SIMULATIONS OF THE KETTLE REBOILER SHELL SIDE THERMAL-HYDRAULICS WITH DIFFERENT TWO-PHASE FLOW MODELS

by

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A computational fluid dynamics approach is presented for the simulation and analyses of the kettle reboiler shell side thermal-hydraulics with two different models of two-phase flow – the mixture and two fluid model. The mixture model is based on solving one momentum equation for two-phase mixture flow and a closure law for the calculation of the slip between gas and liquid phase velocities. In the two fluid modeling approach the momentum balance is formed for each phase, while the gas-liquid interaction due to momentum exchange at the interface surface is predicted with an empirical correlation for the interface friction coefficient. In both approaches the two-phase flow is observed as two inter-penetrating continua. The models are solved for the two-dimensional geometry of the kettle reboiler shell side vertical cross section. The computational fluid dynamics numerical method based on the SIMPLE type algorithm is applied. The results of both liquid and vapour velocity fields and void fraction are presented for each modeling approach. The calculated void fraction distributions are compared with available experimental data. The differences in the modeling approaches and obtained results are discussed. The main finding is that the void fraction distribution and two-phase flow field strongly depends on the modeling of the slip between liquid and gas phase velocity in mixture model or on the interface friction model in two fluid model. The better agreement of the numerically predicted void fraction with the experimental data is obtained with the two fluid model and an interfacial friction model developed for the conditions of two-phase flows in large volumes of kettle reboilers or different designs of steam generators.

Key words: kettle reboiler, thermal-hydraulics, numerical simulation, computational fluid dynamics

Introduction

Shell and tube heat exchangers are among the most widely used types of heat exchangers. Various shell and tube heat exchangers are designed for vapour generation on the shell side. They are widely applied in chemical, process, and energy power industry, in refrigerations and air-conditioning equipments, and they are applied such as reboilers, steam generators, and evaporators. It has been estimated that more than 50% of
all heat exchangers employed in process industries are used to boil fluids and involve two-phase flow on the shell side [1]. In process industry they are known as reboilers, while kettle reboilers are one of the most common reboiler types [2]. Also, some developments of horizontal steam generators for nuclear power plants are based on the kettle reboiler design [3].

A typical design of the kettle reboiler applied in the process industry is shown in fig. 1. The evaporating fluid flows on the shell side, across a horizontal tube bundle. The heat is transferred to the boiling two-phase mixture from a hot fluid that circulates inside the tubes. The liquid level is controlled by a weir, so that the bundle is always submerged in liquid. The gap between the bundle and the shell allows internal recirculation of liquid. The liquid enters the bundle at its bottom only. The mass velocity of fluid across the bundle is increased by the recirculation of liquid, affecting the global heat transfer coefficient.

Previous investigations of the kettle reboiler shell side thermal-hydraulics have been performed with experimental and analytical models of various levels of complexity regarding the multidimensionality and thermal-hydraulic complexity of boiling two-phase flow conditions. Void fractions and pressure drops in one-dimensional upward two-phase flows across the tube bundles with various tubes’ arrangements are presented in [4, 5]. One dimensional investigations were performed first, because the process of evaporation is complex and the vertical flow across the tube bundle is dominant. But, reboiler shell side thermal-hydraulics is strongly influence by multidimensional effects. It was shown that the vertical pressure change is not constant along the bundle, causing a lateral pressure change, which must be satisfied by a lateral flow [6]. In [7] a more realistic two-dimensional investigation is presented with information how variation of heat flux, weir height, bundle size and pressure affect the kettle reboiler processes. Two-dimensional numerical models of the kettle reboiler shell side thermal-hydraulics are presented in [8-10]. The main findings in performed researches are: (a) the homogeneous model of two-phase flow provides too high values of the void fraction which means that the gas and liquid phase velocity slip should be taken into account in a kettle reboiler de-
sign or analyses procedures, and (b) the liquid phase circulation is organized on the reboiler shell side, where the intensity of circulation influences the heat transfer coefficient and the void fraction distribution.

This paper presents the possibilities of two commonly applied two-phase flow models for the prediction of the kettle reboiler shell side thermal-hydraulics. These are (a) the mixture model of two-phase flow with the application of the closure law for the prediction of the gas and liquid phase slip velocity (for instance presented in [11]), and (b) the two fluid model of two-phase flow with the closure law for the prediction of the gas and liquid phase interfacial friction (applied in [10]).

**Modelling approaches**

Several assumptions are introduced in modeling the kettle reboiler shell side thermal-hydraulics:

(a) The shell side flow in the slab of the kettle reboiler vertical cross section (as presented with the left scheme in fig. 1) is two-dimensional;
(b) Steady-state conditions are modelled;
(c) The shell side two-phase mixture is saturated;
(d) The surface tension at the gas-liquid interface is neglected, as it is not important for bulk two-phase flow phenomena. Hence, pressure is the same for both phases within the numerical control volume;
(e) Flow governing equations are written in the non-viscous form, while the turbulent viscosity effects are taken into account indirectly through friction coefficients for the tube bundles flow resistance and two-phase interfacial friction force; and
(f) The porous medium concept is used in the simulation of two-phase flow within tube bundles. In the applied mixture model it is assumed that the porous media is 100% open to the fluid flow, while in the two-fluid model the real volumes of liquid and gas phase are taken into account. In both models, the resistance of the tube bundle to the two-phase flow is taken into account through the appropriate volumetric force.

