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Numerical Simulations of Gas-Liquid Boiling Flows Using OpenFOAM

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Abstract

The present work is aimed at development of an experimentally verified computational model based on OpenFOAM for the simulations of gas-liquid boiling flows. The open source CFD code OpenFOAM was developed further to include $k$-$\varepsilon$ turbulence model, different inter-phase coupling forces and energy transport accompanied with phase change. The most commonly used wall heat flux partitioning model, proposed by Kurul and Podowski, was implemented in the OpenFOAM to simulate two-phase boiling. The predicted axial and radial vapor volume fraction distribution, liquid temperature distribution and wall temperature profiles were compared with the DEBORA measurements. A good agreement between the predictions and measurements was observed. The experimentally verified model was used to understand the effects of various interfacial closures e.g. lift force, turbulent dispersion force and wall force, on the vapor volume fraction distribution. The effects of bubble induced turbulence and nucleation site density on the hydrodynamics of the gas-liquid boiling flows were studied. Such an experimentally verified open source CFD code will be useful to simulate boiling under different regimes and in complex geometries.

1. Introduction

Gas-liquid boiling flows have wide spread applications e.g. in Boiling Water Reactors (BWR) and in coal fired boilers for generation of electric power. Sub-cooled flow boiling occurs in most of these reactors which requires large heat transfer coefficients for effective heat exchange. Critical heat flux poses a limitation to this heat transfer mechanism because in such conditions, there is a very sharp decline in the value of heat transfer coefficient causing a rapid increase in heater temperature which may lead to heater melting and destruction. The critical heat flux is found to depend on the flow parameters and the geometrical design of the fuel rod assemblies. While experiments can be used to evolve design improvements and investigate their effects on critical heat flux, they are very expensive. Therefore, use of CFD tools for numerical analyses of these reactors is of high interest to the research community.

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Owing to complex design and operation of the aforementioned process equipment/reactors, a significant research activity is focused on development of computational models capable of predicting vapor volume fraction and temperature distribution in gas-liquid boiling flows. While some research groups have used the commercial solvers (e.g. Ansys CFX\textsuperscript{3,4}, STAR CD\textsuperscript{5} etc.) for simulations of the gas-liquid boiling flows, several research groups have developed their own in-house solvers (e.g. COBRA\textsuperscript{6}). In most of these works, an Eulerian-Eulerian two-fluid model\textsuperscript{3,4,5} coupled with phase change models has been widely used. Different researchers have shown that interphase-coupling forces e.g. drag force, lift force, turbulent dispersion force, virtual mass and wall force affect the vapor volume fraction, phase velocity and temperature distributions. While various interphase coupling force formulations have been used by different researchers to simulate boiling flows under a widely varying operating conditions, there are no conclusive guidelines on suitability of a certain set of interfacial closures to simulate boiling under different regimes. Several experimental investigations have been carried out on measurements of void fraction and liquid/wall temperature distributions for boiling flows in simplified geometries\textsuperscript{3,4,5} like tube, annular channel and complex geometries\textsuperscript{6,7} consisting of multiple fuel rods to understand the flow, void fraction and temperature distribution in boiling flows.

Kurul and Podowski\textsuperscript{1} wall heat flux partitioning model has been used widely along with various correlations that are available in the literature for bubble departure diameter, bubble departure frequency and nucleation site density. These parameters are highly dependent on flow conditions. Most of the simulations performed using commercial solvers have been carried out for simple geometries e.g. tube, annular channel\textsuperscript{3,4,5} with a few cases for multiple tubes\textsuperscript{6,7}. Also, most of the numerical analyses available in literature is for high pressure boiling flows\textsuperscript{2,3}. There is an increased interest in simulations of low pressure sub-cooled boiling to perform safety analysis of low pressure
reactors\textsuperscript{4}. While most efforts were focused on development of commercial/in-house codes, the present work is aimed at developing further the open source CFD code OpenFOAM to simulate boiling flows under different operating conditions and verify the predictions using the data available in the literature\textsuperscript{2}.

