RPE | **Radiation Physics & Engineering**
A Peer-Reviewed Journal
Published by K.N. Toosi University of Technology
http://rpe.kntu.ac.ir
Research Article

Radiation Physics and Engineering 2025; 6(3):35–40

Simulation of pool boiling for surfaces with various wettability

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HIGHLIGHTS

- The Rensselaer Polytechnic Institute (RPI) model, is used to simulate surfaces with different wettability
- With some modifications, the RPI model be employed to simulate pool boiling heat transfer and CHF.
- The modified RPI model has a good ability to accurately predict the heat flux for the pool boiling stage.
- The critical heat flux results from the simulation showed an error of less than 5% compared to the experimental results.

ABSTRACT

A boiling model, specifically the Rensselaer Polytechnic Institute (RPI) model, is utilized by Computational Fluid Dynamics (CFD) code to calculate the pool boiling behavior on surfaces with varying wettability characteristics. The RPI model is an accurate method for predicting the heat transfer coefficient of nucleate boiling, which is based on a component-by-component heat flux analysis. With some modifications, the RPI model can also be employed to simulate pool boiling heat transfer and CHF. To validate the modeling approach, the calculated heat flux for the pool boiling regime is compared to experimental data from the literature. The results indicate that the modified RPI model has a good ability to accurately predict the heat flux for the pool boiling stage. Furthermore, this modified RPI model demonstrates close agreement with the experimental results obtained for surfaces exhibiting diverse wettability properties. This suggests the model's capability to effectively capture the impact of surface wettability on pool boiling heat transfer. The successful application and validation of the modified RPI model for pool boiling simulations, particularly its ability to account for varying surface wettability characteristics, represents a valuable contribution to the existing knowledge on computational modeling of boiling heat transfer phenomena.

KEYWORDS
RPI model
Pool boiling
Wettability characteristics
Boiling heat transfer
CHF

HISTORY
Received: 10 September 2024
Revised: 6 January 2025
Accepted: 20 January 2025
Published: Summer 2025

1 Introduction

Device performance in many applications increasingly depends on the ability to dissipate large amounts of heat while maintaining material temperatures below regulatory limits. These include supercomputers, computer data centers, power electronics for hybrid vehicles, heat exchangers for hydrogen storage, advanced radar, medical X-ray equipment, avionics for aircraft, satellites and spacecraft, laser- and microwave-guided energy weapons, which are collectively categorized as relatively low temperature applications, and nuclear power plants (Liang and Mudawar, 2019).

One of the efficient heat transfer mood in the nuclear power plants is the nucleate boiling. In this heat transfer regime, the high heat flux can be transferred with smaller wall superheat than other heat transfer regimes. The nucleate boiling regime in the heat transfer systems is limited by the onset of nucleate boiling (ONB) and critical heat flux (CHF).

The boiling process is a very complex phenomenon and a lot of research is being done to understand the concept of boiling heat transfer. The value of the critical heat flux (CHF) determines the maximum heat transfer that is possible in the nucleate boiling process under a certain condition. Most research on boiling has focused on increasing the CHF value and boiling heat transfer coefficient. It is very difficult to set specific conditions to achieve a higher CHF value because the heat transfer during boiling in the tank depends on many parameters such as: the operating pressure, the type of working fluid, the structure of the heated surface, the surface tension between the heated surface and working fluid, surface roughness, and etc. (Rahimian et al., 2020c).

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https://doi.org/10.22034/rpe.2025.477700.1242

Boiling phenomena serves as a critical heat transfer mechanism within nuclear reactors, especially in the cooling systems associated with the reactor core. This process facilitates the effective dissipation of the substantial heat produced in the reactor core during both standard operational conditions and potential accident scenarios. Furthermore, it plays a vital role in cooling the nuclear fuel rods, thereby preventing overheating, which is essential for preserving the structural integrity of the fuel and averting the release of radioactive substances. Numerous advanced nuclear reactor designs incorporate passive safety systems that leverage the principles of boiling for emergency core cooling, thereby enhancing the reactor's inherent safety features. The investigation of boiling heat transfer is fundamental to the comprehensive thermal-hydraulic analysis and modeling of nuclear reactor systems, which is essential for ensuring optimal design, safety, and performance (Rahimian et al., 2020a; Hadad et al., 2013; Rahimian et al., 2022, 2019, 2020b; Sharma et al., 2015).

