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A comparison of models for the evaporation of the Lennard-Jones fluid

Paolo Barbante [a], Aldo Frezzotti [b,*]

[a] *Politecnico di Milano, Dipartimento di Matematica, Via E. Bonardi 9, 20133 Milano, Italy*
[b] *Politecnico di Milano, Dipartimento di Scienze e Tecnologie Aerospaziali, Via La Masa 34, 20156 Milano, Italy*

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ABSTRACT

The evaporation of a thin liquid film is studied by a diffuse interface model whose thermodynamic and transport properties are consistent with those of the Lennard-Jones fluid. Solutions are obtained for various liquid film temperatures and downstream vapor flow velocities. The results are compared with reference molecular dynamics simulations of a system of atoms interacting by the 6-12 Lenard-Jones potential. It is shown that the diffuse interface model underestimates the temperature drop across the non-equilibrium vapor region next to the liquid–vapor interface but overestimates the density drop, thus predicting smaller evaporation rates. Results indicates that the discrepancies between molecular dynamics and diffuse interface model predictions become smaller when the liquid film temperature approaches the critical temperature and the vapor becomes a dense, non-ideal gas. Further successful comparisons of molecular dynamics results with the predictions of a hybrid model, combining the continuum description of the liquid with the kinetic description of the vapor, suggest that the observed discrepancies can be attributed to poor description of the Knudsen layer provided by the diffuse interface model when the vapor phase is dilute.

1. Introduction

Diffuse interface models (DIMs) provide an interesting and rapidly developing approach to the study of multiphase flows [1,2]. In the case of a fluid with coexisting liquid and vapor regions, DIMs are capable of a unified description of both phase bulks and interfacial regions, thanks to the presence of an additional contribution in the static part of the stress tensor, which is made to depend on the spatial derivatives of the density field [1,2], following Korteweg theory of capillary phenomena [3]. Non-equilibrium effects are taken into account by adding viscous stresses, in the classical form of Navier–Stokes constitutive law, to static ones. Similarly, the fluid internal energy and Fourier law expression for heat flux are modified by terms depending on density gradients [1,2]. In principle, DIMs treatment of multiphase flows offers several advantages. A single mathematical model, based on a small number of PDEs, describes the liquid, vapor and interface regions. Any need to adopt boundary conditions at vapor–liquid interface to take into account evaporation/condensation phenomena [4,5] is eliminated. Moreover, no interface tracking technique is necessary in DIMs based numerical simulations, since the finite thickness interfacial regions are part of the flowfield. Such attractive features have been exploited to study liquid jets instabilities, spinodal decomposition, boiling and bubble dynamics [6–8]. DIMs studies, specifically addressing evaporation/condensation flows, are scant and limited to qualitative analysis of flow properties [9,10].

Although attractive, DIMs description of evaporation or condensation phenomena is not automatically accurate. As a matter of fact, when the vapor phase is dilute a kinetic layer (Knudsen layer) [11,12] is always formed in the vicinity of the vapor–liquid interface, during evaporation or condensation. This kinetic region extends into the vapor for a few mean paths, depending on the intensity of the mass flow rate. Macroscopic flow properties suffer rapid changes which are not well described by hydrodynamic equations. Since DIMs adopts Navier–Stokes and Fourier constitutive laws, some deviations from the correct fluid behavior are to be expected. The present work aims at extending a preliminary investigation about the accuracy of DIMs in describing evaporation flows [13]. The evaporation of a planar liquid film is used as test problem. Accurate Molecular Dynamics (MD) simulations of the Lennard-Jones fluid are performed to obtain the benchmark flowfield structure in the liquid, vapor and interface regions, without any additional assumption beyond those intrinsic in the classical MD simulation of fluids.

In conducting the comparison of MD computed flow properties with DIMs results, particular care has been taken in constructing

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* Corresponding author.
E-mail address: aldo.frezzotti@polimi.it (A. Frezzotti).

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a diffuse interface model matching the thermodynamic [14] and transport properties [15,16] of the Lennard-Jones fluid. In order to highlight the role of kinetic effects in the Knudsen layer, MD and DIM results are also compared with computations based on a hybrid model (HM) in which the liquid region is described by hydrodynamic equations, whereas the vapor is governed by the Boltzmann equation [17]. The liquid and vapor phase are separated by a structureless interface, replaced by kinetic boundary conditions [4]. According with the above considerations, the paper content is organized as follows: Section 2 describes the test problem characteristics; MD simulations are described in Section 3, whereas DIM structure, its numerical implementation and results are described in Section 4. The kinetic model structure and numerics are described in Section 5, along with results and comparisons with the reference MD calculations.