2. Model test cases

DEBORA experiments\textsuperscript{2} were used to validate the modified CFD code. A detailed description of the test facility can be found in Garnier et al.\textsuperscript{2} In DEBORA experiments, R12 (Dichlorodifluoromethane) was used as working fluid instead of water. The geometry consisted of a vertical heated tube having an inner diameter of 19.2 mm and heated length of 3.5 m. The experiments were conducted at mass fluxes of 2000-3000 kgm\textsuperscript{-2}s\textsuperscript{-1} instead of water. The measurements of the radial profiles for vapor volume fraction, vapor velocity, liquid temperature and bubble size at the end of heated length reported by Garnier et al.\textsuperscript{2} were used for verifications of simulations. 1.46-2.62 MPa. The measurements of the radial profiles for vapor volume fraction, vapor velocity, liquid temperature and bubble size at the end of heated length reported by Garnier et al.\textsuperscript{2} were used for verifications of simulations. While most e

3. Computational model

In the present work, Eulerian-Eulerian approach coupled with phase change was used, in which each phase is considered as continuum, which can interpenetrate with the other phases. In this approach, Reynolds averaged mass, momentum and energy conservation equations are solved. In OpenFOAM, the continuity equation is written in conservative form. So, only one equation needs to be solved. The continuity equation is solved for the dispersed phase (vapor) and the continuous phase fraction is calculated using $\alpha_l + \alpha_g = 1$. The final equation is given as:

$$\frac{\partial \alpha_g}{\partial t} + \nabla \cdot \alpha_g \vec{V} + \nabla \cdot \alpha_g \vec{V}_r (1 - \alpha_g) = \frac{\Gamma_g}{\rho_g}$$  \hfill (1)

where, $\vec{V} = \alpha_g \vec{U}_g + \alpha_l \vec{U}_l$ and $\vec{V}_r = \vec{U}_g - \vec{U}_l$. Similarly, the Reynolds averaged momentum conservation equations coupled with sources terms for momentum exchange due to bubble evaporation and condensation were solved for each phase as follows:

$$\frac{\partial \left( \alpha_l \rho_l \vec{U}_l \right)}{\partial t} + \nabla \cdot \alpha_l \rho_l \vec{U}_l \vec{U}_l = -\alpha_l \nabla p - \nabla \cdot \vec{f}_l + \alpha_l \rho_l \vec{g} + M_{lk} + \Gamma_k \vec{U}_k - \Gamma_{kl} \vec{U}_l$$  \hfill (2)

For incompressible fluids as in present case, the stress tensor is given as $\bar{\tau}_i = -\alpha_l \mu_{eff} \left( \nabla \vec{U}_i + \nabla \vec{U}^T_i \right)$ where $\bar{M}_{ik} = -\bar{M}_{ki}$ are the inter-phase momentum exchange terms. Since vapor phase is assumed to be saturated, so Reynolds averaged energy equation was solved only for the liquid phase as:

$$\frac{\partial \left( \alpha_l \rho_l H_l \right)}{\partial t} + \nabla \cdot \alpha_l \rho_l \vec{U}_l H_l = -\alpha_l \nabla \cdot \left( q_l + q'_l \right) + \alpha_l \frac{Dp}{Dt} + \Gamma_k H_k - \Gamma_{kl} H_l + Q_{lg}$$  \hfill (3)

where, $q_l = (\lambda_l / c_{pl}) \nabla H_l$, $q'_l = (\lambda'_l / c_{pl}) \nabla H_l$ and $\lambda'_l = c_{pl} \nu'_l / \rho_l \nu'_l$.

