**A Lattice Boltzmann Framework for the Simulation of Boiling Hydrodynamics in BWRs**

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## INTRODUCTION

Multi phase and multi component flows are ubiquitous in nature as well as in many man-made processes. A specific example is the Boiling Water Reactor (BWR) core, in which the coolant enters the core as liquid, undergoes a phase change as it traverses the core and exits as a high quality two-phase mixture. Two-phase flows in BWRs typically manifest a wide variety of geometrical patterns of the co-existing phases depending on the local system conditions. Modeling of such flows currently relies on empirical correlations (for example, in the simulation of bubble nucleation, bubble growth and coalescence, and inter-phase surface topology transitions) that hinder the accurate simulation of two-phase phenomena using Computational Fluid Dynamics (CFD) approaches. The Lattice Boltzmann Method (LBM) is in rapid development [1-2] as a modeling tool to understand these macro-phenomena by coupling them with their underlying micro-dynamics.

This paper presents a consistent LBM formulation for the simulation of a two-phase water-steam system. Results of initial model validation in a range of thermo-dynamic conditions typical for BWRs are also shown. The interface between the two coexisting phases is captured from the dynamics of the model itself, i.e., no interface tracking is needed. The model is based on the Peng-Robinson (P-R) non-ideal equation of state and can quantitatively approximate the phase-coexistence curve for water at different temperatures ranging from 125 to 325 $^{o}$C. Consequently, coexisting phases with large density ratios (up to ~1000) may be simulated. Two-phase models in the 200-300 C temperature range are of significant importance to nuclear engineers since most BWRs operate under similar thermodynamic conditions. Simulation of bubbles and droplets in a gravity-free environment of the corresponding coexisting phase until steady state is reached satisfies Laplace law [3] at different temperatures and thus, yield the surface tension of the fluid. Comparing the LBM surface tension thus calculated using the LBM to the corresponding experimental values for water, the LBM lattice unit (*lu*)

can be scaled to the physical units. Using this approach, spatial scaling of the LBM emerges from the model itself and is not imposed externally.

## PENG-ROBINSON (P-R) EQUATION OF STATE

An equation of state (EOS) describes the relationship between temperature, pressure and density (volume) of a fluid. One such EOS was proposed by Peng and Robinson (P-R) [3]. It is widely used for determining the state of various fluids categorized by different accentric factors. The accentric factor ($\omega$) depends on the molecular structure of the fluid and is determined from its critical properties. Values of $\omega$ are tabulated in thermodynamic tables for various fluids. P-R EOS, which is a three-parameter ($T_c$, $p_c$ and $\omega$, defined below) cubic equation, fairly accurately captures the saturated densities over most of the liquid-vapor equilibrium curve. For water and steam, accentric factor $\omega = 0.3443$ leads to predicted values of saturated densities that agree very well with experimental data. This comparison is shown in Fig. 1.
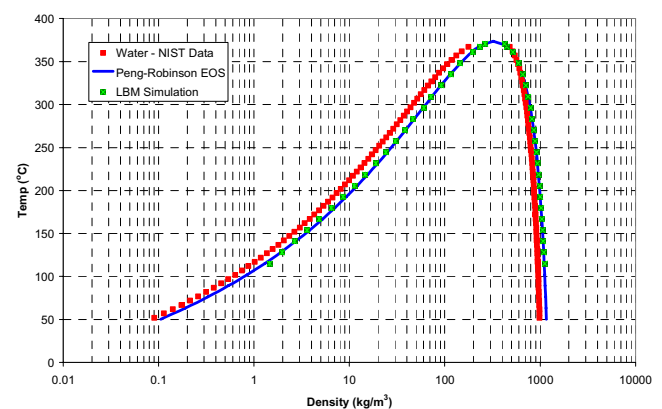


Figure 1. Comparison of the theoretical coexistence curve and the corresponding LBM simulation for Peng-Robinson (P-R) equation of state. Saturated water and vapor densities from NIST tables [4] are also shown.

Although more sophisticated equations of state —fitted to experimental data— can be developed and

implemented in the LBM model, P-R EOS is chosen due to its flexibility in changing the type of fluid by varying the accentric factor ω.

