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EMPLOYMENT OF A COMPUTATIONAL MODELING FOR SIMULATION OF CONVECTION HEAT TRANSFER WITH NUCLEATE POOL BOILING

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Abstract. *In this work, a numerical study of heat transfer with phase change is presented. This process occurs in several technologies in the refrigeration sector, e.g. in condensers and evaporators heat exchangers. In operation, this equipment has internal and external flows with thermal exchange and the occurrence of boiling and/or condensation. In this sense, this work aims to develop a model that allows the study of heat transfer in boiling flows for future analysis on devices design framework. The Volume Of Fluid (VOF) method and Lee's evaporation–condensation model were used to estimate volumetric fractions and to calculate interfacial mass transfer, respectively. The conservation equations of mass, momentum and energy, in addition to the transport equation of the volume fraction, were solved using the Finite Volume Method (MVF), more precisely with the ANSYS–FLUENT software. The model was validated with a correlation of the reference case of nucleated boiling in a pool. The results of the numerical simulation showed good agreement with the one obtained by correlation. The comparison of heat flux between correlation and simulation led to differences lower than 5%. Results of volume fraction and velocity fields also demonstrated that the model was able to predict qualitatively the fluid flow behavior, predicting adequately the bubbles formation and their growth along the domain.*

Keywords: *Numerical Model, Heat Convection, Phase Change, Pool Boiling, Turbulent Flow*

1. INTRODUCTION

Several engineering applications involve heat exchange, fluid movement and the presence of physical phenomena associated with convection. In many projects of interest for applications in industrial sectors, mainly refrigeration, equipments with intensive heat exchange are characterized with boiling convective flows.

In this work, the physical phenomenon of nucleated boiling that occurs in many equipment such as heat exchangers is investigated. The understanding of the physical mechanisms involved and the modeling of the phase change processes become essential in the scenario that allows the optimization of different applications. According to Tanguy et al. (2014), this type of flow is present in several technologies to be improved such as fluid storage in micro gravity, cryogenic applications and heat exchangers. This fact is directly related to the vast and growing industrial applicability, for example, in the automobile industry, refrigeration and in residential air conditioning systems (Li et al., 2012).

Saw et al. (2018) stated that in the semiconductor industry, for example, boiling flow in microchannel heat sinks is seen as one of the ideal solutions for removing high heat fluxes. In this sense, it is desirable to operate in a nucleated boiling regime, since, in this regime, high transfers are associated with small values of excess temperature.

In addition, in applications considered environmentally sustainable, Machado and Cabral (2017) stated that water heating systems that make use of solar collectors assisted by thermosyphons are also important technologies that present

flow with phase change. These systems have great potential for both residential and industrial applications. Inside the thermosiphons, a complex flow is verified due to the presence of two phases and the equipment can operate in different boiling regimes.

Recent literature recognizes the great difficulty in predicting the behavior of boiling convection heat transfer, as well as, the convection heat transfer coefficient. This fact was presented in the work of Mudawar and Qu (2003), in which the authors discussed the results of an experimental approach of boiling flow in a rectangular microchannel heatsink. The study carried out revealed that, due to the exclusive nature of the flow and the operational conditions, many empirical correlations that are recommended are unable to predict, with quality, the correct trend of the heat transfer coefficient.

According to Machado and Cabral and Cabral (2017), dimensionless parameters such as the heat transfer coefficient can be used. However, the large number of variables involved in determining this parameter and the way they are physically related makes it difficult to predict the phenomenon as well as to develop empirical correlations.

For this reason, numerical models for predicting phase change processes are limited (Tanguy et al., 2014). This fact is described as a challenge and the development of new numerical models is of interest to recent studies such as the one presented by Ferrari et al. (2018). The authors developed a model capable of predicting the complex flow with boiling in cross sections of the geometry of a square microchannel and compared it with results found in the literature for circular microchannel under the same configurations. A slug-flow regime was simulated using the Volume Of Fluid (VOF) method to estimate the volume fractions in the interface dynamics and, according to the authors, the study carried out presented fundamental analyzes for applications in microchannel heat exchangers that have non-circular channels.

