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# Development, verification and application of a new model for active nucleation site density in boiling systems

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## ABSTRACT

A new model for active nucleation site density in boiling systems has been developed and preliminarily applied in Computational Fluid Dynamics (CFD) simulations of subcooled boiling in a vertical heated tube. The new model is based on a parametric analysis of existing experimental data. It is a function of three variables: wall superheat, pressure, and contact angle; and is applicable in a wide range of pressures: 0.101 MPa–19.8 MPa. A preliminary study of the temperature dependence of the contact angle has been performed during the development process. The new model is intended to improve the predictions of: (i) interfacial area concentration in two-fluid models, and (ii) wall temperature in subcooled boiling simulations. For the active nucleation site density itself, the verification results showed that the values predicted by the newly developed model are in good agreement with various published experimental data. The model also demonstrated improvements of other existing models. The new model was utilized in CFD simulations of subcooled boiling in a vertical heated tube. The predicted void fraction and wall temperature in subcooled boiling flow agree well with the experimental data.

## 1. Introduction

Subcooled boiling, in Light Water Reactors (LWRs), has been drawing increasing attention for its significant enhancement on the heat transfer and its close relation to the critical heat flux. In Pressurized Water Reactors (PWRs), subcooled boiling may take place in the reactor core (fuel assemblies) and the steam generator, both highly related to the reactor safety.

Recently, increasing efforts have been made to utilize the two-fluid model coupled with the wall boiling model to simulate subcooled boiling. In the two-fluid model, the liquid and vapor phases are modeled by separate sets of equations for convention of mass, momentum, and energy; and interfacial items are used to calculate the mass, moment and energy transfer between the phases. The wall boiling model is concerned with the wall sources induced by the nucleate boiling near the heated wall. The most widely used wall boiling model, the so-called RPI wall boiling model, in which the wall heat flux is split into three parts was developed by Kurul and Podowski (1991). Hibiki and Ishii (2003) found theoretically that active nucleation site density has a great influence on the prediction of interfacial area concentration. The active nucleation site density is an important sub-model within the RPI wall boiling model as well. Krepper and Rzehak (2011) showed that active nucleation site density has a significant impact on the calculation of the wall temperature when using the wall boiling model. Therefore, it is desirable to develop a reliable model for the prediction of the active nucleation site density, as both the interfacial area concentration and the wall boiling model are of great importance in the simulation of subcooled boiling.

A model developed by Lemmert and Chawla (1977); which is only related to the wall superheat based on the experimental data with a coolant in a pressure range of 0.1 to 0.2 MPa, is widely used in the subcooled boiling simulation for its simplicity and good convergence characteristics. Wang and Dhir (1993) proposed an empirical correlation, which takes into account the effects of contact angle and critical cavity size on the basis of their experimental data in atmospheric pressure. Basu et al. (2002) proposed an empirical correlation on the wall superheat and contact angle based on their convective and pool boiling experimental data in atmospheric pressure. While most of the models focus on the atmospheric pressure, Kocamustafaogullari and Ishii (1983) proposed a model that is applicable to pressure as high as 19.8 MPa by means of a parametric study. Their model is a function of the contact angle and critical cavity size. Hibiki and Ishii (2003) then

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**Nomenclature**

| | |
|---|---|
| $A$ | parameter and function of pressure |
| $B$ | parameter and function of pressure |
| $C$ | parameter |
| $D$ | tube diameter |
| $c$ | parameter |
| $f(P)$ | function of pressure |
| $f_1(\theta)$ | function of contact angle |
| $f_2(P)$ | function of pressure |
| $f_3(\Delta T_{sup})$ | function of wall superheat |
| $G$ | mass flow rate |
| $h_{gl}$ | latent heat |
| $K$ | parameter |
| $m$ | exponent |
| $N$ | number of experimental data |
| $N_0$ | constant |
| $N_w$ | active nucleation site density |
| $P$ | system pressure |
| $P_f$ | system pressure |

| | |
|---|---|
| $q_w$ | wall heat flux |
| $Q$ | wall heat flux |
| $R$ | gas constant |
| $R_c$ | critical cavity radius |
| $T_g$ | gas temperature |
| $T_{sat}$ | saturation temperature |
| $T_c$ | critical temperature at which contact angle becomes 0 |
| $T_w$ | wall temperature |
| $T_0$ | room temperature |
| $\rho_l$ | density of liquid |
| $\rho_g$ | density of gas |
| $\gamma$ | exponent |
| $\sigma$ | surface tension |
| $\sigma_1, \sigma_2$ | prediction error |
| $\theta$ | contact angle |
| $\theta_0$ | contact angle at room temperature |
| $\Delta T_{sup}$ | wall superheat |
| $x_i$ | the ith data point |
| *cal.* | calculated values |
| *exp.* | experimental values |

developed a new mechanistic model for a wide range of operation conditions, including high pressures. Hibiki and Ishii claimed that their model produced more accurate results when compared with the Kocamustafaogullari and Ishii's model. However, the model gives extremely high values of the active nucleation site density in high heat flux conditions, which leads to convergence issues in the simulation of subcooled boiling (Star-CCM+, 2013), especially in high pressure conditions.

