A numerical scheme for including surface tension effects in hydrodynamic simulation: a full Korteweg type model without parasitic flows

Wangyi Liu[1], John Barnard[2], Alice Koniges[1], David Eder[2], Nathan Masters[2], Aaron Fisher[2], Alex Friedman[2]
[1]LBNL, USA, [2]LLNL, USA

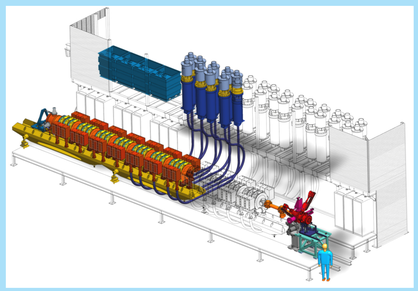
This work was part of the Petascale Initiative in Computational Science at NERSC, supported by the Director, Office of Science, Advanced Scientific Computing Research, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231. This work was performed under the auspices of the U.S. Department of Energy by LBNL under Contract DE-AC02-05CH11231 and by LLNL under Contract DE-AC52-07NA27344. This research used resources of the National Energy Research Scientific Computing Center, which is supported by the Office of Science of the U.S. Department of Energy under Contract No. DEAC02-05CH11231.

Introduction

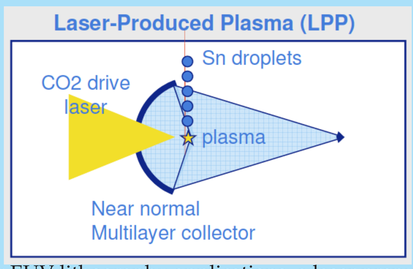
We consider a single-fluid diffuse interface model to simulate surface tension effects. Parasitic flow is a widely-faced unwanted numerical effect for surface tension models. It is a small velocity field caused by an unbalance between numerically calculated stresses in the interfacial region[1]. In this simulation we consider the full model instead of the isothermal case, and we use a technique similar to that of [1] that completely removes parasitic flow. We show the benchmark of this model against Laplacian equation and its parasitic flow removal performance, then show a droplet breakup scenario.

Application

Our goal is to accurately simulate the droplet breakup with a proper surface tension model. Its application includes NDCX-II experiment and an EUV lithography using laser heated tin droplets.



NDCX-II is an ion beam accelerator that can be used to study warm dense matter regime For certain targets, metal droplets are formed, requiring surface tension effects in modeling.



For EUV lithography applications, a laser prepulse causes Sn droplets to flatten followed by main pulse, which vaporizes the Sn producing EUV radiation.

Model

Out single fluid diffuse interface model is based on the full(nonisothermal) Korteweg model. In conservation form for mass, momentum and entropy we have

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{v}), \tag{1}$$

$$\frac{\partial (\rho \vec{v})}{\partial t} = -\nabla \cdot (\rho \vec{v} \otimes \vec{v}) - \nabla p + \nu \Delta \vec{v} + K \rho \nabla \Delta \rho, \tag{2}$$

$$\frac{\partial S}{\partial t} = -\nabla \cdot (S \vec{v}) + k \frac{\Delta T}{T} + \nu \frac{\nabla \vec{V} :: \nabla \vec{V}}{T} \tag{3}$$

Here S is entropy per volume, ν is viscosity coefficient. K is a parameter related to the strength of surface tension. A Van der Waals EOS closes the system.

Numerical simulation

The main technique is similar to that of [1], but we extend it to non-isothermal case. Instead of using $\nabla \rho$, we use $S \nabla T + \rho \nabla \mu$. Here T denotes temperature and μ is the chemical potential. These will make sure that total energy

$$E = \int e(\rho, T) + \frac{1}{2} \rho |\vec{V}|^2 + \frac{K}{2} |\nabla \rho|^2 \tag{4}$$

is conserved. This formulation can be derived directly from the Hamiltonian fluid mechanics. This will produce wrong equilibrium condition in the case with no surface tension, but only because normal Navier-Stokes equation cannot handle evaporation and condensation well. We use 4th order explicit Runge-Kutta for time discretization.