Many contributions, which include numerical studies on phase change, are available as a reference for simulations and use the VOF method. The method is widely used because it allows the modeling of two or more immiscible fluids and can be associated with other methods as shown in the work by Tomar et al. (2005). The authors used the Level Set and VOF methods in a coupled manner and presented an approach for modeling two-phase flow with surface tension. The use of the methodology resulted in a two-dimensional simulation of the bubble growth, in water, close to critical pressure and in refrigerant type R134 subjected to almost critical and very critical pressure. The effects of overheating on the periodic nature of boiling were studied, i.e., on the dynamics of vapor bubbles that include formation, growth and detachment from the solid surface. It was found that the frequency of formation and dynamics of vapour bubbles detachment is a function of the amount of energy transferred (degree of overheating).

It is noted in the various studies that, only with the volume fraction equations of the VOF method, it is not possible to quantify the heat and mass transfer through the interfaces. The method developed by Hirt and Nichols (1981) solves a single set of equations to track the volume fraction of each fluid. The formulation of the method is based on the fact that for each phase a variable is introduced: the volume fraction, α , of the phase in the computational cell. According to Kandlikar and Perez-Raya (2016), in the interface tracked by the method there is mass transfer from one phase to another. However, the method does not quantify this transport and other effects such as heat flow in the normal direction and effects due to surface tension. Therefore, a phase change model is necessary for this purpose.

The model proposed by Lee (1980) is widely used and cited in the literature, for example, in the numerical work conducted by Sun et al. (2014). This and other models were implemented to model the phase change from liquid to vapour of water. Authors presented a new model of phase change for simulation of flow with boiling and condensation. The work aimed to develop computational modeling with improvements made in the evaporation–condensation model proposed by Lee.

In the view of above mentioned aspects, the development of computational modeling for prediction of convection heat transfer with phase of change is still an important subject. The above mentioned studies related the development of modeling to estimate the heat flux between surfaces and phase change flow, interfacial mass exchange, reconstruction of liquid/gas (or vapour) interfaces in the formation of steam bubbles and reliable representation of multiphase flow in different flow regimes. In the present work, it is performed an initial attempt of a computational model development for prediction of convection heat transfer considering a boiling flow, allowing its application in future studies of geometric evaluation in this kind of problem.

The objective of this work is the development of a numerical modeling for the predictions of heat convective flows with nucleated boiling to use in the future to investigate the influence of the geometry of the lower surface of a reservoir on the heat flow in a similar domain. In the present study, the nucleated boiling process is studied using the VOF method and evaporation-condensation model of Lee (1980). The study includes both qualitative analyzes of volume fractions, regarding the dynamics of the formation of vapour bubbles characteristic of the boiling regime, and quantitative analyzes of the heat fluxes on the surface of the domain. The validation of the model is performed by comparison between the heat flux in a plate subjected to boiling obtained with the present model and that predicted in the Rohsenow (1951) correlation.

2. PROBLEM DESCRIPTION

The equations used in modeling the physical phase change mechanism presented in this work were deduced through the fundamental principle of conservation of continuity, momentum and energy.

The behavior of a fluid changing phase on a heated horizontal surface is investigated in this work. The fluid is heated by the solid surface, a polished copper material, subjected to a constant temperature and higher than the liquid saturation temperature of 373.15 K until the boiling process occurs. In this problem, it is considered that the initial phase is liquid water in the saturated condition, i.e., a state in which most of the liquid slightly exceeds the saturation temperature.

The computational domain is a rectangular fluid region, as illustrated in Fig. 1. The dimensions of the domain are 0.04 m (in x -direction) and 0.08 m (in y -direction). The total region of the domain occupied by liquid water has the following properties: density, $\rho_l = 957.9$ [kg/m³]; dynamic viscosity, $\mu_l = 279 \times 10^{-6}$ [N.s/m²]; specific heat, $C_{p,l} = 4.217$ [kJ/kg.K]. The property of the phase that appears on the solid surface with the phase change, superheated water vapour: $\rho_v = 0.5956$ [kg/m³]; dynamic viscosity, $\mu_v = 1.34 \times 10^{-5}$ [N.s/m²]. Also considered are: surface tension, $\sigma = 58.9 \times 10^{-3}$ [N/m] and gravitational acceleration, $g = 9.81$ [m/s²].

