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

Wangyi Liu, John Bernard, Alex Friedman,
Nathan Masters, Aaron Fisher, Velemir Mlaker,
Alice Koniges, David Eder

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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 in a bunch 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 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 be corporated into the code.

We discuss a surface tension model that has been implemented and applied to WDM experiments. It is based on a single-fluid diffuse interface model that allows droplet formation behaviors and is described in the following section. It will be followed by the numerical results.

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. See for example [1].

We choose this model for two reasons. Firstly, it is easy to be adapted into the current full-scale fluid simulation. The only change necessary is an additional term to the stress tensor, see next section for details. Secondly, this model does not require explicit physical state of the two phases. It will be more convenient for running the same code over different materials and more importantly, when temperature changes.

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 only have 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 it 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, surface tension coefficient still depends on temperature. Temperature changes the density and pressure of the two phases, thus affect 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 add it to the original stress tensor. The differential operators are approximated by finite difference methods. The grid is irregular most of the times, 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. For the initial condition, the droplet has a radius of 0.1 μm, density $1.5 g/cm^3$, with temperature $9000K$. The surroundings have a density $0.1 g/cm^3$ and temperature $6000K$. 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 tension model respectively. See figure for result. 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.

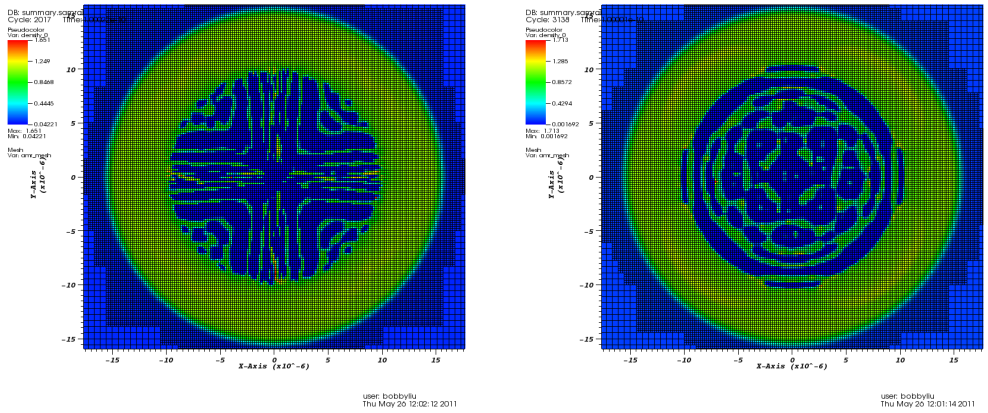

Figure 1: Result of an expanding Aluminum drop without the use of surface tension model(left) and with the use of surface tension model(right). The result with surface tension model forms droplets while the other does not. The colorbar is shown on a linear scale from 0 to 1.7.

4 Conclusions

We combine the diffuse interface model with ALE-AMR code and get good results. This model behaves reasonably in terms of droplet breakup. Improvement of this model is still necessary, e.g., have an additional parameter so that both interfacial width and surface tension coefficient can be changed simutaneously.

References

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