3.1. Inter-phase momentum exchange terms

The inter-phase momentum exchange was accounted through the forces acting on the dispersed bubbles as:

$$M_{ki} = -\bar{M}_{ik} = \bar{M}_D + \bar{M}_L + \bar{M}_{TD} + \bar{M}_W$$  \hfill (4)
where $\bar{MD}, \bar{ML}, \bar{MTD}, \bar{MW}$ are inter-phase momentum transfer contributions from drag, lift, turbulent dispersion and wall forces respectively. The volumetric source of the momentum exchange between the two phases due to the drag force exerted by the liquid is given by

$$\bar{MD} = \frac{3}{4} \rho_l \alpha_l \frac{C_D}{d_b} \left| \vec{U}_g - \vec{U}_l \right| \left( \vec{U}_g - \vec{U}_l \right) \left( \vec{U}_g - \vec{U}_l \right)$$

(5)

The drag coefficient $C_D$ was calculated using the correlation of Tsuchiya et al. The lift force that is experienced by bubbles due to velocity gradients in continuous phase was estimated as:

$$\bar{ML} = C_L \frac{\alpha_l \rho_l}{d_b} \left( \vec{U}_g - \vec{U}_l \right) \times \nabla \times \vec{U}_l$$

(6)

The $C_L$ was calculated using the model proposed by Tomiyama et al. The liquid phase turbulence influences the vapor distribution and it was accounted by the turbulent dispersion force model of Bertadano et al. as $\bar{MTD} = -C_{TD} \rho_l \alpha_l \sqrt{\alpha_g}$ where, $C_{TD}$ is turbulent dispersion coefficient which may vary from 0-10. The wall force acts opposite to the lift force and forces the bubbles to move towards pipe center. Under the present conditions, wall force was found to have negligible effect and was thus ignored as confirmed by Krepper and Rzhak.

### 3.2. Wall boiling model

According to Kurul and Podowski wall flux partitioning model, the heat flux between the heated wall and liquid is exchanged via three mechanisms

$$q = q_q + q_e + q_c$$

(7)

where $q_q, q_e, q_c$ are convective, evaporative and quenching heat respectively. At the heated walls, bubbles are formed due to vaporisation of liquid at the nucleation sites and the part of the wall heat used for this is called evaporation flux. Once bubbles reach critical bubble size they detach from the wall, cold liquid replaces the space occupied by bubbles and receives heat from the wall. This flux is called quenching heat flux. The rest of the area of the wall, that is not covered with the bubbles, is used for the single phase convective heat transfer. The quenching heat flux is given by

$$q_q = A_q h_q (T_w - T_l)$$

(8)

The area available for quenching heat transfer is $A_q = \pi N d_{dep}^2$. The quenching heat transfer coefficient was calculated as $h_q = 2 \lambda_l f \sqrt{t/\pi \kappa}$. The bubble waiting time is given as, $t = 0.8 f_{dep}$. The evaporation heat flux is given by

$$q_e = \frac{\pi}{6} d_{dep}^3 \rho_l f_{dep} N h_{fg}$$

(9)

where, nucleation site density $N$ was calculated as $N = N_{ref} \left| (T_w - T_{sat}) \right|^{1.805}$ and bubble departure frequency was calculated as $f_{dep} = \sqrt{4g (\rho_l - \rho_g) / 3 \rho_l d_{dep}}$. The convective heat flux was calculated using following correlation

$$q_c = (1 - A_q) \frac{\rho_l C_p u^*}{T^*} (T_w - T_l)$$

(10)

where $T^*$ is the non-dimensionless temperature.

### 3.3. Condensation and evaporation including boiling at the heated wall

Since bulk of the liquid is below the saturation temperature, bubbles formed at the wall start condensing when they move inside. Similarly, evaporation can take place in the bulk of the liquid. This interphase mass transfer was accounted by including appropriate source and sink terms into the continuity equation. The rate of evaporation is given by

$$\Gamma_{lg} = \frac{h_{lg} A_{lg} (T_l - T_g)}{h_{fg}}$$

(11)
The rate of condensation is given by
\[
\Gamma_{gl} = \frac{h_{lg} A_{lg} (T_g - T_l)}{h_{fg}}
\] (12)

Further, \(\Gamma_{lg} + \Gamma_{gl} = 0\). The interfacial heat transfer \(Q_{lg}\) is given by \(Q_{lg} = h_{lg} A_{lg} (T_{sat} - T_l)\), where \(h_{lg}\) is heat transfer coefficient calculated as \(h_{lg} = Nu \lambda_l / d_l\) and \(Nu\) is Nusselt number given by \(14\ Nu = 2 + 0.6 Re^{0.5} Pr^{0.3}\). The interfacial area is calculated as \(A_{lg} = 6 \alpha_g / d_b\). For present work, since bubble size was found to be almost constant, a constant mean bubble diameter was used in the simulations. An additional source term active only at the near wall cells was included to account for the vapor generation at the heated wall. It was calculated using wall heat flux partitioning model as \(\Gamma_g = q_e A_s / h_{fg} V_{cv}\) where \(V_{cv}\) is control volume and \(A_s\) is heated wall area.