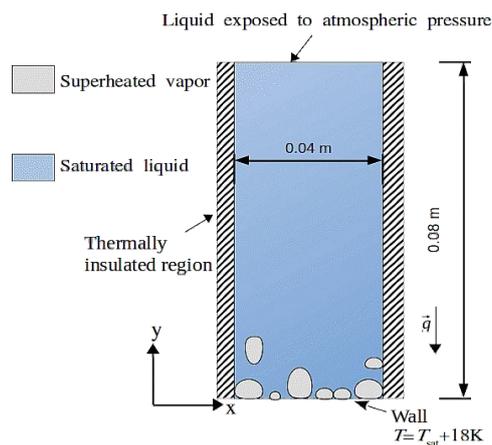


Figure 1. Schematic domain studied in the present problem.

It is considered that lateral and lower surfaces of the domain have non-slip and impermeability boundary conditions, i.e., velocities in x and y -directions are null ($u = v = 0$ m/s).

Concerning the thermal boundary conditions, the lateral surfaces are modeled as thermally insulated, i.e., $dT/dx = 0$ (where x represents a spatial coordinate).

In the top region, a null pressure gauge and locally parabolic condition is assumed, while in the bottom region, heated solid surface, was modeled so as to have an initial temperature, $t = 0$, constant of 18 K more than the saturation temperature:

$$T = T_{sat} + 18 K \quad (1)$$

Where $T - T_{sat}$ is the excess temperature (ΔT_e).

3. VOF METHOD AND LEE MODEL

According to Hirt and Nichols (1981), authors of the method used, the volume fraction of all phases add up to the unit in the computational cell. Depending on its value, the specific properties and variables of each problem will be assigned to each control volume within the domain. The volume fraction, α , can be found in three different situations:

$$\alpha_l = 1 \quad (2)$$

$$\alpha_l = 0 \quad (3)$$

$$\alpha_l + \alpha_v = 1 \quad (4)$$

The first situation, Eq. (2), the cell would be filled by one phase. Equation (3) represents the situation in which the cell would not be filled by a given phase considered and in Eq. (4), the cell contains the interface between one or more fluids, in this case, the cell would contain a volumetric fraction of the certain phases, $0 < \alpha_l < 1$, where the subscripts l e v represent the liquid and vapour phases, respectively.

In the interface tracking process, a continuity equation is solved for the volume fraction in each phase. In this work, the process is performed using the VOF method. For any phase, l , the ANSYS® FLUENT code solves the VOF equation and estimates the evolution of the volume fractions field, α , using an algorithm based on the following equation (Hirt and Nichols, 1981):

$$\frac{1}{\rho_l} \left[\frac{\partial}{\partial t} (\alpha_l \rho_l) + \nabla \cdot (\vec{v}_l \alpha_l \rho_l) = S_{\alpha l} + \sum_{v=1}^n (\dot{m}_{vl} - \dot{m}_{lv}) \right] \quad (5)$$

where ρ is the density of the fluid [kg/m^3]; \dot{m}_{vl} is the mass transfer from phase v to phase l and \dot{m}_{lv} mass transfer from phase l to phase v .

If l and v represent the liquid and vapour phases, respectively, \dot{m}_{vl} it would correspond to the condensation process and \dot{m}_{lv} to the boiling process. This equation represents the time advance of the volume fraction, α , and the idea that it moves with the fluid due to the product with the flow velocity, \vec{v} .

To quantify the mass transfer through the interfaces in Eq. (5), the model proposed by Lee (1980) was used. In this model, the process of transferring liquid-vapour mass is governed by the following equations and temperature regimes:
 if $T_l > T_{sat}$ the process is one of evaporation.

$$\dot{m}_{lv} = coef \cdot \alpha_l \rho_l \frac{(T_l - T_{sat})}{T_{sat}} \quad (6)$$

if $T_v < T_{sat}$ the process is of condensation.

$$\dot{m}_{vl} = coef \cdot \alpha_v \rho_v \frac{(T_{sat} - T_v)}{T_{sat}} \quad (7)$$

where *coef* is the coefficient interpreted as a relaxation factor of mass transfer in unit of time [1/s].

