Computational Solutions of the Equations for a Multi-dimensional Diffuse-Interface Model of Compressible Fluid Flow with Capillary Effects

Diane Denny, Ph.D. †

Abstract

We study the initial-value problem for a system of equations arising from a diffuse-interface model of low-speed flows of compressible fluids with capillary stress effects. We compute solutions to an initial-value problem with suitable initial data and boundary conditions on a bounded domain. We also compute solutions to a related stochastic system of differential equations for the mean and fluctuation of the flow variables.

Background

Many scientists are interested in the problem of explaining and predicting the behavior of fluids near the liquid-vapor critical point. Near the critical point, many of the thermophysical properties of a fluid exhibit a singular behavior. For instance, the isothermal compressibility and the isobaric thermal expansion coefficients, as well as the isobaric specific heat, all diverge at the critical point. Critical enhancement effects are also encountered in the behavior of the thermal conductivity and the viscosity in the vicinity of the critical point. Near the critical point, the divergence of the compressibility leads to macroscopic density gradients (upon which microscopic density fluctuations are superimposed). It has been shown that temperature changes in a near-critical fluid can occur rapidly via a mechanism which creates adiabatic pressure changes in the bulk of the fluid [2]. Although early adiabatic processes act rapidly to accomplish most of the temperature changes (in seconds), most of the alteration of the density variations is a non-adiabatic process, driven by the much slower (hours-long) process of heat diffusion. Studies have shown that large density variations slow down the dynamics and reduce the effectiveness of the adiabatic mechanism; however, the adiabatic effect is still responsible for most of the temperature changes [2]. These conclusions drawn by previous researchers were based on results derived from one-dimensional models. No studies of how three-dimensional flow effects alter the overall dynamics, or how the capillary effects contribute to the energy, have been performed so far.

Simulation of the three-dimensional flow of a near-critical fluid using a diffuse interface model (which includes the effect of viscosity, heat conduction, and capillary stresses on fluid properties) and analysis of the results obtained, are the main focus of this paper. Previous studies of near-critical fluids have concentrated on studying models of one-dimensional flows in which the interface is modelled as a free boundary, with separate systems of equations describing the flow on each side of the interface. The sharp interface model, which utilizes a free boundary description of the interface between two fluids, breaks down as a physical model when the interfacial thickness is comparable to the length scale of the phenomena being examined. For example, in a near-critical fluid the thickness of the interface diverges at the critical point, and consequently the representation of the interface as a zero thickness boundary may no longer be appropriate. Another difficulty associated with the free-boundary formulation arises in its use in

computational settings when the free boundary shape becomes complicated or self-intersecting. Diffuse interface models, which use a single set of equations to model the fluid flow and which incorporate capillary stresses in fluid flow equations, provide an alternative description in the face of these difficulties [1]. Local and global existence of unique solutions to the diffuse-interface model equations has been proven by a number of researchers (for example, Hattori and Li [3], [4], [5]). Few numerical studies of these particular diffuse-interface model equations have been performed; those studies which have been conducted considered only one-dimensional versions of the model equations.

For the purpose of this paper, we use the diffuse-interface model equations (given below) for the flow of a compressible, viscous, heat-conducting fluid near the critical point. Our objective is to study how multi-dimensionality affects the flow variables. An additional objective is to develop stochastic partial differential equations based on the diffuse-interface model which incorporate the effect of uncertainty in the data, and then numerically compute solutions to the equations thus obtained.

We consider the low-speed flow of compressible, viscous, heat-conducting fluid. The equations of motion include forces due to capillary stresses that arise from a contribution made by strong density gradients to the free energy. The diffuse-interface model we are considering consists of the following system of equations:

$$\rho \frac{D\vec{v}}{Dt} = -\nabla p + m\rho\nabla\Delta\rho + \mu\Delta\vec{v}$$

$$\frac{D\theta}{Dt} = (1-\frac{c_v}{c_p})\alpha_p^{-1}\nabla\bullet\vec{v} + (\rho c_v)^{-1}\kappa\Delta\theta$$

$$\frac{D\rho}{Dt} = -\rho\nabla\bullet\vec{v}$$

where ρ is the density, θ is the temperature, and $\vec{v}$ is the velocity. Here, κ is the coefficient of thermal conductivity, m is the capillary stress coefficient (which is a constant), and μ is the viscosity coefficient. Also, α_p is the isobaric thermal expansion coefficient, and c_p, c_v are the specific heat capacities at constant pressure and at constant volume, respectively. The equation of state for the pressure is $p = \hat{p}(\rho,\theta)$. The material derivative $\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v}\bullet\nabla$.