Recent studies of boiling heat transfer have shown that the nanofluids can significantly improve the CHF (Hadad et al., 2013, 2015). Further studies have shown that these changes in the nanofluid boiling phenomenon and CHF are not due to the intrinsic nature of the nanofluids but are due to the deposition of the nanoparticles on the heating surfaces and change of surface texture and morphology (Rahimian et al., 2022, 2019, 2020b). Therefore, several studies carried out on the coating of heating surfaces with nanoparticles. The major focus on the surface modification to augment CHF and boiling heat transfer has been on the microscale modifications. Recent studies are almost experimental. A large number of published articles in this field are experimental studies and less simulations of coated surfaces have been performed.

In this article, fluent software has been utilized to simulate the heat transfer of Nano-coated surfaces. This software employs the Eulerian-Eulerian framework to model boiling flow, specifically implementing the Rensselaer Polytechnic Institute (RPI) model. Although the RPI method is primarily intended for flow boiling simulations, it can be slightly modified for applications in pool boiling. The first phase involves verifying the calculations and equations related to this model. This modeling is accomplished by varying boiling parameters such as nucleation site density and bubble departure frequency. The parameters selected for this analysis are based on experimental data from this study as well as previous research.

2 General governing equations

In the Eulerian-Eulerian method, the dispersed phase is also considered as a continuous phase. All phases can interpenetrate when moving through the solution domain. Continuity is expressed as Eq. (1):

$$\frac{1}{\rho_{rq}}\Big(\frac{\partial}{\partial t}(\alpha_q\rho_q) + \nabla.(\alpha_q\rho_q\vec{v}) = \sum_{p=1}^{n}(\dot{m}_{pq} - \dot{m}_{qp})\Big) \tag{1}$$

where ρ_{rq} is the phase reference density, or the volume averaged density of the q phase in the solution domain Ishii and Mishima (Ishii and Mishima, 1984). The momentum balance is in the form of an Eq. (2):

$$\begin{aligned}\frac{\partial}{\partial t}(\alpha_q\rho_q\vec{v}_q) + \nabla.(\alpha_q\rho_q\vec{v}_q\vec{v}_q) = -\alpha_q\nabla p + \nabla.\bar{\tau}_q \\ + \alpha_q p_q\vec{g} + \sum_{p=1}^{n}(\vec{R}_{pq} + \dot{m}_{pq}\vec{v}_{pq} - \dot{m}_{qp}\vec{v}_{qp}) \\ + (\vec{F}_q + \vec{F}_{lift,q} + \vec{F}_{vm,q})\end{aligned} \tag{2}$$

Using the law of conservation of momentum, the equations of motion governing the fluid are obtained, which are used to calculate the speed and pressure. In Eq. (2), the terms of stress tensor, lift force, virtual mass force are expressed as Eqs. (3) to Eq. (5):

$$\bar{\tau}_q = \alpha_q\mu_q(\nabla\vec{v}_q + \vec{v}_q^T) + \alpha_q(\lambda_q - \frac{2}{3}\mu_q)\nabla.\vec{v}_q\bar{I} \tag{3}$$

$$\vec{F}_{lift} = -C_l\rho_q\alpha_p(\vec{v}_q - \vec{v}_p)\times(\nabla\times\vec{v}_q) \tag{4}$$

$$\vec{F}_{vm} = 0.5\alpha_p\rho_q\Big(\frac{\mathrm{d}_q\vec{v}_q}{\mathrm{d}t} - \frac{\mathrm{d}_p\vec{v}_p}{\mathrm{d}t}\Big) \tag{5}$$

Here μ_q and λ_q are the shear and bulk viscosity of phase q, $\vec{F}_q$ is an external body force, $\vec{F}_{lift,q}$ is a lift force, $\vec{F}_{vm,q}$ is a virtual mass force and p is the pressure shared by all phases. The lift force acting on a secondary phase p in a primary phase q is computed from Drew and Lahey (Drew and Lahey, 1993). Here C_l is the lift coefficient, which typically takes a value of 0.5 for inviscid flow.