To improve the prediction capability of the active nucleation site density in a wide range of operating conditions, especially in high pressure conditions such as PWR systems, a new model has been developed in both empirical and theoretical ways. The new model is utilized in Computational Fluid Dynamics (CFD) simulation of subcooled boiling flow in a vertical heated tube. The obtained results are presented in this paper.

## 2. Modeling of active nucleation site density

### 2.1. Parametric analysis

To model the active nucleation site density, which simply counts the average number of gas-filled cavities in a heated wall, a number of flow parameters, including heat flux, fluid properties and wall conditions, should be taken into account as they are directly related to the generation of the gas-filled cavities.

Several studies have been performed on the active nucleation site density, $N_w$, as a function of the wall heat flux, $q_w$, the wall superheat, $\Delta T_{sup}$ , or the critical cavity radius, $R_c$. Gaertner and Westwater (1960) found that $N_w$ has an exponential dependence on the wall heat flux:

$$N_w \propto q_w^{2.1}. \tag{1}$$

A similar tendency was observed in the Sakashita's experiment (Sakashita, 2011) on nickel foil surface. Moreover, Sakashita also found that when other conditions are maintained, the wall heat flux and wall superheat follow the relationship: $q_w \propto \Delta T_{sup}^m$. Thus, the effect of $q_w$ can be represented by the effect of wall superheat.

Wang and Dhir (1993), Kocamustafaogullari and Ishii (1983), Hibiki and Ishii (2003) proposed their correlations based on $R_c$, or rather, $R_c^{-1}$. $R_c$ can be written as:

$$R_c = \frac{2\sigma\{1 + (\rho_g/\rho_l)\}/P_f}{\exp\{h_{gl}(T_g - T_{sat})/(RT_g T_{sat})\} - 1}, \tag{2}$$

where $\sigma$, $\rho_g$, $\rho_l$, $P_f$, $h_{gl}$, $T_g$, $T_{sat}$ and $R$ are the surface tension, gas density, liquid density, system pressure, latent heat, gas temperature, saturation temperature and gas constant, respectively. When $\rho_g << \rho_l$ and $h_{gl}(T_g - T_{sat})/(RT_g T_{sat}) << 1$, $R_c$ can be simplified as:

$$R_c \approx \frac{2\sigma T_{sat}}{(T_g - T_{sat})h_{fg}\rho_g}. \tag{3}$$

In boiling systems, usually the wall temperature instead of the gas temperature is used in Eq. (3). Thus,

$$R_c^{-1} \propto \Delta T_{sup}. \tag{4}$$

This simplification may not be suitable for relatively low and high pressures, but $R_c^{-1}$ can still be approximated as a linear function of $\Delta T_{sup}$ within a certain range of wall superheat. In the $R_c^{-1}$ correlation, other parameters are liquid properties, which are all pressure related in water systems. Therefore, $R_c^{-1}$ can be represented as a function of the wall superheat and pressure. From the above analysis, it is implied that $q_w$, $\Delta T_{sup}$ and $R_c$ are correlated, thus in this work $\Delta T_{sup}$ is selected as a variable because of its more direct relation to the active nucleation site density. $R_c^{-1}$ is pressure related. Therefore pressure may also affect the active nucleation site density. Sakashita (2011) proved experimentally the pressure effect on the active nucleation site density. Higher pressure induces higher active nucleation site density. The positive influence of pressure can also be found in the Hibiki and Ishii (2003) and in the Kocamustafaogullari and Ishii (1983). To develop a model that suits PWR conditions, pressure is also regarded as one of the main variables. In the new model, the properties of liquid are implicitly included in the function of pressure, bringing some convenience in calculating the value as there is no need to obtain the complex properties.

In addition to the wall superheat and pressure, the surface conditions, such as the material of the heated surface and its roughness, also have a significant effect on the generation of gas cavities. Basu et al., Hibiki and Ishii, Wang and Dhir all used the contact angle θ to describe the influence of the heated wall, as it represents the wettability of the surface and relates to the surface roughness (Kandlikar and Steinke, 2002).

Other flow parameters, such as the mass velocity and liquid subcooling, are not considered in this work, because it is believed that for a given wall superheat the active nucleation site density has no significant dependence on these parameters, as experimentally proved by Basu et al. (Basu et al., 2002).

As a result, the wall superheat, pressure and contact angle are chosen as the variables that have the largest influence on the prediction of active nucleation site density. These three variables also cover most