Some empirical values for the coefficient were presented by Sun et al. (2014), as well as theoretical formulations obtained from Fourier's law that can be used to overcome the limitations found by the use of expressions and empirical coefficients. In the numerical study by Machado and Cabral (2017), results of seven combinations for the coefficients were tested and presented. The authors highlighted the values of 0.1 s^{-1} for evaporation and 1.0 s^{-1} for condensation as the ideal combination for the nucleated boiling problem in a thermosyphon.

4. GOVERNING EQUATIONS WITH VOF

Considering a incompressible, two dimensional convective flow with phase of change, the momentum equation for the mixture liquid/vapour of water can be given by (Bejan, 2013):

$$\frac{\partial}{\partial t} (\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + \rho \vec{g} + F_v \quad (8)$$

where ρ is the density of the mixture [kg/m^3]; \vec{v} e \vec{g} are the velocity [m/s] and gravitational acceleration [m/s^2] vectors, t the time [s], p is the pressure [N/m^2] and F_v is the force per unit volume caused by surface tension [N/m^3].

The mixture density is given by the following equation:

$$\rho = \alpha_v \rho_v + (1 - \alpha_v) \rho_l \quad (9)$$

In the VOF method, the surface tension is calculated using the Continuum Surface Force (CSF) model proposed by Brackbill et al. (1992). The divergence theorem is used to express the surface force in terms of a volumetric force. This force appears as a source term and is expressed using the following simplified equation for two phases:

$$F_v = \sigma_{lv} \frac{\rho k_l \nabla \alpha_l}{\frac{1}{2}(\rho_l + \rho_v)} \quad (10)$$

where σ_{iv} is the surface tension coefficient and k is the surface curvature of the interface, calculated by local gradients of the volume fraction from the normal phase to the surface, given by the following relationships:

$$n = \nabla \alpha_v \quad (11)$$

$$\hat{n} = \frac{n}{|n|} \quad (12)$$

$$k = \nabla \hat{n} = \nabla \cdot \left(\frac{\nabla \alpha_v}{|\nabla \alpha_v|} \right) \quad (13)$$

where $k_l = -k_v$.

For all phases, a single energy equation is solved in the estimation of the temperature field, as shown in the following equation for each phase:

$$\frac{\partial}{\partial t} (\rho E) + \nabla \cdot (\vec{v} (\rho E + p)) = \nabla \cdot (\lambda \nabla T) + S_T \quad (14)$$

The thermal conductivity denoted by λ and the term S_T contains contributions from the heat source. The energy, E , evaluated in the method is described as follows for any phase q :

$$E = \frac{\sum_{q=1}^n \alpha_q \rho_q E_q}{\sum_{q=1}^n \alpha_q \rho_q} \quad (15)$$

For the two phases considered, liquid-vapour, Eq. (15) is in the form:

$$E = \frac{\alpha_l \rho_l E_l + \alpha_v \rho_v E_v}{\alpha_l \rho_l + \alpha_v \rho_v} \quad (16)$$

where E_l and E_v for each phase is a function of specific heat and temperature. In the work developed by Sun et al. (2014) an expression is found for each of these variables, described as follows:

