concentration. The solid lines in these figures represent the values predicted by the Chapman-Enskog analysis.

One possible application of our model is the simulation of two-fluid miscible displacement in a Hele-Shaw cell[14, 20]. The Hele-Shaw cell is an analog for the study of two-dimensional two-phase flow in porous media[19, 13]. A qualitative feature of miscible displacements which our model should reproduce is the instability phenomenon known as "viscous fingering". We test the feasibility of our model for simulating such flows by performing a simulation of a flow consisting of two layers of fluid of the same density, initially with a random perturbation on the interface, and subsequently accelerated towards each other. The body forces on the fluids can be incorporated by simply adding a term of the form $\frac{t_p}{c_s^2} \rho_r c_{pi\alpha} f_{r\alpha}$, where $f_{r\alpha}$ is the force per unit volume, to the r.h.s of (13). It can be shown easily that this term reproduces the required body force term in the Navier-Stokes equation. Figure 4 shows the concentration field after the two fluids have penetrated into each other for some time. It is seen that the diffusive dynamics furnished by the model, coupled with a Rayleigh-Taylor-like instability mechanism, has led to the growth of viscous fingers and bubbles. A more detailed comparison of our numerical results with those obtained using other methods and with physical experiments will be done in the future.

4 Conclusion

We have introduced a simple generalization of the LBGK model for the simulation of multiphase miscible fluids. A Chapman-Enskog analysis of the model shows that the component diffusivities and viscosities are adjustable through the use of different relaxation parameters for each component. The theoretical ex-

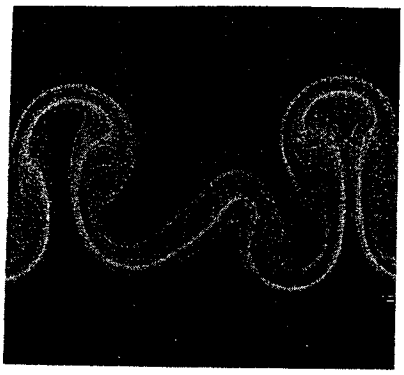

Figure 4: A gray-scale contour plot of the concentration field of two layers of fluid, of the some density and initially superposed one on the other with a random perturbation imposed on the interface, are accelerated towards each other. The size of the grid is 64×64 and $\omega_1 = \omega_2 = 1.7$.

pressions for the shear viscosity and diffusivity are found to agree with numerical experiment. A possible application of the model is demonstrated with a preliminary simulation of two-dimensional two-phase miscible fingering.

Acknowledgment

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