We consider a fluid layer with rigid horizontal boundaries and periodic boundary conditions on the remaining sides. First, we apply the diffuse-interface model equations to fluid flow near the liquid-vapor critical point and compute numerical solutions to these equations with the "no-flux" conditions , $\nabla\rho\bullet\vec{n} = 0, \nabla\theta\bullet\vec{n} = 0,$ for the density and

temperature, and the "no-slip" condition $\vec{v} = 0$ for the velocity at the horizontal boundaries (z=0,z=1). Then we will incorporate uncertainty in the data into the model equations and compute solutions.

Scaling and Non-dimensionalization

We non-dimensionalize and scale the variables in a manner appropriate to a typical experiment for the fluid xenon near the liquid-vapor critical point. We obtain the following non-dimensional equations (non-dimensional quantities are indicated by an asterisk, *):

$$\rho^* \frac{D\vec{v}^*}{Dt^*} = -M^{-2}\nabla p^* + c\rho^*\nabla\Delta\rho^* + \mathrm{Re}^{-1}\mu^*\Delta\vec{v}^*$$

$$\frac{D\theta^*}{Dt^*} = (1-\Gamma^{-1}\frac{c_v^*}{c_p^*})(\alpha_p^*)^{-1}\nabla\bullet\vec{v}^* + D_T(\rho^* c_v^*)^{-1}\kappa^*\Delta\theta^*$$

$$\frac{D\rho^*}{Dt^*} = -\rho^*\nabla\bullet\vec{v}^*$$

where the gradient and the divergence are taken with respect to the non-dimensional spatial variable, and $\frac{D}{Dt^*} = \frac{\partial}{\partial t^*} + \vec{v}^*\bullet\nabla$ Here D_T is a non-dimensional diffusivity, M is a small parameter proportional to the characteristic velocity, Re is the Reynolds number, and c is proportional to the constant coefficient m of capillarity. Γ is a ratio of specific heat capacities. The dimensionless constants $M^2, \mathrm{Re}^{-1}, D_T, \Gamma^{-1}$, and c are estimated as follows:

$$D_T = 6\times10^{-5}, M^2 = 3\times10^{-7}, \Gamma^{-1} = 1.8\times10^{-4}, c = 4.44\times10^{-3}, \mathrm{Re}^{-1} = 4.5\times10^{-2}$$

Computational solutions

To compute the solutions, a finite difference scheme was employed. The Douglas-Rachford method was used in discretizing the diffusion term in the temperature equation and also in discretizing the viscosity term in the momentum equation. A second-order Adams-Bashforth method was used to discretize the remaining terms in the temperature and momentum equations, and was also used for the continuity equation. Periodic boundary conditions were applied in the x,y directions. The "no-flux" conditions $\nabla\rho\bullet\vec{n} = 0, \nabla\theta\bullet\vec{n} = 0,$ were used for the density and temperature, and the "no-slip" condition $\vec{v} = 0$ was used for the velocity at the horizontal boundaries (z=0,z=1). The following initial data was used to study a problem in which the density ranges continuously from a lower bound of ρ =1.09 at the z=1 boundary to an upper bound of ρ =1.1 at the z=0 boundary. The initial data for temperature ranges from θ =1.102 at

z=1 to θ =1.1 at z=0. The initial data for velocity ranges from values of 0 to 1 in each velocity component (u,v,w).