$$E_l = C_{p,l} (T - 298,15) \quad (17)$$

$$E_v = C_{p,v} (T - 298,15) \quad (18)$$

5. NUMERICAL PROCEDURES

In the numerical solution of the described problem, the conservation equations of mass, momentum and energy, as well as, the volume fraction transport equation are solved with the Finite Volumes Method (FVM) that is implemented in the commercial software used ANSYS–FLUENT 14.5. Concerning the numerical procedures used, the methods of discretization and main parameters for transient simulation are (ANSYS–FLUENT User Guide, 2013; Versteeg and Malalasekera, 2007): Initialized fluid is liquid water at a temperature equal to the saturation temperature of 373.15 K; operating pressure of 101.325 kPa; the second order Upstream Differencing Scheme (Upwind) spatial interpolation scheme was adopted for the momentum and energy equations. The Geo-Reconstruct scheme is used to tackle with the reconstruction of interface distribution. Moreover, residuals of 1.0×10^{-6} are used for all solved equations in order to achieve the convergence at each time step. For the pressure-velocity coupling solution, the SIMPLE algorithm and the explicit first order scheme for advancing time with interval, Δt , were adopted, based on the Courant number of 0.25. For the two-phase turbulence treatments, the standard model $k-\varepsilon$ was adopted because it is the model most commonly used in the literature, see for example the works of Wu et al. (2007) and Heynderickx et al. (2009). In addition, it was pointed out in the numerical study by Su et al. (2015) that the $k-\varepsilon$ model led to better agreement with experimental results when compared with other models, as the $k-\omega$. In the modeling of turbulence of the regions close to the wall the enhanced treatment method Enhanced Wall Treatment ε -Equation (EWT- ε) was used, in these regions the most refined mesh element has y^+ equal to 1.29×10^{-2} . Moreover, the $coeff = 0.1 \text{ s}^{-1}$ and $coeff = 1.0 \text{ s}^{-1}$ is used for the mass transfer

coefficient, described in Eq. (6) and Eq. (7), respectively, of the evaporation–condensation model. This value is recommended in the numerical evaporation studies carried out by Machado and Cabral (2017).

6. RESULTS

For numerical simulation of the case of nucleated boiling in a pool, the time step initially used is 10^{-4} [s]. The choice is based on the convergence of the problem and on experiences reported in the literature that indicate the tendency to reduce the magnitude of errors using small time steps. It is considered 2.5×10^4 number of time steps totaling a simulated real time of 2.5 [s].

Concerning the spatial discretization, two different meshes are investigated: an unstructured mesh containing 17,726 volumes (rectangles and triangles) and a structured mesh with 23,000 rectangular volumes and a higher refinement near the inferior and superior walls. Figure 2 illustrates the structured mesh employed in the present simulations. The simulations are performed on a computer with Intel Core i7 processor of 3.30 GHz and memory of 16 GB RAM. The computational effort for each simulation is nearly 8.64×10^5 s.

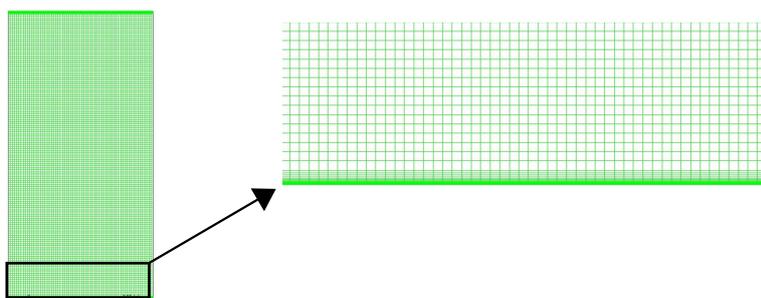


Figure 2. Structured mesh used in the present study.

Comparison results between the two meshes show that both follow similar trends for the total heat transfer rate obtained in the bottom surface of the domain, as illustrated in Fig. 3. However, the value of the rate obtained with the unstructured mesh is noticeably higher in the first time steps compared to the structured mesh.

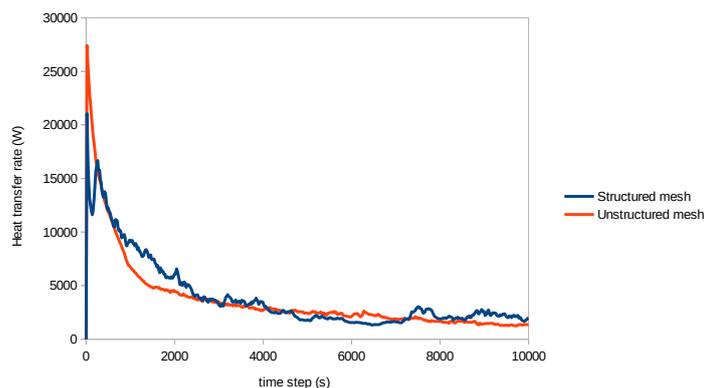


Figure 3. Heat transfer rate obtained in the lower surface as a function of time for different studied grids.

