CrossMark

# Electrically charged interfacial interaction based on thermodynamic jump condition

Yukihiro Yonemoto [a,*], Tomoaki Kunugi [b]

[a] Priority Organization for Innovation and Excellence, Kumamoto University 2-39-1, Kurokami, Chuo, Kumamoto 860-8555, Japan
[b] Department of Nuclear Engineering, Kyoto University C3-d2S06, Kyoto Daigaku-Katsura, Nishikyo-ku, Kyoto 615-8540, Japan

## ARTICLE INFO

## ABSTRACT

At a gas–liquid interface, there are many unknown physical and chemical phenomena related to thermodynamics, electromagnetics, hydrodynamics, and heat and mass transfer. It is very difficult to understand all these mechanisms in detail; therefore, modeling the gas–liquid interface is one of the key issues in interfacial phenomena of multiphase flows. In our previous study, we developed a new gas–liquid interfacial model based on thermodynamics and a mathematical approach. In that study, we derived a new equation of free energy based on the lattice gas model, including the influence of an electric double layer on the interface caused by contamination. Then, an interfacial jump condition at the gas–liquid interface treated by thermodynamics was derived on the basis of our interfacial model. In this study, we analytically discuss the interfacial interaction on the basis of the thermodynamic jump condition on the macroscopic scale. Finally, we reveal the force vector fields on the gas–liquid interface depending on an electric potential. The result implies that contamination at the interface is very important to interfacial interaction.

## 1. Introduction

The mechanism of bubble coalescence/repulsion is still unknown, although it is a superficially simple behavior. Experimental research on bubble coalescence/repulsion has mainly focused on the effects of electrolyte concentration on the behavior and coalescence threshold of bubbles in a liquid (Bredwell & Telgenhoff, 1995; Craig, 2004; Giribabu & Ghosh, 2007; Henry & Craig, 2008; Marčelja, 2004; Riberio & Mewes, 2007; Spyridopoulos & Simons, 2004; Tsang, Koh, & Koch, 2004). These studies have revealed that the ions adsorbed at the gas–liquid interface, combination of these ions, and electrolyte concentration are important factors in bubble coalescence/repulsion. Contamination at the interface could greatly influence bubble coalescence/repulsion because contamination may be related to the heat and mass transfer and electrochemistry around the interface (Auster, Gunde, Mader, & Windhab, 2009; Joshi et al., 2009; Martin, Montes, & Galan, 2007). A coalescence model for a combination of simple ions has been theoretically proposed. It focuses on determining the impact of repulsive interaction, which results from the formation of an electric double layer around the interface, on bubble coalescence (Marčelja, 2000, 2006). However, a detailed mechanism has not yet been elucidated. On the other hand, from numerical research on the interfacial interaction, it is known that bubble coalescence occurs easily (non-realistic coalescence) (Matsumoto, Fukami, Kunugi, & Serizawa, 2001). This has been determined because the conventional interfacial model has been mainly constructed only on the basis of the mechanical energy balance (Brackbill, Kothe, & Zemach, 1992; Tryggvason et al., 2001).

---

* Corresponding author. Tel./fax: +81 963423690.
  E-mail address: yonemoto@mech.kumamoto-u.ac.jp (Y. Yonemoto).

Interfacial phenomena such as evaporation, condensation, and heat and mass transfer are complicated because such phenomena are characterized by various time and space scales. Because these phenomena are mainly related to thermodynamics, they are difficult to understand from a mechanical point of view. In our previous study, a gas–liquid interfacial model was developed to promote an understanding of bubble interaction such as coalescence and repulsion. The interfacial model was based on the phase field theory (Cahn & Hilliard, 1958), and a multiscale multiphase flow equation was finally derived. In the derivation, the multiscale concept with respect to the time and space scales was applied to the Navier–Stokes equation on the basis of the Chapman-Enskog expansion. From this equation, an interfacial jump condition was derived mathematically and thermodynamically (Yonemoto & Kunugi, 2011, chap. 4). The interfacial jump condition is a macroscopic interfacial equation in which the interface is characterized by a curvature (a mathematical interface). Therefore, our new interfacial model theoretically supports gas–liquid interfacial phenomena ranging from microscopic to macroscopic scales. The jump condition of physical parameters at the interface has been studied since early times (Delhaye, 1974; Scriven, 1960). In particular, the interfacial jump condition with respect to momentum has been mathematically derived considering the mechanical energy balance. In the derivation, the Stokes theorem, Gauss divergence theorem, and differential geometry were mainly used. An interfacial model based only on the mechanical energy balance cannot treat detailed physical and chemical phenomena occurring at the interface. In particular, contamination at the interface is an important aspect of interfacial interaction. In the present study, on the basis of the interfacial jump condition derived from the multiscale multiphase flow equation, interfacial interaction is analytically discussed to gain a deeper understanding of bubble coalescence and repulsion.