For multiphase flows, this model includes the "virtual mass effect" that happens when a secondary phase p accelerates relative to the primary phase q. The inertia of the primary-phase mass encountered by the accelerating particles (or droplets or bubbles) exerts a "virtual mass force" on the particles Drew and Lahey (Drew and Lahey, 1993).

The energy balance is in the form of Eq. (6):

$$\begin{aligned}\frac{\partial}{\partial t}(\alpha_p\rho_q h_q) + \nabla.(\alpha_q\rho_q\vec{u}_q\vec{h}_q) = \alpha_q\frac{\partial p_q}{\partial t} + \bar{\tau}_q : \nabla\bar{u}_q \\ - \nabla.\bar{q}_q + S_q + \sum_{p=1}^{n}\Big(Q_{pq} + \dot{m}_{pq}h_{pq} - \dot{m}_{qp}h_{qp}\Big)\end{aligned} \tag{6}$$

where h_q is the specific enthalpy of the q^{th} phase, $\vec{q}_q$ is the heat flux, S_q is a source term that includes sources of enthalpy (e.g., due to chemical reaction or radiation), Q_{pq} is the intensity of heat exchange between the p^{th} and q^{th} phases, and h_{pq} is the interphase enthalpy.

3 RPI model

This model is one of the most popular and accurate methods for predicting the heat transfer coefficient of nucleate boiling, which is based on the component-by-component heat flux (the so-called RPI method). This model is based on Bowring's design (Bowring, 1962) and in it different boiling mechanisms are investigated separately. The RPI model was initially developed to investigate boiling flow, but in this study it was studied to investigate pool boiling. The heat that is removed by the boiling flow is expressed in the following three categories.

Heat that is used for evaporation and latent heat and creates bubbles. The heat used to re-form the thermal boundary layer, which is called the quench heat flux. The heat that is transferred to the liquid phase in areas far from the bubble due to turbulent natural convection. The total boiling heat flux is obtained from the sum of this heat flux and is expressed as:

$$\begin{aligned}\dot{q}_w &= \dot{q}_c + \dot{q}_Q + \dot{q}_E \\ \dot{q}_w &= h_c(T_w - T_L)(1 - A_b) + \frac{2k_l}{\sqrt{\pi \lambda_l T}}(T_w - T_l) \\ &\quad + V_d N_w \rho_v h_{fv} f\end{aligned} \tag{7}$$

The heated wall surface is divided into area A_b , which is covered by nucleating bubbles and a portion $(1 - A_b)$, which is covered by the fluid. In convective heat flux (q_C), h_C is the single phase heat transfer coefficient, and T_w and T_l are the wall and liquid temperatures, respectively. The quenching heat flux (qQ) models the cyclic averaged transient energy transfer related to liquid filling the wall locality after bubble detachment. In quenching heat flux, k_l is the conductivity, T is the periodic time, and $\lambda_l = \frac{k_l}{\rho_l c_{pl}}$ is the diffusivity. In the evaporative flux (q_E), V_d is the volume of the bubble based on the bubble departure diameter, N_w is the active nucleate site density, ρ_v is the vapor density, and h_{fv} is the latent heat of evaporation, and f is the bubble departure frequency. These equations need closure for the following parameters: Area of Influence description is established on the departure diameter and the nucleate site density:

$$A_b = \min(1, k\frac{N_w \pi D_w^2}{4}) \tag{8}$$

The value of the empirical constant k is usually set to 4 or computed based on Del Valle and Kenning's relation.

