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A COUPLED MOLECULAR-CONTINUUM FRAMEWORK FOR MULTISCALE SIMULATIONS OF BOILING

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1. ABSTRACT

Boiling is a perfect example of a multiscale process where molecular-level physics giving rise to bubble nucleation interact with larger-scale boundary layers determined by the outer system boundary conditions. We present a novel multiscale simulation method which merges Molecular Dynamics (MD) and Computational Fluid Dynamics (CFD) descriptions into a single modelling framework, where MD resolves the near-wall region where molecular interactions are important, and a CFD solver resolves the bulk flow. We model the progressive heating of a Lennard-Jones fluid via contact with a solid wall until a vapour bubble nucleates in the MD region of the domain and grows by entering in the CFD domain. Our results show that an incompressible CFD flow model based on the Volume Of Fluid (VOF) method with interphase mass transfer calculated via the Hertz-Knudsen-Schrage equation is sufficient to obtain seamless coupling of phase fraction, velocity and temperature fields, with the hybrid MD-CFD framework yielding bubble dynamics closely matching those of MD alone.

2. INTRODUCTION

The next generation of science depends on solving the problem of linking simulations at different scales. In many physical processes, phenomena happening at the molecular scale determine the large-scale dynamics of the system. For example, near-wall turbulence in fluid mechanics depends on the wall-fluid molecular interaction, bubble/droplet nucleation in heating/cooling processes depend on the thermal fluctuations at the nanoscale, the wear of interacting surfaces in tribology depends on the viscoelastic properties of materials at localised points of contact. These molecular-level physics are implemented via empirical closure models in state-of-art continuum-scale simulation methods, which often limit the reliability of simulation outputs. Coupled algorithms have the potential to revolutionise the simulation of engineering systems allowing them to retain the full molecular detail [1]. In domain decomposition coupling, Molecular Dynamics (MD) captures the near-wall region whereas a continuum Computational Fluid Dynamics (CFD) description based on the Navier-Stokes equations resolves the bulk flow; flux and/or state properties are directly exchanged in an overlap region, without intermediate models. While this technique is well established for wall-bounded single-phase flows, its adoption in multiphase flows is still in its infancy. In this work, we present our progress in developing a coupled MD-CS framework using a full open-source platform and show that coupled framework is capable of reproducing the bubble growth rate over time from nucleation until a bubble size of about 70 nm, demonstrating the accuracy and robustness of the

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coupling architecture, and that the fluid dynamics description based on the Navier-Stokes equations is capable of correctly capturing the main heat and mass transfer mechanisms responsible for bubble growth at the nanoscale.

3. METHODOLOGY

The methodology is based on two computer simulation software running concurrently. The MD simulation uses the opensource software flowMol [2] whereas the CFD simulation is based on the opensource toolbox OpenFOAM. A schematic of the domain decomposition architecture is provided in Fig. 1(a). The MD solver simulates the solid wall, through which heat is provided, and a fluidic region above it which is sufficiently thick to enable nucleation. The CFD mesh partially overlaps the MD domain, but does not capture the wall and near-wall region which is handled exclusively by the MD, so that no contact line models are necessary. On the MD → CFD domain boundary, MD fields of density, velocity and temperature are converted into CFD fields of phase fraction, velocity and temperature, to provide boundary conditions for the CFD. The transfer of information is one-way from MD to CFD, and thus the MD evolves agnostic of the CFD. The MD model is based on the simple and widely used Lennard-Jones potential which is representative of fluids such as Argon. The CFD model is based on the solution of the continuum Navier-Stokes equations as implemented in the opensource toolbox OpenFOAM v2106. The liquid-vapour two-phase boiling flow is simulated by means of a VOF interface capturing method, using our self-developed library boilingFoam [3]. The liquid-vapour phase change rate is evaluated using the Hertz-Knudsen-Schrage equation:

$$\dot{m} = \frac{2\gamma}{2-\gamma}\left(\frac{M}{2\pi R_g}\right)^{1/2}\frac{\rho_v h_{lv}(T-T_{sat})}{T_{sat}^{3/2}} \qquad (1)$$

where γ is the accommodation coefficient, M is the molecular mass, R_g is the universal gas constant, ρ_v is the vapour density, h_{lv} is the latent heat, T_{sat} is the saturation temperature and T is the local interface temperature. A full description of the numerical framework is provided by Gennari et al. [4]. We simulate the boiling of Argon, which fills the computational domain at an initial temperature of 108 K (0.9 in MD units) which is approximately equal to the saturation temperature of the fluid. The bottom of the solid wall is set to 126 K (1.05 in MD units). The computational domain is a two-dimensional box of 160×160 nm^2 (476×476 in MD units). The CFD side of the domain is meshed with a regular grid made of squares of size of 1 nm. The fluid properties in the CFD are set according to the NIST database, except for the liquid and vapour densities that are calculated from the MD.