Initial data:

$$\rho|_{t=0} = 1.1 - 0.01\cos^2(2\pi x)\cos^2(2\pi y)(0.5z^2 - z^3/3)$$
$$\theta|_{t=0} = 1.1 + 0.01\cos^2(2\pi x)\cos^2(2\pi y)(0.5z^2 - z^3/3)$$
$$u|_{t=0} = \cos^2(2\pi x)\cos^2(2\pi y)(z - z^2)$$
$$v|_{t=0} = \cos^2(2\pi x)\cos^2(2\pi y)(z - z^2)$$
$$w|_{t=0} = \cos^2(2\pi x)\cos^2(2\pi y)(z - z^2)$$

Solutions were computed for each of the flow variables at z=0.5, after 800 time steps, which corresponds to approximately 10 seconds of elapsed time. The results demonstrate that there is a variation in the values of the flow variables, which depends on the values of x and y. The density values ranged from 1.08 to 1.13, with the largest variation occurring near the boundaries, and averaging around 1.1 away from the boundaries. The temperature values ranged from 0.6 to 1.2, averaging at about a value of 0.9, with the largest values occurring near the center at (x,y)=(0.5,0.5). Although the initial data for the velocity components was positive, after 800 time steps the u,v components had both negative and positive values, ranging from -0.02 to 0.04 in the u component, and ranging from -0.02 to 0.04 in the v component. The largest changes in the values of the u component occurred in the direction of the x-axis. The largest changes in the values of the v component occurred in the direction of the y-axis. The w component values were positive, remaining at nearly a constant value of 0.01.

The Stochastic Model Equations

We considered the effect of uncertainty in the model equations' parameters and in the initial data. The boundary data was considered to be deterministic; the same boundary conditions were employed as were used for the deterministic model. The random variables were expanded in a perturbation series, and then solutions to the zero-order and first-order equations were computed. The solutions to the first-order equations yielded an estimate of the zero-mean fluctuation of each random flow variable.

The perturbation expansions were:

$$\rho = \rho^0 + \rho^1 + \rho^2 + \ldots$$
$$\theta = \theta^0 + \theta^1 + \theta^2 + \ldots$$
$$\vec{v} = \vec{v}^0 + \vec{v}^1 + \vec{v}^2 + \ldots$$

where the zero-order variables are approximately the mean of each random flow variable. The equations for the zero-order and first-order equations are as follows:
Zero-order equations:

$$\rho^0 \frac{D\vec{v}^0}{Dt} = -M^{-2}\nabla p^0 + c\rho^0 \nabla \Delta\rho^0 + \mathrm{Re}^{-1}\langle\mu\rangle\Delta\vec{v}^0$$

$$\frac{D\theta^0}{Dt} = \left\langle (1-\Gamma^{-1}\frac{c_v}{c_p})(\alpha_p)^{-1} \right\rangle \nabla \bullet \vec{v}^0 + \left\langle D_T(\rho c_v)^{-1}\kappa \right\rangle \Delta\theta^0$$

$$\frac{D\rho^0}{Dt} = -\rho^0 \nabla \bullet \vec{v}^0$$

First-order equations:

$$\rho^0 \frac{D\vec{v}^1}{Dt} = -\rho^1 \frac{D\vec{v}^0}{Dt} - M^{-2}\nabla p^1 + c\rho^0 \nabla \Delta\rho^1 + \mathrm{Re}^{-1}\langle\mu\rangle\Delta\vec{v}^1$$

$$+ c\rho^1 \nabla \Delta\rho^0 + \mathrm{Re}^{-1}(\mu - \langle\mu\rangle)\Delta\vec{v}^0$$

$$\frac{D\theta^1}{Dt} = \left\langle (1-\Gamma^{-1}\frac{c_v}{c_p})(\alpha_p)^{-1} \right\rangle \nabla \bullet \vec{v}^1 + \left\langle D_T(\rho c_v)^{-1}\kappa \right\rangle \Delta\theta^1$$

$$\left((1-\Gamma^{-1}\frac{c_v}{c_p})(\alpha_p)^{-1} - \left\langle (1-\Gamma^{-1}\frac{c_v}{c_p})(\alpha_p)^{-1} \right\rangle \right) \nabla \bullet \vec{v}^0$$

$$\left(D_T(\rho c_v)^{-1}\kappa - \left\langle D_T(\rho c_v)^{-1}\kappa \right\rangle \right) \Delta\theta^0$$

$$\frac{D\rho^1}{Dt} = -\rho^0 \nabla \bullet \vec{v}^1 - \rho^1 \nabla \bullet \vec{v}^0$$