### 3.4. Turbulence model

The liquid phase turbulence was simulated by solving a standard k-\(\epsilon\) model (model equations are not provided here). The liquid phase turbulent kinematic viscosity was calculated as \(\nu_{t,l} = C_\mu k^2 / \epsilon\). The bubble induced turbulence was accounted as \(\nu_{t,b} = (1/2) C_{\mu b} d_b \alpha_g \| \vec{U}_g - \vec{U}_l \|\); Where \(C_{\mu b} = 1.2\). Following Krepper and Rzehak, the turbulence in the vapor phase was neglected owing to the small density.

### 4. Model set-up and numerical solution

The simulations were carried out for an axis-symmetric geometry. A velocity inlet condition was specified at the bottom and pressure boundary condition was imposed at the top outlet. The no slip velocity boundary condition was specified at the wall for the vapor and liquid phase. For vapor phase, some researchers have argued that free slip condition is best suited and thus effect of free slip BC for vapor phase was also investigated. For momentum exchange, the models described in Section 3.1 were used. The k-\(\epsilon\) turbulence model with bubble induced turbulence source term (Sato et al. 15) was used to simulate turbulence in the continuous phase.

The solution algorithm PISO was used to solve pressure-velocity coupling. In this work, a combination of Gauss upwind, Gauss linear and Gauss limited Linear schemes were used for discretization of spatial derivatives. For the time derivative, first order accurate Euler implicit method was used. The set of discretized equations was solved by the generalised geometric-algebraic multi-grid (GAMG) solver with Diagonal incomplete-Cholesky (symmetric) smoother for pressure and the preconditioned bi-conjugate gradient (PBiCG) solver with Diagonal incomplete-LU (DILU) pre-conditioner for the rest of the variables. The existing two phase solver twoPhaseEulerFoam available for isothermal gas-liquid flows was further developed to account for phase change phenomenon.

### 5. Results and discussion

#### 5.1. Validation of results

Fig. 1(a) and 1(b) show the snapshots of the predicted vapor volume fraction distribution for the two selected cases DEBORA5 and DEBORA7, respectively. Comparing the snapshots, the shift from wall peak (DEBORA5) to core peak (DEBORA7) can be clearly observed. A possible mechanism for the transport of the vapor bubbles towards the center of the pipe is the lift force which changes its direction for the larger bubbles. For R12, this change occurs for bubble size 1.5 mm at 1.46 MPa and 1.0 mm at 2.65 MPa respectively. The measured bubble size (DEBORA5 - 0.452 mm and DEBORA7 - 1.00 mm) shows the presence of larger bubble in the DEBORA tests. This may be one of the reason behind the transport of larger bubbles in centre of the pipe leading to wall peaking in DEBORA7. Fig. 1(c) and 1(d) shows the snapshots of the instantaneous liquid temperature for DEBORA5 and DEBORA7. Fig. 2(a) shows the comparison of the measured and predicted vapor volume fraction distribution for DEBORA5. It can be seen that the predicted vapor volume fraction is in a good agreement with the measurements at the centre of the pipe but the predicted vapor volume fraction profile exhibited a sudden increase near the wall. Since a considerable bubble size distribution along the pipe radius was observed in the experiments, one of the possible
reason for observed disagreement could be the use of constant bubble size in the simulations. In case of DEBORA7 (Fig. 2(b)), the predicted vapor volume fraction distribution was in a qualitative agreement with the measurements, but the predictions were better than that of Krepper and Rzeňák.\(^3\)

The comparison of measured and predicted liquid temperature for DEBORA5 showed overprediction of the liquid temperature in the center of the pipe (see Fig 3(a)). The difference observed between the cross-sectional averaged measured temperature (359.3 K) and predicted temperature (359.7 K) was 0.1 %. Similarly, the predicted cross-sectional averaged vapor volume fraction (0.173) is very close to the measurements (0.217) (results not shown here). The predicted vapor and liquid velocity profiles for DEBORA5 were in a qualitative agreement with the measurements (results not shown here).