Application of the RPI model generally uses the frequency of bubble departure as the one based on inertia controlled growth (not really applicable to subcooled boiling).

$$f = \frac{1}{T} = \sqrt{\frac{4g(\rho_l - \rho_v)}{3\rho - lD_w}} \tag{9}$$

The nucleate site density is frequently signified by a correlation based on the wall superheat.

$$N_w^* = f(\rho^*) r_c^{*-4.4} \tag{10}$$

Here

$$N_w^* = N_w D_w^2 \tag{11}$$

$$r_c^* = \frac{2r_c}{D_w} \tag{12}$$

$$r_c^* = \frac{2\sigma T_{sat}}{\rho_v h_{fv} \Delta T_w} \tag{13}$$

$$\rho^* = \frac{\rho_l - \rho_v}{\rho_v} \tag{14}$$

where w_D is the bubble departure diameter and $D_w = 0.0012(\rho^*)^{0.9} 0.0208\phi\sqrt{\frac{\sigma}{g(\rho_l - \rho_v)}}$ with ϕ existence the contact angle in degrees. The density function is defined as:

$$f(\rho^*) = 2.157 \times 10^{-7} \rho^{*-3.2}(1 + 0.0049\rho^*)^{4.13} \tag{15}$$

4 Boundary conditions

The geometry and dimensions used in this modeling are identical to those in the experimental study conducted by Gerardi et al. (Gerardi et al., 2010). Furthermore, the Reynolds-stress is modeled using the standard $k-\varepsilon$ model based on the eddy-viscosity approach and constant intensity turbulence, equal to 5%, is inserted. On the walls, the non-slip conditions are executed, while both turbulent kinetic energy and dissipation of turbulent kinetic energy are equal to zero. Surface heat flux from heated surface is supposed to be constant along its length at each heating step. Operational pressure is atmospheric.

5 Numerical validation

In order to validate a part of the RPI model for the simulation of pool boiling and also because of the simplicity in the simulation, the experimental results of Gerardi et al. (Gerardi et al., 2010) have been used. Figure 1 shows a diagram of Gerardi et al.'s experimental equipment system, Fig. 2 also shows the modeled geometry and created mesh.

The accuracy of finite volume method is directly related to the quality of the discretization used. A comprehensive mesh sensitivity study was done to check on the influence of the mesh resolution on the results and to minimize numerical influences introduced by the size of meshes and their distributions. For mesh sensitivity analysis, four meshes of differing size were used ranging from 15000 to 35000 for the geometry. The mesh refinement ratio (MRR) is defined as the ratio between consecutive meshes of mesh refinement. The number of 32000 mesh appears to be satisfactory to ensure the accuracy of numerical results as well as their independency with respect to the number of nodes used. The boiling curve depicts the variation of heat flux from the surface to the liquid with wall superheat (wall temperature minus liquid saturation temperature).

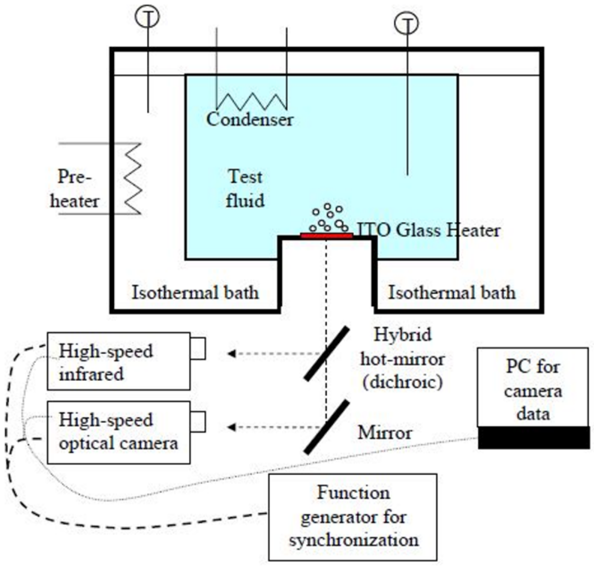

Figure 1: A schematic of the boiling heat transfer measurement system by Gerardi et al. (Gerardi et al., 2010).