2. Test problem description

A simple test problem is used to assess the capabilities of DIM and HM in describing the evaporation of a simple Lennard-Jones liquid (see Fig. 1). A liquid film, in the form of an infinite planar slab of finite thickness Δz_l, is initially in equilibrium with its vapor phase at temperature T_l. The vapor occupies two regions, symmetrically located with respect to the liquid slab center. Each of them is delimited by the adjacent liquid–vapor interface and an impermeable and adiabatic piston, whose planar surface is kept parallel to the vapor–liquid interface. The left and right pistons are initially located in the vicinity of the vapor–liquid interface at positions $-z_p(0)$ and $z_p(0)$, respectively. Evaporation flow is then started by withdrawing both pistons with constant opposite speeds $\mp v_p$. During evaporation, the center of the liquid slab is kept at constant temperature T_l to avoid excessive cooling of the liquid slab. The resulting flow is unsteady, because of the interfacial motion and the time evolution of the non-uniform temperature profile in the liquid. However, the receding interfaces common temperature $T_I(t)$, after an initial rapid transient cooling, reaches a minimum followed by a slow monotonic increase. If the initial slab thickness is large enough, the part of the $T_I(t)$ curve following the minimum is so slowly increasing to be considered a constant plateau. In this phase of the system evolution, the temperature profile in the liquid takes an approximately linear shape evolving self-similarly. If the duration of the temperature plateau is long enough with respect to the time sound waves in the vapor take to travel through the gap between the piston and the interface, then the vapor flow becomes quasi-steady. Its structure is relatively simple, consisting in a kinetic region (Knudsen layer) next to the interface, followed by a uniform equilibrium region where the vapor moves with the piston speed. Vapor density and temperature are dictated by the proper kinetic jump relationships [4,11,12,18], determined by the microscopic mechanisms governing molecular emission from the liquid phase into the vapor and vapor molecules scattering from the liquid surface [19,20,5]. Hence, the present test problem represents a good probe of the capabilities of a model to reproduce transport properties at the vapor–liquid interface.

3. Molecular dynamics simulations of a liquid film evaporation

The role of molecular dynamics (MD) [21] simulations is to provide the most fundamental description of the test problem and the reference flowfield properties. It is assumed that the fluid is composed by N_a identical atoms of mass m, interacting pairwise through forces derived from the following Lennard-Jones (LJ) 6−12 potential $\phi_{LJ}(r)$ [22]:

$$\phi_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]. \tag{1}$$

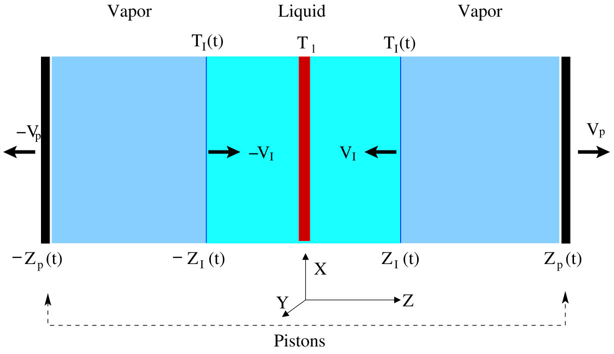

Fig. 1. Sketch of test problem set up.

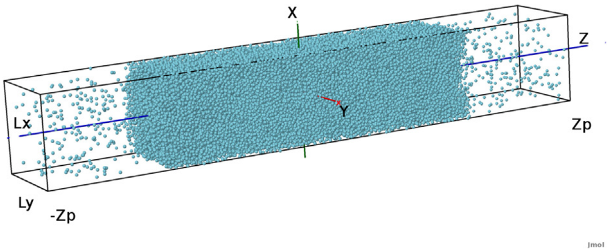

Fig. 2. Scheme of molecular dynamics simulation domain geometry.

In Eq. (1), r the distance between two interacting atoms, ϵ is the depth of the potential well, whereas the length σ defines the effective range of atomic forces. More precisely, $r_m = 2^{1/6}\sigma$ is the position of the potential minimum.

The atomic mass and the LJ potential parameters have been adopted as natural units for all fluid properties defined in the paper. Accordingly, length, time and mass are normalized with respect to the natural space, time and mass scales of atomistic simulations, namely σ, $\sqrt{\frac{m\sigma^2}{\epsilon}}$ and m, respectively. Temperature is normalized to $\frac{\epsilon}{k_B}$, being k_B the Boltzmann constant. Throughout the paper, the symbol ρ is associated with the fluid reduced density $n\sigma^3$, being n the fluid number density. The described normalizations has been also used in the Diffuse Interface Model and in the hybrid continuum–kinetic model described below.

Atomic motions are computed numerically by integrating Newton's equations by the velocity Verlet scheme [21]. The time step, in LJ units, has been varied between 2.0e−03 and 5.0e−03. The infinite system is constructed as the union of periodic replicas of the finite fluid column sketched in Fig. 2. The MD computational domain has fixed side lengths L_x and L_y along the two directions x and y, where periodic boundary conditions [21] are applied, being parallel to the liquid surface. Along the direction normal to the liquid surface, spanned by the coordinate z, the column height is delimited by the piston positions. Forces have been computed according to the minimum image convention [21], after truncating atomic interactions of pairs whose relative distance r exceeds a specified cut-off radius r_c. The latter been set equal to 3.0σ to keep the computational time within reasonable limits. A spatial grid, with a cell size of r_c, has been used to index atoms and make the search of nearest neighbors more efficient. Although intrinsically three-dimensional, the adopted MD setup guarantees that *ensemble* averaged macroscopic quantities will depend only on z and t, thus approximating the infinite system described in Section 2 in a statistical sense.

Each computation has been started from an initial state in which a liquid slab, located in the center of the computational box, is in equilibrium with its vapor at a specified temperature T_l. The vapor occupies the two symmetrical gaps located between the vapor–liquid interfaces and the box walls at $z = \mp z_p(t)$, consisting

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