In the first step of time, the percentage difference in the heat transfer rate between the meshes was 23.17%. However, it can be observed that the average value of the total heat transfer rate in the 2.5×10^4 time steps was 3964.5 W with the structured mesh higher than the value obtained with the unstructured mesh of 3700.8 W. In spite of differences found, at the steady state condition, the magnitudes of heat transfer rates are similar.

In numerical simulation, an essential step to verify the accuracy of the model and the applicability of the numerical scheme, according to Kandlikar and Perez-Raya (2016), is the validation step. The validation of the developed model is carried out by comparing the results obtained in the numerical simulation with the correlation of Rohsenow (1951) and qualitative behavior described in Incropera et al. (2008) and Bejan (2013). In this sense, to obtain the comparison with theoretical predictions, the numerical simulation of the case of nucleated pool boiling was developed using the properties of liquid water and steam obtained experimentally and available in Incropera et al. (2008).

The first fractions of steam appeared on the wall at a constant temperature of around $t = 0.055$ s, and after few instants of time, the first generated bubbles associate with others and detaches from the bottom surface towards the upper region of the pool domain. Figure 4 shows the nature and dynamics of the formation of vapour bubbles, characteristic of pool boiling. In Figure 4 the vapour is represented in light blue color while the liquid is represented in dark blue color.

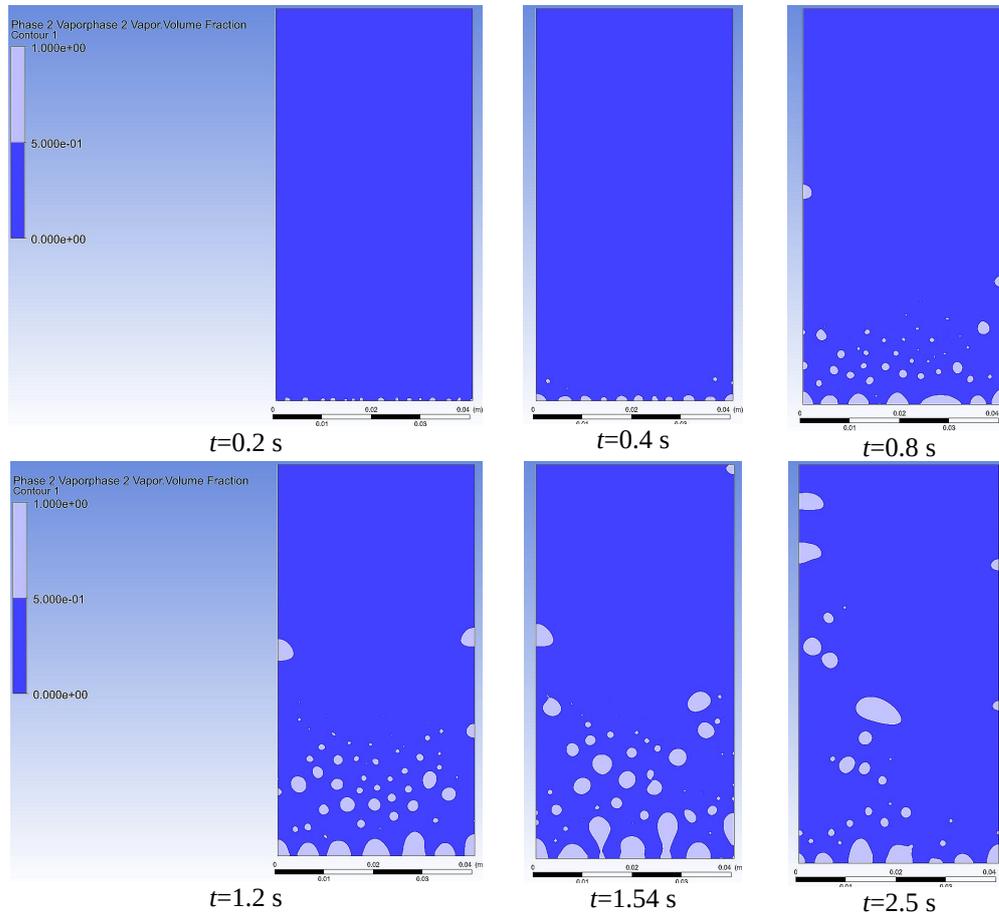


Figure 4. Volumetric fraction in pool boiling for $\Delta T_e = 18$ K.