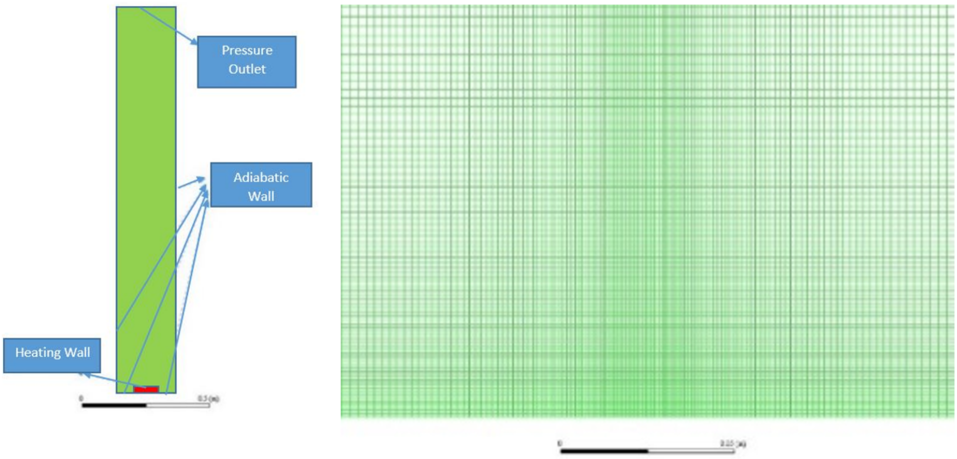

Figure 2: A view of the geometry and mesh to simulate the studies of Gerardi et al. (Gerardi et al., 2010).

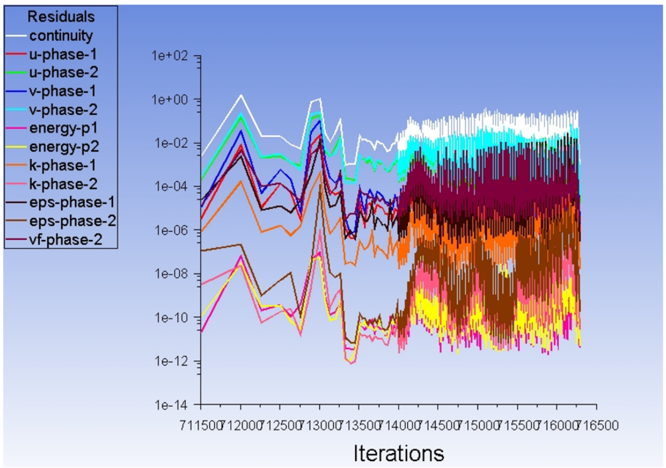

Figure 3: Residual of the basic equations.

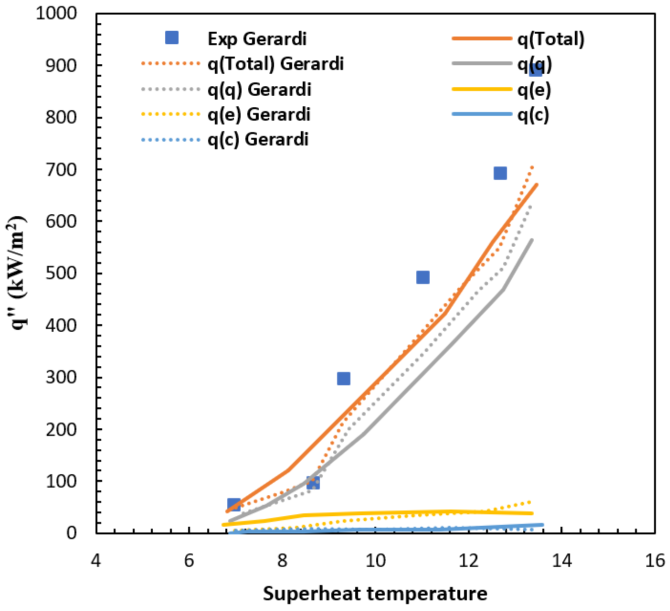

Figure 4: Simulation of pool boiling and comparison of its results with the experimental results of Gerardi et al. (Gerardi et al., 2010).