5.2. Effect of interphase momentum exchange and turbulence models

The previous investigations showed that the lift force affects the hydrodynamics of the gas-liquid flows. In case of DEBORA5, the effect of lift force was found to be marginal. While increasing the lift force coefficient \(C_L\) from 0.01 to 0.1, vapor volume fraction profiles were marginally affected as seen in Fig. 4(a). The effect of lift force was found to be more prominent in case of DEBORA7. As shown in Fig. 4(b), increasing \(C_L\) from 0.05 to 0.3 led to...
an improvement in the vapor volume fraction profile. In case of DEBORA7, since bubbles were larger, the lift force pushes them towards the centre of the pipe causing core peaking phenomenon.

The turbulent dispersion force has been also shown to have a significant contribution in determining the radial profiles of vapor volume fraction and liquid temperature as can be seen in the literature\(^3\,\text{,}^{13}\). The effect of the turbulent dispersion force was studied by performing simulations with dispersion coefficients \(C_{TD} = 0.25\) and \(0.4\). However as shown in Fig. 5(a), the effect of turbulent dispersion force showed marginal effect on the predicted vapor volume fraction distribution. In case of DEBORA7 (Fig. 5(b)), similar results were obtained.

The influence of bubbles on liquid turbulence was studied by using bubble induced turbulence model (Sato et al.\(^{15}\)). The model showed marginal change in the vapor and liquid velocities with bubble induced turbulence model (results not shown here).

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Fig. 3. Effect of reference nucleation site density on (a) liquid temperature (b) wall temperature (DEBORA5)

Fig. 4. Effect of lift force on vapor volume fraction distribution for (a) DEBORA5 (b) DEBORA7

Fig. 5. Effect of turbulent dispersion force on vapor volume fraction distribution for (a) DEBORA5 (b) DEBORA7
5.3. Effect of nucleation site density

The nucleation site density $N$ was found to have a strong influence on the vapor volume fraction and temperature distribution, specifically on the wall superheat ($T_{W} - T_{sat}$). There are no conclusive guidelines on the use of a specific value of nucleation site density $N_{ref}$. In the present work, simulations were performed at different values of reference nucleation site density ($N_{ref}$). The predicted vapor volume fraction distributions were much closer to the measurements for $N_{ref} = 4 \times 10^5$ (results not shown here). Further increase in the value of $N_{ref}$ led to over-prediction of the vapor volume fraction. The $N_{ref}$ was found to have negligible effect on the liquid temperature profile as shown in Fig 3(a). The wall superheat was found to have a significant influence on the wall temperature predictions as shown in Fig 3(b). A good agreement was found between the measured and predicted wall temperature was obtained at $N_{ref} = 0.5 \times 10^7$. Although use of the higher $N_{ref}$ was advised by researchers$^3$, but in the present case this led to severe overprediction of the vapor volume fraction.

6. Summary and conclusions

In the present work, existing OpenFOAM solver was developed further by implementing various boiling correlations, wall heat flux partitioning model and energy equation. Also, different inter-phase coupling forces and bubble turbulence terms were included in the code. The modified code was used to simulate the boiling and predictions were

terms for $N_{ref} = 4 \times 10^5$ (results not shown here). Further increase in the value of $N_{ref}$ led to over-prediction of the vapor volume fraction. The $N_{ref}$ was found to have negligible effect on the liquid temperature profile as shown in Fig 3(a). The wall superheat was found to have a significant influence on the wall temperature predictions as shown in Fig 3(b). A good agreement was found between the measured and predicted wall temperature was obtained at $N_{ref} = 0.5 \times 10^7$. Although use of the higher $N_{ref}$ was advised by researchers$^3$, but in the present case this led to severe overprediction of the vapor volume fraction.

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