4. RESULTS

At the onset of the simulation, the wall is heated up in the MD region of the domain and heat progressively diffuses across the fluidic domain. After about 4000 MD time-units, corresponding to about 8.6 ns, nucleation occurs in the MD. Figure 1(b) shows a plot of the bubble mass over time for the MD-only simulation and the hybrid MD-CFD model and emphasises an almost linear dependence with time. Since T_{sat} and γ are not defined in MD, two curves are shown for the hybrid model, one for $T_{sat} = 0.9$ (108 K) and $\gamma = 0.2$ and one for $T_{sat} = 0.92$ (110 K) and $\gamma = 1$. The value $\gamma = 0.2$ yields the best agreement of the MD-only and MD-CFD growth rates when $T_{sat} = 0.9$, whereas $T_{sat} = 0.92$ is the saturation temperature that yields the best agreement when setting $\gamma = 1$. Note that values of $\gamma \approx 0.7$ were reported in the literature for Argon in these conditions [5], and a best agreement with MD-only results would be achieved by a $T_{sat} = 0.9 - 0.92$, consistently with the present results. Figure 2(c) illustrates the density fields obtained by the MD-only and coupled framework side-by-side for $T_{sat} = 0.9$ and $\gamma = 0.2$. The figure confirms the good match of bubble size and shape between the two solutions, and emphasises that the bubble interface transitions well from the MD to the CFD domain without spurious effects. Additional systematic simulations performed by varying γ in the range $\gamma = 0.1 - 1$ reveal that reducing γ has the effect of reducing the phase-change rate at the interface, due to the prefactor $2\gamma/(2-\gamma)$ in Eq. (1). However, the range of variation of

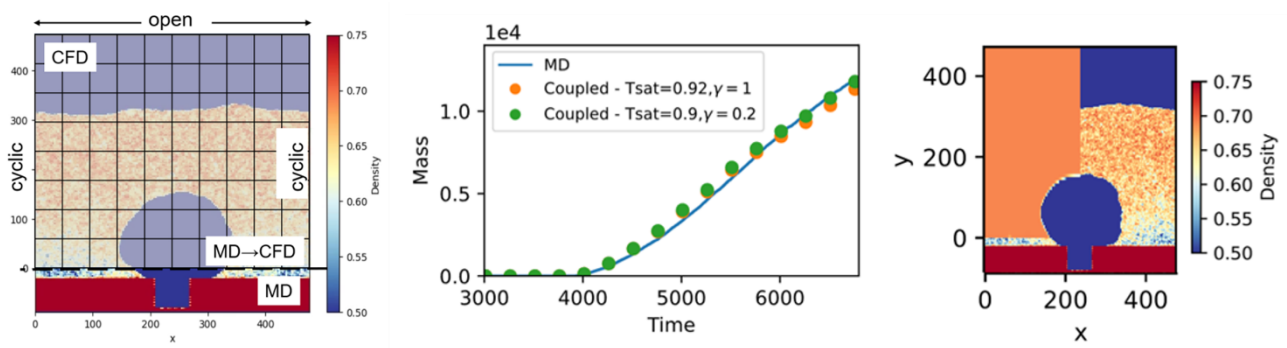

Figure 1. (a) Schematic of the coupled domain. (b) Comparison of MD and coupled MD-CFD results in terms of bubble mass over time. (c) Comparison of CFD (left-half) and MD (right-half) density field. All units are expressed in MD reduced units, with a unit length being 0.34 nm, unit time 2.15 ps, unit temperature 120 K, unit mass 6×10^{-26} kg. An MD density of 0.7 corresponds to 1160 kg/m^3.

the bubble mass at the end of the simulation is narrower than those of γ and of the prefactor, because increasing γ causes a reduction of the temperature at the interface owing to a larger amount of latent heat being dissipated.

5. CONCLUSIONS

We have developed a hybrid atomistic-continuum framework to perform coupled MD-CFD simulations of heterogeneous boiling over a superheated solid surface. We showcase the model by simulating the nucleate boiling of Argon over a superheated surface and we demonstrate that the hybrid framework yields a bubble growth rate that agrees well with the MD-only simulation up to a bubble diameter of 70 nm, emphasising that the continuum formulation of the interphase mass transfer based on the Hertz-Knudsen-Schrage equation leads to phase-change rates in agreement with the molecular-level description. This provides opportunities for multiscale simulations of boiling, where fundamental nucleation processes are retained in a CFD description.

The simulation code is publicly available in Github: https://github.com/Crompulence/CPL_APP_OPENFOAM

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