**Mixture model**

The mixture model solves the continuity equation for the mixture, the momentum equation for the mixture, and the volume fraction equation for the secondary phases, as well as algebraic expressions for the relative velocities (if the phases are moving at different velocities) [11]. The energy equation for the mixture is also a constituent of the mixture model, but here it is not included since the saturated liquid and two-phase flows on the reboiler shell side are considered.

The continuity equation for the two-phase mixture is:

\[ \nabla \cdot (\rho_m \bar{v}_m) = 0 \]  

(1)
where $\bar{v}_m$ is the mass-averaged velocity:

$$
\bar{v}_m = \frac{\sum_{k=fg} \alpha_k \rho_k \bar{v}_k}{\rho_m}
$$

(2)

and $\rho_m$ is the mixture density:

$$
\rho_m = \sum_{k=fg} \alpha_k \rho_k
$$

(3)

$\alpha_k$ is the volume fraction of phase $k$ (liquid phase $k = f$ or gas phase $k = g$).

The momentum equation for the mixture can be obtained by summing the individual momentum equations for both phases:

$$
\nabla \cdot (\rho_m \bar{v}_m \bar{v}_m) = -\nabla p + \rho_m \ddot{\bar{v}} + \nabla \cdot (\rho_g \bar{v}_g \bar{v}_g) = -\bar{F}_{wm}
$$

(4)

where $\bar{v}_{dr,g}$ is the drift velocity of the dispersed vapour phase:

$$
\bar{v}_{dr,g} = \bar{v}_g - \bar{v}_m
$$

(5)

Introducing eq. (2) in eq. (5) the following expression for the vapour drift velocity is derived in which the slip velocity between the vapor and liquid phase figures (also referred to as the relative velocity):

$$
\bar{v}_{fg} = \bar{v}_g - \bar{v}_f
$$

(6)

The slip velocity is calculated with the following semi-empirical correlation:

$$
\bar{v}_{fg} = \frac{(\rho_m - \rho_g) d_g^2}{18 \mu_f f_{drag}} \ddot{\bar{a}}
$$

(7)

where $d_g$ is the bubble diameter and $\ddot{\bar{a}}$ is the mixture acceleration. The drag coefficient $f_{drag}$ is calculated with the empirical relations of Schiller and Naumann:

$$
f_{drag} = \begin{cases} 
1 + 0.15 \text{Re}^{0.678}, & \text{Re} \leq 1000 \\
0.0183 \text{Re}, & \text{Re} > 1000 
\end{cases}
$$

(8)

and the acceleration $\ddot{\bar{a}}$ is of the form:

$$
\ddot{\bar{a}} = \ddot{\bar{g}} - (\nabla \cdot \bar{v}) \bar{v} - \frac{\partial \bar{v}}{\partial t} = \ddot{\bar{g}} - \frac{D\bar{v}_m}{Dt}
$$

(9)

The volumetric force of tube bundle resistance to two-phase mixture flow $\bar{F}_{wm}$ is calculated as:

$$
\bar{F}_{wm} = \sum_{e=1}^{2} \zeta_e \frac{\rho_m v_m^2}{2} \frac{\bar{g}}{\Delta e}
$$

(10)
where \( \mathbf{e} \) is a unit vector in the direction of the Cartesian coordinate axis, and \( \Delta e \) is the width of the computational cell. The coefficient of the local pressure drop in \( e \) direction \( \zeta_e \) is calculated according to [12].

The vapour volume fraction is calculated from the continuity equation:

\[
\nabla \cdot (\alpha_g \rho_g \nabla \rho) = -\nabla \cdot (\alpha_g \rho_g \vec{v}_g)
\]  \( (11) \)

**Two fluid model**

Here applied two-fluid model of two-phase flow consists of the continuity and momentum equations for each phase and corresponding closure laws.