The P-R equation of state is:

$$p = \frac{\rho RT}{1-b\rho} - \frac{a\alpha(T)\rho^2}{1+2b\rho-b^2\rho^2} \qquad (1)$$

where

$$\alpha(T) = [1+(0.37464+1.54226\omega-0.26992\omega^2)(1-\sqrt{T/T_c})]^2$$

and $a = 0.45724R^2T_c^2\big/p_c$ , $b = 0.0778RT_c\big/p_c$ . Here, $T_c$ and $p_c$ represent critical temperature and critical pressure of the fluid under consideration, respectively. For water, $T_c$ is 647.1 $K$ and $p_c$ is 22.064 $MPa$. In simulations reported here, the constants $a$, $b$ and $R$ are set to be 2/49, 2/21 and 1, respectively [5]. Critical properties of the LBM fluid are then evaluated in terms of these constants. Using the law of corresponding states [3], reduced properties of lattice fluid can then be converted to real fluid properties.

P-R EOS can be written as a cubic equation in $V$ (replace $\rho$ by $1/V$ in Eq. (1)) and thus, have three real roots for $T < T_c$. The benefit of the cubic nature is that it can describe both the gaseous and the liquid phases of a fluid. Plotting $p$ vs. $V$ at constant $T$ and then applying the so-called *Maxwell equal-area construction* [3] yields the phase-coexistence curve. Figure 1 compares theoretical coexistence curve with the one obtained using the LBM simulations. It can be seen that the LBM results agree well with the theoretical results. Moreover, in Fig. 1, saturated water and vapor densities from NIST tables [4] are also plotted for comparison. It is observed that, when compared to the water-steam data at a selected saturation temperature, P-R EOS slightly over-predicts the saturated vapor and water densities. However, the calculated density ratio of saturated liquid and vapor matches very well with the water-steam data at different temperatures as shown in Fig. 2.

**RESULTS AND DISCUSSIONS**

The LBM simulations are performed for a *xy*-periodic domain of size 200 x 200 lattice-units (*lu*). Initially, a water drop (or vapor bubble) of 20 x 20 *lu* radius is placed at the center of the domain surrounded by the corresponding coexisting phase (saturated vapor for liquid *drop at the centre* and saturated liquid for vapor *bubble at the centre*). Simulation is supposed to have reached the steady-state [6-8] when the difference in simulation observables (velocities, densities etc.) for each consecutive 1000 time-steps reaches below $10^{-6}$ units. For the results reported here, steady-state is reached after 40,000 time steps. Using Laplace law, the surface tension

of water-steam system may be estimated. A series of bubbles of various sizes (20 to 50 *lu* radius) are simulated at different temperatures. After 40,000 time steps, the steady-state radii and inside/outside densities of the bubble are evaluated. Densities are then converted to the corresponding pressures using P-R EOS and the difference between the inside and the outside pressure $\Delta P$ of the bubble is computed. According to the Laplace law, for a 2D droplet/bubble, the pressure difference is given by

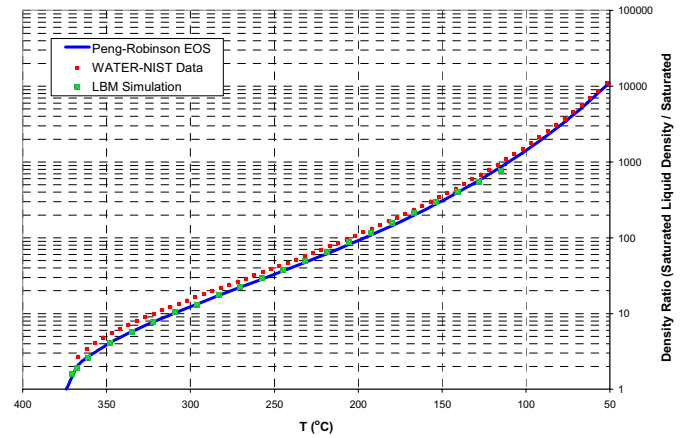$$\Delta P = \frac{\sigma}{R} \qquad (2)$$



Figure 2. Comparison of density ratios (saturated water / saturated vapor) obtained from Peng-Robinson EOS, NIST saturated property tables [4], and from corresponding LBM simulations at different temperatures.