Surface tension coefficient

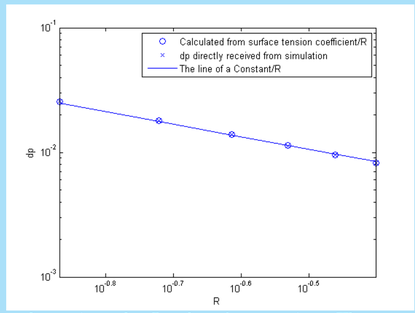
Equivalent surface tension coefficient

$$\alpha = K \int_{-}^{+} (\frac{d\rho}{dz})^2 dz, \tag{5}$$

where z is the normal direction of the interface and the integration is done across the interface [2]. If we write interfacial width as ϵ, then $\alpha \sim K \frac{\delta \rho^2}{\epsilon}$.

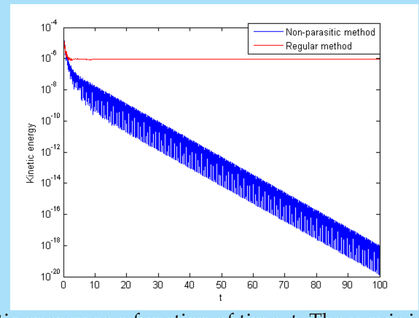
Benchmark-Laplace's equation

To benchmark the result against the Laplace's equation, we use a droplet surrounded by vapor of the same material, temperature, and similar pressure. Then we run the simulation until it reaches equilibrium, recording the difference of pressure between two sides of the interface. We measure the actual pressure difference and compare it against the Laplace equation $\delta p = \frac{\sigma}{R}$ where σ is the surface tension coefficient measured as in Eq. 5.



Benchmark against the Laplace's equation. The x-axis is the radius of droplet R, and the y-axis is the pressure difference dp. Circle denotes the theoretical δp from Laplace's equation, and cross is the δp measured from simulation. The line is $\delta p = C/R$ where C is a constant for comparison.

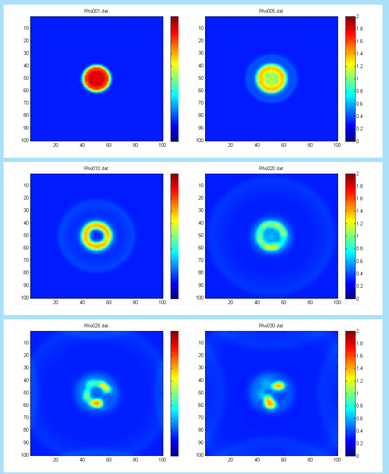
Another test problem shows the reduction in parasitic flow. We run the previous simulation out to longer time with same initial condition, comparing the two schemes with and without parasitic flow removal. Since parasitic flow is characterized by a non-zero velocity, the simulation with parasitic flow will not converge to a full equilibrium state. Kinetic energy is used as a measure of the remnant of the parasitic flow in the plot below.



Kinetic energy as a function of time, t. The x-axis is time, and y-axis is the kinetic energy. Blue curve has parasitic flows reduced, red curve is the unaltered method. Parasitic flow remains significant even as the simulation moves towards equilibrium in the unaltered case.

Droplet breakup simulation

Droplet breakup is simulated as example for many other numerical models, but most of those simulations has an explicitly specified external force or shear flow that causes the breakup. In this section we present a droplet breakup scenario caused only by heating. We start with a droplet in vapor setting as previous simulation, then heat the droplet to a higher temperature. Depending on the temperature of heated droplet, 1) if it is higher than a threshold temperature T_0, the droplet will completely evaporize; 2) if it is lower than T_0, it will expand before the decrease of pressure cause it to extract back. We initialize the heated droplet to a temperature with perturbation around T_0, and when it expands part of the droplet will tend to expand and part will tend to retract. These two effects combined will cause the droplet to breakup.



Sample of a droplet breakup simulation

References

[1] Jamet, D., Torres, D., and Brackbill, J. On the theory and computation of surface tension: The elimination of aprasitic currents through energy conservation in the second-gradient method In *J. Comp. Physics, 2002*

[2] Nadiga, B. T. and Zaleski, S. Investigations of a Two-Phase Fluid Model In *Contributions to Mineralogy and Petrology 1995*

[3] Prosperetti, A. Motion of two superposed viscous fluids In *Phys. Fluids, 1981*