Physica A 392 (2013) 3863–3868

Contents lists available at SciVerse ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Numerical simulation of pool boiling of a Lennard-Jones liquid

Hajime Inaoka *, Nobuyasu Ito

[a] Department of Applied Physics, Graduate School of Engineering, The University of Tokyo, Tokyo 113-8656, Japan

HIGHLIGHTS

- Successful numerical simulation of pool boiling by a molecular dynamics model.
- The change in regimes of boiling from nucleate boiling to film boiling is reproduced.
- The pool boiling curve by the model is consistent with experimental observations.

ARTICLE INFO

Article history:
Received 26 December 2012
Received in revised form 2 May 2013
Available online 11 May 2013

Keywords:
Pool boiling
Molecular dynamics simulation
Lennard-Jones particle system

ABSTRACT

We performed a numerical simulation of pool boiling by a molecular dynamics model. In the simulation, a liquid composed of Lennard-Jones particles in a uniform gravitational field is heated by a heat source at the bottom of the system. The model successfully reproduces the change in regimes of boiling from nucleate boiling to film boiling with the increase of the heat source temperature. We present the pool boiling curve by the model, whose general behavior is consistent with those observed in experiments of pool boiling.

1. Introduction

Boiling of a liquid is an important physical phenomenon for industrial applications related to energy production and energy transportation such as boilers, heat engines, and heat exchangers. Thus it is very significant to develop a technique to simulate behavior of a boiling liquid numerically in detail under a given condition. Boiling of a liquid is, however, a highly complex, nonequilibrium process involved with a phase transition from the liquid to the gas. Our knowledge of basic physics to deal with such an extreme process is, unfortunately, still very limited. Especially, there are many unknown factors in the dynamics of a gas–liquid interface and the transfer processes of the mass and the energy across the interface in a nonequilibrium environment. In spite of such a situation, there have been attempts to simulate boiling numerically by combinations of known physics and models of gas–liquid interfaces.

One of straightforward approaches to simulate boiling is directly solving equations of the dynamics of a fluid, such as a Navier–Stokes equation and various conservation laws of physical quantities, with a model of gas–liquid interfaces. Juric and Tryggvason simulated film boiling by coupling a finite difference approximation of a Navier–Stokes equation and a front tracking method with phase changes through liquid–vapor interfaces [1]. Dhir discussed conservation laws of mass, momentum, and energy for vapor and gas phases with continuously evolving vapor–liquid interfaces, and presented results of a numerical simulation of nucleate boiling and film boiling focusing on the difference of the conservation laws between these boiling regimes [2]. Tomar, Biswas, Sharma, and Agrawal simulated boiling of two types of fluids [3] with a combination

* Corresponding author. Tel.: +81 358416808.
E-mail address: inaoka@serow.t.u-tokyo.ac.jp (H. Inaoka).

0378-4371/$ – see front matter © 2013 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.physa.2013.05.002

of a volume-of-fluid method [4] and an interface capturing method called a level-set method [5]. A three-dimensional simulation of nucleate boiling was performed by Shin, Abdel-Khalik, and Juric using a model based on a combination of conservation laws and a construction method of gas–liquid interfaces [6].

Another approach to simulate boiling is based on a lattice Boltzmann method. A technique to simulate gas–liquid flows numerically by a lattice Boltzmann method with models of gas–liquid interfaces has been developed in the 1990's [7], and there have been attempts to simulate boiling by numerical models based on the technique. Seta and Okui simulated pool boiling in two-dimensional space and reproduced nucleate boiling [8]. Their simulation is, however, as the authors admitted, limited to cases with an unrealistically small density difference between the vapor and the liquid. Márkus and Házi also simulated two-dimensional boiling in microscale and discussed the relation between the heat source temperature and the heat flux from the source [9]. Though there was no comparison of the simulation result with experimental results, they discussed the heat conduction quantitatively in relation to the surface geometry of the heat source. Ryu and Ko performed a two-dimensional simulation of bubble nucleation of a superheated liquid by a free energy based multiphase lattice Boltzmann method [10]. They tried to validate their method by comparing the simulation result with analytical and experimental results.