The boiling curve is highly effective for identifying the different heat transfer regimes encountered at different levels of wall superheat. They are comprised of (a) the single-phase liquid cooling regime (b) the nucleate boiling (N_B) regime (c) the transition boiling (T_B) regime. Figure 3 shows the nucleate boiling regime of boiling curve. The total partitioned heat flux, q_{total}, is shown along with the component heat fluxes: evaporation (q_e); quench, (q_q); and convection, (q_c).

The convergence values and residual plot have been shown in Fig. 2. Figure 4 shows the comparison between the experimental results and the simulation of Gerardi et al. (Gerardi et al., 2010) and the numerical simulation of pool boiling in this study. The simulation results presented in this study are similar to those of Gerardi et al. (Gerardi et al., 2010) and closely match the experimental results, following the same trend. At partial heat fluxes, the quench flux demonstrates the highest heat removal capacity. In general, the modeling of pool boiling exhibits an error of less than 5% (Gerardi et al., 2010).

6 RPI Modeling Enhancement

As mentioned in Section 4, the bubble departure diameter depends on the contact angle of the droplet with the surface. By altering the bubble departure diameter, the nucleation site density and the frequency of bubble departure also change. Therefore, by modifying the contact angle, all boiling parameters are affected. Considering that the deposition of nanoparticles alters the contact angle of the droplet with the surface (Rahimian et al., 2022, 2019, 2020b), it is sufficient to obtain the aforementioned boiling parameters with new contact surfaces and perform modeling with them. Thus, by changing the contact angle provided by the coating, the boiling phenomenon of coated surfaces can be simulated.

7 Results

In this article, by changing boiling parameters in the RPI method, such as Bubble departure diameter, bubble departure frequency, and nucleation site density, simulation of surfaces with various wettability has been done (Fig. 4). One of the most important areas of boiling is the critical heat flux, which can be predicted at surfaces with various wettability only by using empirical correlations. Therefore, creating the possibility of simulating boiling as well as critical heat flux for surfaces with different wettability will be very useful.

In this study, varying the contact angle affects the bubble departure diameter and, consequently, other boiling parameters. The analysis begins with a low heat flux, which is then increased in step increments (see Fig. 5). This process continues until a sudden increase in superheat temperature is observed, indicating the critical heat flux. In this article, some experimental correlations of critical heat flux are introduced, and at the end, simulation results and experimental relations are compared with each other.

The CHF or the boiling crisis refers to the maximum heat flux that a significant portion of the solid-liquid contact is not lost on a heating surface. The nucleate boiling is the heat transfer regime used in many industries, and the CHF represents the upper limit of the safe operation of thermal systems.

The CHF was modeled by Zuber et al. (Zuber, 1959) assuming that the hydrodynamic stability is the main factor in this process. According to this model, the ability of the hydrodynamic system to prevent the formation of large dry areas is a controlling factor for the CHF. This correlation is expressed as follows.

$$q''_{CHF} = K\rho_g h_{fg}\Big[\frac{g\sigma(\rho_f-\rho_g)}{\rho_g^2}\Big]^{1/4} \tag{16}$$

Here K depends on the system geometry. Therefore, this relation is related only to fluid parameters and has no dependence on the surface parameters.

One of the models that includes the surface effects on the CHF is the Kandlikar (Kandlikar, 2001) model. This model analyses the mechanism of the CHF phenomenon using the hydrodynamic behavior of a bubble interface on a heating surface. The Kandlikar model investigates the parallel forces with the heating surface, which is the result of evaporation at the interface of the liquid-vapor near the heating surface. In this model, the CHF occurs when the momentum force due to evaporation at the bubble base exceeds the sum of the forces holding the bubble, including inertia, pressure and buoyancy forces.