Figure 4 also shows the evolution of vapour formation and bubbles displacement from the lower region towards the upper one in the rectangular fluid domain considering 6 different instants of time: 0.2 s, 0.4 s, 0.8 s, 1.2 s, 1.54 s and 2.5 s. The formation of vapour bubbles can be observed on the heated bottom surface and the release of these bubbles towards the upper region of the rectangular domain of the problem. It was then possible to attest that nucleate pool boiling occurred characterized by the rise of jets or columns of bubbles. According to Bejan (2013), this regime occurs in the range of temperature excesses from 10°C to 30°C and the confirmation of this boiling mode can be done by evaluating the heat flux from the heated surface to the fluid.

Table 1 shows the comparison between the value of the thermal flux on the surface obtained by numerical simulation and the magnitude predicted using the Rohsenow correlation (Rohsenow, 1951).

Table 1. Comparison of thermal flux obtained by numerical simulation and correlation for $\Delta T_e = 18$ K

Case	Heat Flux (W/m^2)	Error (%)
Simulated heat flux	685257.5	4.03
Heat flux of Rohsenow correlation	714035.1	

Errors obtained between flow calculated by numerical simulation and the Rohsenow correlation for nucleated boiling is expected and reported in the literature according to Incropera et al. (2008). The difference obtained of 4.03% can be considered quite satisfactory because the prediction of turbulent flows with change of phase is extremely

complex to be performed. The two-dimensional approximation of the proposed numerical model could have contributed to obtain the difference in the results. However, the adoption of this simplification is necessary here since the use of three-dimensional meshes can make the computational effort to be excessively large and unviable in this problem. In addition, the simulation of two-dimensional domains can be considered suitable when considering the idealization of sufficiently large lengths in the normal plane to the figure (z direction). In this sense, more refined meshes in a two-dimensional domain to capture different scales of space and time of flow is an alternative.

In the dynamics of bubble formation, coalescence is also experimentally predicted by Mukherjee and Dhir (2004) and also presented in Bejan (2013). According to the authors, before ascending, the first fractions of steam unite and then form bags of superheated steam. This condition hinders the movement of the liquid in the region close to the surface due to the agglomeration of the bubbles.

The developed modeling allowed the prediction of the phenomenon through numerical simulation of the case in which the excess temperature, ΔT_e , was equal to 18 K. However, simulations were also carried out with excess temperatures of 5 K and 25 K allowing the realization of qualitative comparisons regarding the global behavior of the problem, that is, the analogous process of formation of vapour bubbles in the nucleated pool boiling at different temperature excesses as shown in Fig. 5.

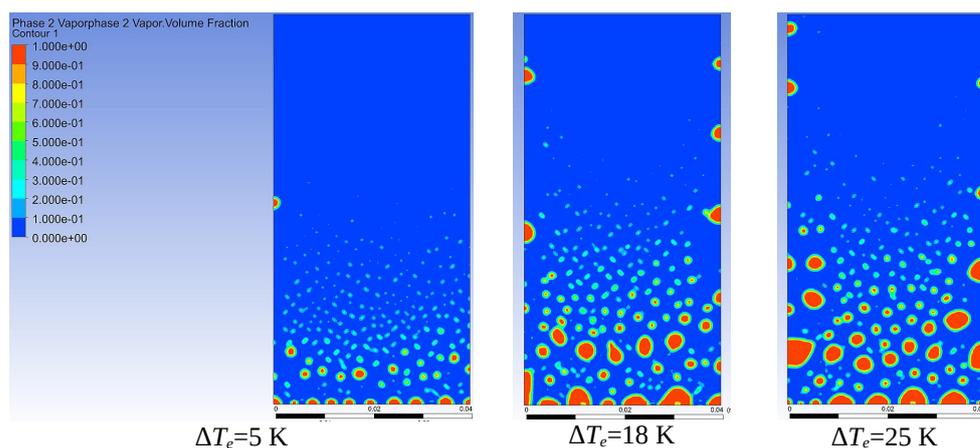


Figure 5. Volume fractions in the pool boiling for different excess temperatures.