Though there have been many works to reproduce boiling numerically as we partly mentioned above, the physical validity of these works is still uncertain. Many of the works related to numerical simulations of boiling published so far, more or less, involve models of gas–liquid interfaces and the transport of the mass and the energy through the interfaces based on assumptions of local equilibrium or linear nonequilibrium conditions. Such assumptions are, however, still to be tested in an extreme nonequilibrium environment of boiling.

Under such circumstances, a molecular dynamics (MD) simulation is one of the most promising methods to reproduce boiling numerically. In a case of an MD model, the liquid and the gas in a system are composed of a set of particles interacting with each other, and the time evolution of the system is performed simply by integrating an equation of motion. By choosing a mode of the interaction between pairs of particles properly, we expect that the boiling of the liquid is naturally reproduced without introducing any artifacts in the model. The only hardship to realize a simulation of boiling by an MD model is that it requires a lot of computer power to deal with the motion of particles with a sufficient number to compose the liquid and the gas in the system. The recent progress of computers has gradually made it possible to perform such a numerical simulation. In fact, the authors and a coworker studied an explosive gas–liquid flow by an MD model with two types of Lennard-Jones (LJ) particles [11,12]. We successfully reproduced major flow regimes of gas–liquid flows, such as a bubble flow and a spray flow. This work proved that complex behavior of a gas–liquid flow is simulated by an MD model with the capability of present computers.

In this paper, we present a molecular dynamics model of pool boiling of a Lennard-Jones particle system. There were studies of processes related to boiling using MD simulations, such as simulations of bubble nucleation by decompression of a liquid [13,14], and a simulation of evaporation of a gas from liquid surfaces in an annular flow [15]. To the best of our knowledge, however, there has not been any attempt to reproduce pool boiling comprehensively including bubble nucleation by heating of a liquid, growth of the bubble by continuous phase transition from liquid to gas, and detachment of the bubble from the heating surface by buoyancy. Though the system size of our simulation is still small to compare the results with experimental observations directly, it is significant to prove that pool boiling is comprehensively simulated by an MD model.

2. Model

We consider a situation that a liquid is put in a vessel in a uniform, downward gravitational field and it is heated from the bottom of the vessel. Since the vessel is put in a closed environment, the space above the liquid surface is filled by a gas vaporized from the liquid surface.

In our simulation, the liquid and the gas are both composed of Lennard-Jones particles. That is, pairs of particles in the system interact with each other via a 12-6 Lennard-Jones potential with a constant ϕ_0,

$$\phi(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] + \phi_0, \tag{1}$$

where ϵ and σ are constants and set to be unities. We introduce a cutoff r_0 of the potential to avoid long range interaction, that is, $\phi(r) = 0$ for $r \geq r_0$. The value of the constant ϕ_0 is set so that $\phi(r_0)$ is zero. We use $r_0 = 2.5$ in our simulation and ϕ_0 is about $\phi_0 \sim 0.016$ in this case. The time evolution of the system is governed by a Hamiltonian

$$H = \sum_i \frac{1}{2m_i}|\boldsymbol{p}_i|^2 + \sum_{i,j(i<j)} \phi(|\boldsymbol{q}_i - \boldsymbol{q}_j|) + \sum_i V_i, \tag{2}$$

and the numerical simulation is performed simply by integrating an equation of motion with a position-Verlet scheme. In the Hamiltonian, m_i, $\boldsymbol{q}_i$, and $\boldsymbol{p}_i$ denote the mass, the position, and the momentum of the i-th particle, respectively. In our simulation, the mass of all the particles is set as $m = 1$. V_i is the potential of external forces applied to the i-th particle, such as the gravitational force. The sums of the first and the third terms of the Hamiltonian run over all the particles and the second sum runs over all the pairs of the particles in the system. Any mechanical quantity in the system can be measured by