The surface tension on the heater surface is a fluid property that depends on the surface wettability (contact angle). The Kandlikar model is expressed as follows:

$$\begin{aligned} q''_{CHF} &= \rho_g^{1/2} h_{fg}\Big(\frac{1+\cos\beta}{16}\Big) \\ &\times \Big[\frac{2}{\pi}+\frac{\pi}{4}(1+\cos\beta)\cos\phi\Big]^{1/2}\Big[\sigma g(\rho_f-\rho_g)\Big]^{1/4} \end{aligned} \tag{17}$$

Here β is the receding contact angle. As mentioned, the Kandlikar model introduces the CHF as a function of the wettability or contact angle. Figure 6 illustrates the relationship between critical heat flux and contact angle for various conditions. As the contact angle decreases, the critical heat flux increases.

Liao et al. (Liao et al., 2008) represent the Zuber CHF correlation with the effect of orientation and contact angle:

$$q''_{CHF} = \Big[1\frac{55-\theta}{100}(0.56)\Big]\rho_g h_{fg}\Big[\frac{g\sigma(\rho_f-\rho_g)}{\rho_g^2}\Big]^{1/4} \tag{18}$$

Under normal conditions, the contact angle of water on a surface is approximately 90 degrees. In this study, calculations were performed at four distinct contact angles: 90, 60, 30, and 10 degrees. The results were then compared with the critical heat flux correlations proposed by Zuber, Kandlikar, and Liao.

Comparing the simulation results with the experimental correlations shows that the simulation with the RPI method has been able to show the critical heat flux changes well. The simulation results are closer to Liao's results. According to creating the ability to simulate surfaces with different wettability, this method can be used to simulate surfaces with nano coatings, which causes a change in their contact angle.

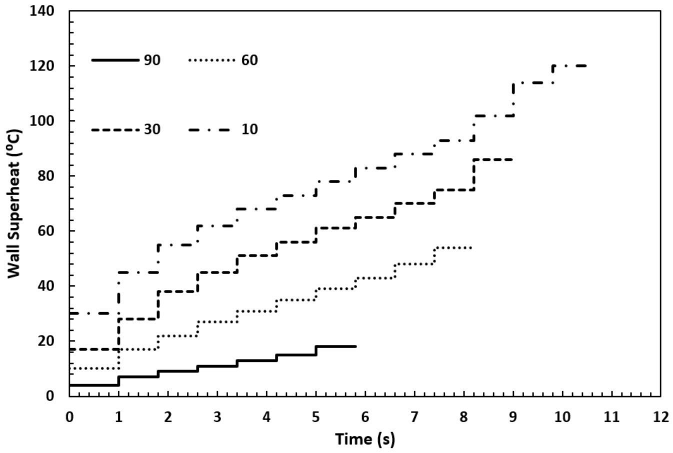

Figure 5: Wall superheat temperature at different times for various contact angles.

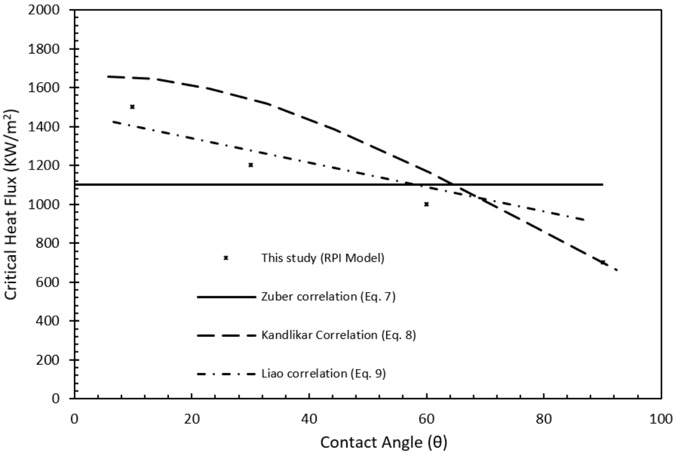

Figure 6: Critical heat flux changes with contact angle to compare experimental and numerical results in this study.

