Modeling droplet breakup effects in warm dense matter experiments with diffuse interface methods in the ALE-AMR code

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Abstract

In this paper we describe an implementation of a single-fluid interface model in the ALE-AMR code to simulate surface tension effects. The model does not require explicit information on the physical state of the two phases. The only change to the existing fluid equations is an additional term in the stress tensor. We show results of applying the model to an expanding Al droplet surrounded by an Al vapor, where additional droplets are created.

1 Introduction

The Neutralized Drift Compression Experiment II (NDCX II) is an induction accelerator planned for initial commissioning in 2012. The final design calls for a 3 MeV, Li+ ion beam, delivered with characteristic pulse duration of 1 ns, and transverse dimension of order 1 mm. The NDCX II will be used in studies of material in the warm dense matter (WDM) regime and

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ion beam/hydrodynamic coupling experiments relevant to heavy-ion-based inertial fusion energy.

Currently the ALE-AMR code is used to model WDM experiments on NDCX II. The code, which combines arbitrary Lagrangian-Eulerian (ALE) hydrodynamics with adaptive mesh refinement (AMR), has physics models that include ion deposition, radiation hydrodynamics, thermal diffusion, anisotropic material strength with material time history, and advanced models for fragmentation. Experiments at NDCX-II will explore the process of bubble and droplet formation (two-phase expansion) of superheated metal solids using ion beams. Thus, a physical model of surface tension needs to be incorporated into the code.

We discuss a surface tension model that has been implemented and applied to WDM experiments and is based on a single-fluid, diffuse-interface model that allows droplet formation behaviors.

2 The Model

2.1 Formation of the model

We base our model on the single-fluid, diffuse interface model described in [3].

$$\frac{d\rho}{dt} = \nabla \cdot (\rho \vec{V}) \tag{1}$$

$$\rho \frac{d\vec{V}}{dt} + \vec{V} \cdot = -\nabla p + \nabla \cdot \sigma_1 + \nabla \cdot \sigma_2 \tag{2}$$

Here, σ_1 represents the viscous stress tensor $\mu(\nabla \vec{V} + (\nabla \vec{V})^T - \frac{2}{3}\nabla \cdot \vec{V} I)$. In addition, we have a new tensor term $\sigma_2 = K((\frac{1}{2}|\nabla \rho|^2 + \rho \Delta \rho) I - \nabla \rho \otimes \nabla \rho)$. This is the Korteweg stress tensor, which represents surface tension force. Some sharp interface arguments link this surface tension term with curvature [1].

We choose this model for two reasons. First, it is easily adapted for the current full-scale fluid simulation. Only one term had to be added to the stress tensor. Second, this model does not require the explicit physical state of the two phases; thus, the same code is easy to run for different materials and, more important, for different temperatures.

2.2 Property of the model

The equivalent surface tension coefficient for this model is $\alpha = K \int_{-}^{+} (\frac{d\rho}{dz})^2 dz$, where z is the normal direction of the interface and the integration is done across the interface [3]. If we write interfacial width as ϵ, then we have $\alpha \sim K\frac{\delta\rho^2}{\epsilon}$. One disadvantage of this model is that since we have only one parameter, K, we cannot adjust ϵ and α individually. Scaling properties show that $\epsilon \sim K^{1/2}$, thus $\alpha \sim K^{1/2}$. An intuitive way of showing this is, if $\rho_0(\vec{x})$ is a stable density distribution at $K = K_0$, then $\rho_0(\vec{x}/2)$ is a stable density distribution at $K = 4K$. The first distribution corresponds to an interface depth twice as much as that of the first distribution.

Even when K is constant, the surface tension coefficient still depends on temperature. Temperature affects the density and pressure of the two phases and thus also affects the surface tension. For example, [2] declares that for Van der Waals fluid $\alpha \sim (T_c - T)^{3/2}$, where T_c is the critical temperature.

3 Results

3.1 Numerical implementation

We added a section of code in ALE-AMR that calculates σ_2 and adds it to the original stress tensor. The differential operators are approximated by finite difference methods. The grid is irregular most of the time, thus we use a similar method as described in [4].

3.2 Results

We use a test problem of an expanding aluminum drop over critical temperature surrounded by aluminum vapor under critical temperature. This simulation is intended to represent the status of material after heavy-ion heating during the NDCX-II experiment. The simulation was run for about 2 hours on the 64-processor NERSC supercomputer Franklin. For the initial condition, the droplet has a radius of 0.1 μ m, density 1.5 g/cm^3, with temperature 9000K. The surroundings have a density 0.1 g/cm^3 and temperature 6000 K. We use the LEOS equation of state, for which aluminum has a critical temperature of about 8400K and critical density of about 0.7 g/cm^3. The value K is taken as 0.001, which leads to a surface tension coefficient of about 1000 erg/cm^2. We run this test problem with and without the surface

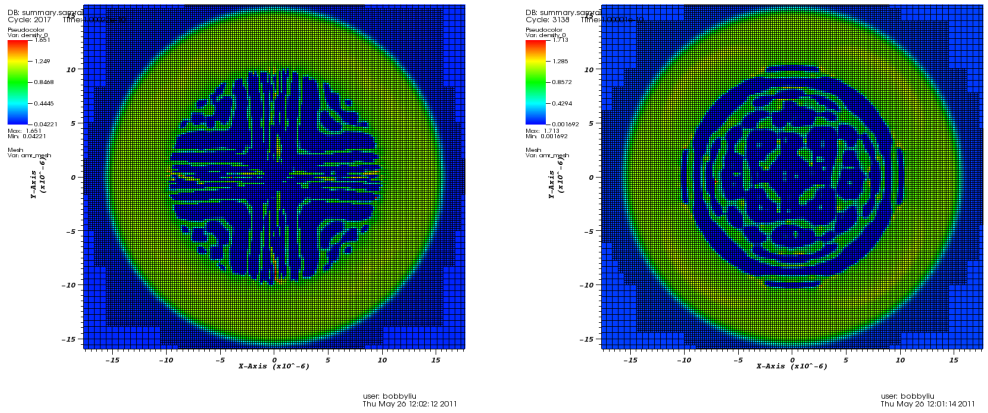

Figure 1: Results of an expanding aluminum drop without the use of surface tension model (left) and with the use of surface tension model (right). The surface tension model forms droplets while the other does not. The colorbar is shown on a linear scale from 0 to 1.7.

tension model, respectively. See Figure 1 for results. Both results show material breakup due to physical instability of spinodal region, but the surface tension model clearly forms droplets while the other one does not.

4 Conclusions

We combined the diffuse interface model with the ALE-AMR code and got good results. This model forms droplets as intended in a test problem resembling the NDCX-II experiment. Improvement of this model is still necessary; for example, ideally this model will have an additional parameter so that both interfacial width and surface tension coefficient can be changed simutaneously.

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