## 2. Interfacial jump condition

### 2.1. Momentum jump condition

Interfacial phenomena are mainly interpreted as discontinuous problems. When the curvature radius is larger than the thickness of an interface, the equilibrium force balance at the interface is given by the following equation expressed in terms of the interfacial coordinate system as defined in Fig. 1.

$$\dot{m}_g \boldsymbol{u}_g + \dot{m}_l \boldsymbol{u}_l - \{(-P_g)\boldsymbol{n}_g + \boldsymbol{\tau}_g \cdot \boldsymbol{n}_g\} - \{(-P_l)\boldsymbol{n}_l + \boldsymbol{\tau}_l \cdot \boldsymbol{n}_l\} - 2H\sigma\boldsymbol{n}_g - \frac{d\sigma}{ds}\boldsymbol{t} = \boldsymbol{0} \tag{1}$$

where $\dot{m}_g$ and $\dot{m}_l$ represent changes in mass, $H$ and $\sigma$ are mean curvature and surface tension coefficient, respectively, $P_i$ and $\tau_i$ ($i = g, l$) are pressure and shear stress, respectively. Eq. (1) is generally known as the momentum jump condition at the interface. The first and second terms on the left-hand side of Eq. (1) represent the change in momentum due to phase change. The third and fifth terms are bulk pressure, which affect the interface. The fourth and sixth terms are viscous force due to fluid motion. The seventh term is surface tension resulting from curvature change. The eighth term is a gradient of the surface tension coefficient along the tangential direction on the interface.

### 2.2. Thermodynamic jump condition

In our previous study, a multiscale multiphase flow equation was derived on the basis of the phase field theory from a viewpoint of thermodynamics, considering the time and space scales from micro to macro. In the present study, macroscopic interfacial phenomena are discussed by assuming that the interfacial jump condition is a measure of the macroscopic interfacial equation. The following equation is the interfacial jump condition derived from the multiscale multiphase flow equation:

$$0 = \underbrace{-\{(-P_g - \varepsilon\pi_g)\boldsymbol{n}_g + \boldsymbol{n}_g \cdot \boldsymbol{\tau}_g\}}_{(a)} \underbrace{-\{(-P_l - \varepsilon\pi_l)\boldsymbol{n}_l + \boldsymbol{n}_l \cdot \boldsymbol{\tau}_l\}}_{(b)} \underbrace{-\boldsymbol{n}_g \varepsilon 2H\sigma}_{(c)}$$

$$\underbrace{-\varepsilon\left(\boldsymbol{t}_1 \frac{1}{2}\frac{\partial\sigma}{\partial s_1} + \boldsymbol{t}_2 \frac{1}{2}\frac{\partial\sigma}{\partial s_2}\right)}_{(d)} \underbrace{-\boldsymbol{n}_g \varepsilon d \int_{-\infty}^{+\infty}\left\{\frac{\partial}{\partial s_1}\left(\frac{\partial\psi}{\partial n}\frac{\partial\psi}{\partial s_1}\right) + \frac{\partial}{\partial s_2}\left(\frac{\partial\psi}{\partial n}\frac{\partial\psi}{\partial s_2}\right)\right\}dn}_{(e)}$$

$$\underbrace{+\boldsymbol{n}_g \varepsilon d \int_{-\infty}^{+\infty}\frac{1}{2}\frac{\partial}{\partial n}\left\{\left(\frac{\partial\psi}{\partial s_1}\right)^2 + \left(\frac{\partial\psi}{\partial s_2}\right)^2\right\}dn}_{(f)} \underbrace{-\varepsilon\int_{-\infty}^{+\infty}\left(\boldsymbol{t}_1 \frac{\partial\psi}{\partial s_1} + \boldsymbol{t}_2 \frac{\partial\psi}{\partial s_2}\right)(-a\psi + b\psi^3)dn}_{(g)} \underbrace{+\varepsilon\int_{-\infty}^{+\infty}\left(\boldsymbol{t}_1 \frac{\partial\pi_i}{\partial s_1} + \boldsymbol{t}_2 \frac{\partial\pi_i}{\partial s_2}\right)dn}_{(h)}$$

$$\underbrace{+\frac{\varepsilon d}{2}\int_{-\infty}^{+\infty}\left\{\boldsymbol{t}_1 \frac{\partial}{\partial s_1}\left(\frac{\partial\psi}{\partial s_1}\right)^2 + \boldsymbol{t}_2 \frac{\partial}{\partial s_2}\left(\frac{\partial\psi}{\partial s_2}\right)^2\right\}d\boldsymbol{n}}_{(i)} \underbrace{+\varepsilon d 2H\int_{-\infty}^{+\infty}\left(\boldsymbol{t}_1 \frac{\partial\psi}{\partial s_1} + \boldsymbol{t}_2 \frac{\partial\psi}{\partial s_2}\right)\left(\frac{\partial\psi}{\partial \boldsymbol{n}}\right)dn}_{(j)}$$

$$\underbrace{+\varepsilon d \int_{-\infty}^{+\infty}\left\{\boldsymbol{t}_1 \frac{\partial}{\partial s_2}\left(\frac{\partial\psi}{\partial s_1}\frac{\partial\psi}{\partial s_2}\right) + \boldsymbol{t}_2 \frac{\partial}{\partial s_1}\left(\frac{\partial\psi}{\partial \boldsymbol{s}_1}\frac{\partial\psi}{\partial s_2}\right)\right\}dn}_{(k)} \underbrace{-\frac{\varepsilon d}{2}\int_{-\infty}^{+\infty}\left\{\boldsymbol{t}_1 \frac{\partial}{\partial s_1}\left(\frac{\partial\psi}{\partial s_2}\right)^2 + \boldsymbol{t}_2 \frac{\partial}{\partial s_2}\left(\frac{\partial\psi}{\partial s_1}\right)^2\right\}dn}_{(l)} \tag{2}$$