Since the blue color, in a dark tone, represents the liquid phase of the fluid, the vapour fraction is identified in red and the other colors, identified between 0.1 and 0.9 in the outline, is the region where the interface is finds.

Figure 6 shows the qualitative comparison between coalescence in the formation of boiling vapour bubbles obtained from numerical simulation with those observed in experiments by Mukherjee and Dhir (2004).

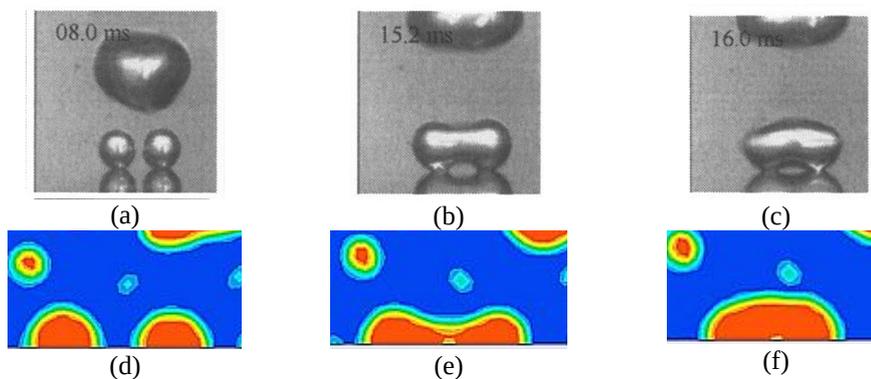


Figure 6. Comparison of the predicted bubble coalescence numerically with experimental data. $\Delta T_e = 5$ K, a - c, experimental (Mukherjee and Dhir (2004)) and $\Delta T_e = 5$ K, d - f, in numerical simulation.

It is worthy to mention that the comparison performed here is based only on the occurrence of the physical phenomenon in a qualitative way, since important differences are noticed in terms of contact angle between vapour bubbles and surface. This fact can be related with some factors as the thermophysical properties of the fluid and nature of liquid-surface combination. Therefore, additional investigations should be performed to investigate the computational model developed in the present work, considering other conditions.

7. CONCLUSION REMARKS

In this research, a numerical study was carried out of the heat transfer by convection with liquid-vapor phase change involved in the nucleated pool boiling process. The main goal here was the development of a computational model for prediction of convection heat transfer with nucleate boiling allowing future studies concerned with geometric assessments.

The basic principle of operation of the method and the modeling that was developed for numerical simulation of the case of nucleated pool boiling were presented. The numerical simulation results presented, obtained with CFD code based on the Finite Volume Method, were evaluated qualitatively by theoretical predictions, comparison with experimental and numerical simulation results and quantitatively by comparison with correlation available in the literature.

Results of initial simulations showed to be consistent with theoretical predictions of the saturated nucleate pool boiling regime presented by Incropera et al. (2008). For the excess of temperature, $\Delta T_e = 18$ K, the the heat flux obtained with the present simulation numerical, $q'' = 685257.5$ [W/m²], is within the expected range of the boiling curve, $10^5 \leq q'' \leq 10^6$, for the occurrence of the modeled regime.

The initial result of numerical simulation of the thermal flow was compared with that obtained through the correlation developed by Rohsenow (1951) for nucleated boiling. The results presented were consistent with a difference lower than 5.0 %. In other words, the qualitative estimative of fluid dynamic of generation and displacement of bubbles, as well as, the magnitude of heat flux indicated that the present computational model is promising for prediction of convective heat transfer in nucleated pool boiling.

In spite of promising behavior, the present code will be further evaluated with other comparisons with results of literature and other conditions. Moreover, it is intended to perform studies related with the influence of the shape of inferior surface over the heat flux and pattern formation of the vapour in the domain.

8. ACKNOWLEDGEMENTS

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