The initial data used for the zero-order equations was the same as was used for the deterministic equations. The following initial data was employed for the first-order equations:

$$\rho^1|_{t=0} = 0.1\sin(2\pi x)\sin(2\pi y)\cos(8\pi z)$$

$$\theta^1|_{t=0} = 0.1\sin(2\pi x)\sin(2\pi y)\cos(8\pi z)$$

$$u^1|_{t=0} = 0.1\sin(2\pi x)\sin(2\pi y)\sin(8\pi z)$$

$$v^1|_{t=0} = 0.1\sin(2\pi x)\sin(2\pi y)\sin(8\pi z)$$

$$w^1|_{t=0} = 0.1\sin(2\pi x)\sin(2\pi y)\sin(8\pi z)$$

Solutions were computed for the zero-mean fluctuation of each of the random flow variables at z=0.5, after 800 time steps, which corresponds to approximately 10 seconds of elapsed time. The results demonstrate that there is a variation in the values of the zero-mean fluctuation of the random flow variables, which depends on the values of x and y.

The values of the zero-mean fluctuation of the density ranged from -0.0002 to 0.0003, with the largest variation occurring in the direction of the x-axis. Although the initial data for the zero-mean fluctuation of the temperature had both positive and negative values, after 800 time steps the values of the zero-mean fluctuation of the temperature were positive, ranging from 0.02 to 0.1, with the largest values occurring near the center at (x,y)=(0.5,0.5). The values of the zero-mean fluctuation of the u component of the velocity ranged from -0.0003 to 0.0005, with the largest variation occurring in the direction of the x-axis. The values of the zero-mean fluctuation of the v component of the velocity ranged from -1.0×10^{-7} to 1.0×10^{-7}, with variation present in both the x and y directions. The values of the zero-mean fluctuation of the w component of the velocity ranged from -3.0×10^{-8} to 1.0×10^{-7}, with variation present in both the x and y directions.

Conclusion

The results of the numerical computation indicate that the flow variables do exhibit variation in both the x and y directions. Previous studies done using one-dimensional models considered variation in the flow variables in only the z direction. As a example, we considered the computed solutions at z=0.5, after 800 time steps (approximately 10 seconds). For this example, it was found that most of the density variation occurred in the boundary layer. Also, the largest temperature values occurred near the center of the domain. The most variation in the values of the velocity components occurred in the u,v components. The results for the zero-mean fluctuations of the random flow variables show that variation in the values of the fluctuations occurred in both the x and y directions. The largest fluctuations after 800 time steps appeared in the values of the zero-mean fluctuations of the temperature. The zero-mean fluctuation of the u component of the velocity was larger than the fluctuations of the v, w components.

This is only a first attempt at studying the effects of multi-dimensionality in the diffuse-interface model equations. Much work remains to be done in the area of simulating multi-dimensional, near-critical fluid flows.

Diane Denny, Ph.D., Texas A&M University-Corpus Christi, Texas, USA.

References

[1] D. M. Anderson, G. B. McFadden and A. A. Wheeler, “Diffuse-interface methods in fluid mechanics”, Ann. Rev. Fluid Mech.,30 (1998), 139-65.

[2] H. Boukari, R. Pego, and R. W. Gammon, “Calculation of the dynamics of gravity-induced density profiles near a liquid-vapor critical point”, Phys. Rev. E 52, 1614-1625 (1995).

[3] H. Hattori and D. Li, “Solutions for two-dimensional system for materials of Korteweg type”, SIAM J. Math. Anal., 25 (1994), 85--98.

[4] H. Hattori and D. Li,“Global solutions of a high dimensional system for Korteweg materials”, J. Math. Anal. Appl., 198 (1996), 84-97.

[5] H. Hattori and D. Li, “The existence of global solutions to a fluid dynamic model for materials for Korteweg type”, J. Partial Diff. Eqs., 9 (1996), 323-342.