In Fig. 3, $\Delta P$ is plotted against the inverse of the bubble radius ($1/R$) which yields straight lines of different slopes at different temperatures. As can be seen from Fig. 3, the spatial grid resolution of the LBM fluid is still in the lattice units (*lu*). Therefore, comparing the LBM surface tension (slope of $\Delta P$ *vs. 1/R*) with experimental surface tension of water may give an approximate measure of the LBM grid size in physical units. Thus, we can write

$$\sigma_{LBM,lu}(MPa.lu) = f\sigma_{Water}(Pa.m) \qquad (3)$$

where $\sigma_{LBM,lu}$ is the LBM surface tension in *MPa-lu* units and $\sigma_{Water}$ is the water surface tension in *Pa-m* units, for example, as given by NIST. Here, $f$ is a scaling factor with appropriate units to relate both the surface tensions. From Eq. (3), the estimate for 1 lattice unit in LBM is obtained as: $1\,lu = f\times10^{-6}\,m$
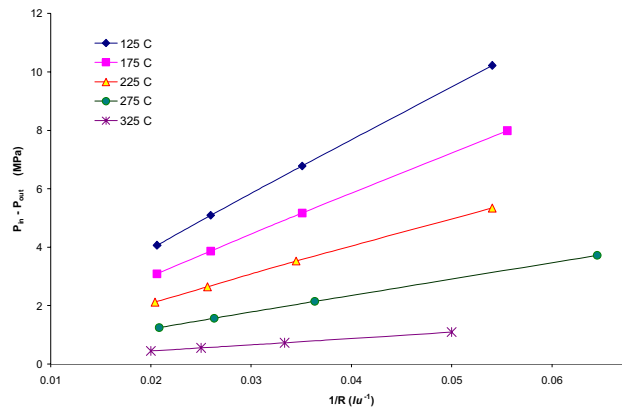
Figure 3. Plot of pressure difference across bubble vs. inverse radius simulated at different temperatures. Simulation domain is *xy-* periodic, and of 200 x 200 lattice unit size.

With *f* close to 1/3000, the LBM surface tension when converted to physical units well predicts the surface tension values in NIST tables for water for different temperatures ranging from 125 C to 325 C. For water, the lattice unit is hence estimated to be close to 0.33 *nm*. Figure 4 shows a comparison of the surface tensions of the LBM fluid and the value tabulated in NIST water property table (after the spatial scaling). Good agreement with macroscopic values suggests that the LBM approach is able to capture the surface tension phenomenon rather well at this scale. However, such a small lattice size is a concern for the computational viability of any realistic simulation and future work will refine the LBM model to allow capturing the correct surface tension while using a coarser lattice.
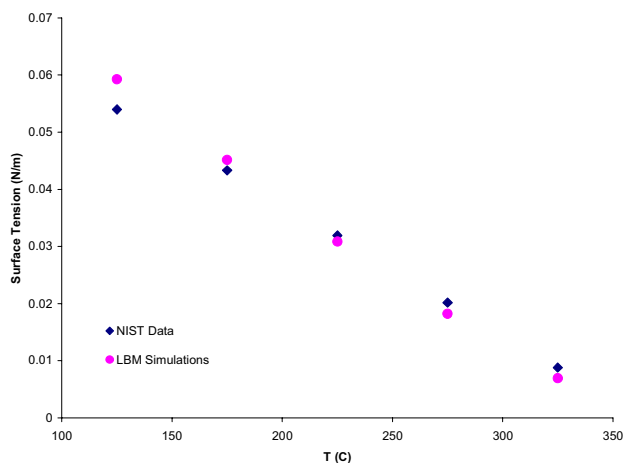


Figure 4. A comparison of surface tension of water (NIST data) with the surface tension values obtained from the LBM simulations, after lattice scaling.

## CONCLUSIONS

A Lattice Boltzmann model for the simulation of two-phase flow phenomena in BWRs is introduced and initial validation results are presented. It is shown that a non-ideal equation of state, such as the Peng-Robinson EOS, may be coupled with the LBGK scheme with single relaxation time to capture the phase-coexistence curve for water and steam in a wide range of temperatures. Simulating a series of isothermal bubbles and droplets suspended in their coexisting phase predicts the surface tension of the LBM fluid in units dependent on the lattice size. Comparing this to the experimental data for water-vapor surface tension provides a way to scale the LBM spatial grid in physical units so that the LBM predicted surface tension closely matches the physical water-vapor surface tension.

## ACKNOWLEDGMENT

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