8 Conclusions

The results of the numerical simulation of nano coatings are as follows:

- The RPI model is used to simulate the boiling flow and with some modifications it can be used to simulate pool boiling;
- The experimental result of Gerardi et al. is used to validate the simulation;
- The critical heat flux results from the simulation showed an error of less than 5% compared to the experimental results;
- The results obtained from the simulation of surfaces with various wettability show the appropriate accuracy of this method to predict the thermal behaviour of nano-coatings.

Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work.

References

Bowring, R. (1962). Physical model, based on bubble detachment, and calculation of steam voidage in he sub-cooled region of a heated channel. Technical report, Institutt for Atomenergi (Norway). OECD Halden Reaktor Prosjekt.

Drew, D. and Lahey, R. (1993). Particulate two-phase flow, Butterworth-Heinemann, Boston. *MA*, pages 509–566.

Gerardi, C., Buongiorno, J., Hu, L.-w., et al. (2010). Study of bubble growth in water pool boiling through synchronized, infrared thermometry and high-speed video. *International Journal of Heat and Mass Transfer*, 53(19-20):4185–4192.

Hadad, K., Rahimian, A., and Nematollahi, M. (2013). Numerical study of single and two-phase models of water/Al_2O_3 nanofluid turbulent forced convection flow in VVER-1000 nuclear reactor. *Annals of Nuclear Energy*, 60:287–294.

Hadad, K., Rahimian, A., and Rabiee, A. (2015). Nanofluid application in post SB-LOCA transient in VVER-1000 NPP. *Annals of Nuclear Energy*, 79:101–110.

Ishii, M. and Mishima, K. (1984). Two-fluid model and hydrodynamic constitutive relations. *Nuclear Engineering and Design*, 82(2-3):107–126.

Kandlikar, S. G. (2001). A theoretical model to predict pool boiling chf incorporating effects of contact angle and orientation. *J. Heat transfer*, 123(6):1071–1079.

Liang, G. and Mudawar, I. (2019). Review of pool boiling enhancement by surface modification. *International Journal of Heat and Mass Transfer*, 128:892–933.

Liao, L., Bao, R., and Liu, Z. (2008). Compositive effects of orientation and contact angle on critical heat flux in pool boiling of water. *Heat and Mass Transfer*, 44:1447–1453.

Rahimian, A., Kazeminejad, H., Khalafi, H., et al. (2019). Boiling heat transfer and critical heat flux enhancement using electrophoretic deposition of sio2 nanofluid. *Science and Technology of Nuclear Installations*, 2019(1):1272156.

Rahimian, A., Kazeminejad, H., Khalafi, H., et al. (2020a). Effect of gamma irradiation on the critical heat flux of nano-coated surfaces. *Nuclear Engineering and Technology*, 52(10):2353–2360.

Rahimian, A., Kazeminejad, H., Khalafi, H., et al. (2020b). Effect of nano-particle coating techniques of SiO2 on improvement of Critical Heat Flux. *Journal of Nuclear Science, Engineering and Technology (JONSAT)*, 41(4):65–73.

Rahimian, A., Kazeminejad, H., Khalafi, H., et al. (2020c). An experimental study of the steel cylinder quenching in water-based nanofluids. *International Journal of Engineering*, 33(1):28–33.

Rahimian, A., Kazeminejad, H., Khalafi, H., et al. (2022). Effect of gamma irradiation on the critical heat flux of sintered nano-coated surfaces. *Radiation Physics and Chemistry*, 199:110297.

Sharma, S. K., Shukla, R., and Sikarwar, B. (2015). Experimental Study for Investigating the Mechanism of Heat Transfer Near the Critical Heat Flux in Nucleate Pool Boiling. *International Journal of Engineering*, 28(8):1241–1250.

Zuber, N. (1959). Hydrodynamic Aspects of Boiling Heat Transfer.

To cite this article:

Rahimian, A. (2025). Simulation of pool boiling for surfaces with various wettability. *Radiation Physics and Engineering*, 6(3), 35-40. doi: 10.22034/rpe.2025.477700.1242

DOI: 10.22034/rpe.2025.477700.1242

To link to this article: `https://doi.org/10.22034/rpe.2025.477700.1242`