Mass conservation equations for liquid and vapour phase are:

\[
\frac{\partial (\alpha_f \rho_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \vec{U}_f) = -\Gamma_e
\]  \( (12) \)

\[
\frac{\partial (\alpha_g \rho_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g \vec{U}_g) = \Gamma_e
\]  \( (13) \)

Liquid and vapour momentum conservation equations:

\[
\frac{\partial (\alpha_f \rho_f \vec{U}_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \vec{U}_f \vec{U}_f) = -\alpha_f \nabla p + \alpha_f \rho_f \vec{g} + \vec{F}_{g_f} - \vec{F}_{w_f} - \Gamma_e \vec{U}_{fi}
\]  \( (14) \)

\[
\frac{\partial (\alpha_g \rho_g \vec{U}_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g \vec{U}_g \vec{U}_g) = -\alpha_g \nabla p + \alpha_g \rho_g \vec{g} + \vec{F}_{g_f} - \vec{F}_{w_g} - \Gamma_e \vec{U}_{fi}
\]  \( (15) \)

Evaporation rate is calculated as:

\[
\Gamma_e = \frac{q_{cell}}{h_{fg}} a_w
\]  \( (16) \)

where

\[
q_{cell} = A_{cell} q_{cell}^e
\]  \( (17) \)

when heat flux at the wall of the shell tube is defined, or:

\[
q_{cell} = h_{tp} A_{cell} \Delta T_{sat}
\]  \( (18) \)

when the temperature of the tube wall is defined.

The heat transfer coefficient calculations in the tube bundle are defined by the Chen type of correlation [13]:

\[
h_{tp} = F h_{conv} + S h_{abh}
\]  \( (19) \)
or
\[
h_{tp} = \frac{0.023k}{D \text{Re}^{0.8} \text{Pr}^{0.4} F} + \\
+0.00122 \frac{k^{0.79} \text{Re}^{0.45} \text{Pr}^{0.49} \mu_f^{0.5} \mu_g^{0.29} \rho_f^{0.24} \rho_g^{0.24} (T_w - T_{sat})^{0.24} (p_w - p)^{0.75} S}{\alpha^{0.5} \rho_f^{0.29} h_{fg}^{0.24} \rho_g^{0.24}}
\]  
\hspace{1cm} (20)

where applied coefficients are defined as:
\[p_w = p_{sat}\]  
\hspace{1cm} (21)

\[
F = 10 \quad \text{for } X_{TR}^{-1} \leq 0.10
\]  
\hspace{1cm} (22)

\[
F = 2.35(X_{TR}^{-1} + 0.213)^{0.736} \quad \text{for } X_{TR}^{-1} > 0.10
\]  
\hspace{1cm} (22)

\[
S = [1 + 0.12(\text{Re} F^{1.25})^{1.14}]^{-1} \quad \text{for } \text{Re} F^{1.25} < 325
\]  
\[
S = [1 + 0.42(\text{Re} F^{1.25})^{0.78}] \quad \text{for } 325 \leq \text{Re} F^{1.25} < 700
\]  
\[
S = 0.1 \quad \text{for } \text{Re} F^{1.25} \geq 700
\]  
\hspace{1cm} (23)

and Martinelli parameter:
\[X_{TR} = \left(\frac{1 - \alpha}{\alpha}\right)^{0.9} \left(\frac{\rho_g}{\rho_f}\right)^{0.5} \left(\frac{\mu_f}{\mu_g}\right)^{0.1} \]  
\hspace{1cm} (24)

and Reynolds number:
\[\text{Re} = \frac{G(1 - X)D_{hy}}{\mu_f} \]  
\hspace{1cm} (25)

The wall drag term can be expressed as a pressure drop due to the tube bundle friction. The pressure drop due to the two-phase mixture flow around tubes in a bundle is determined by taking into account the separate contribution of the each phase to the total pressure drop. The pressure drop of phase \(k\) in \(e\) direction is defined as:
\[
\bar{F}_{we} = \zeta_{ke} \frac{\rho_k}{2} \frac{\hat{u}_k^2}{(1 - \alpha_w)} \frac{\alpha_k}{\alpha_f + \alpha_g} \hat{v}
\]  
\hspace{1cm} (26)

where \(\zeta_{ke}\) is pressure loss coefficient in \(y\) direction and \(\hat{u}_k, k = f, g\) is the maximum velocity of the phase in \(e\) direction.

The interfacial friction terms have influence on void fraction and relative velocity of the phases [14]:
\[
\bar{F}_{gf} = \frac{3}{4} \rho_f \frac{C_{di}}{D_b} \alpha \cdot |\bar{U}_g - \bar{U}_f| |\hat{U}_g - \hat{U}_f|
\]  
\hspace{1cm} (27)
where $C_{di}$ is the interfacial drag coefficient and $D_b$ is the diameter of the bubble. For bubble flow $\phi \leq 0.3$ [14]:

$$C_{di} = 0.267D_b \sqrt{\frac{g \Delta \rho}{\sigma}} \left[ 1 + \frac{\sqrt{1767f(\phi)^6}}{18.67f(\phi)} \right]$$ (28)

where

$$f(\phi) = (1 - \phi)^{1.5}$$ (29)

and

$$\phi = \frac{\alpha_g}{\alpha_f + \alpha_g}$$ (30)

For churn-turbulent flows ($\phi > 0.3$), a new correlation is proposed based on the results proposed in [15]:

$$C_{di} = 1.487D_b \sqrt{\frac{g \Delta \rho}{\sigma}} (1 - \phi)^3 (1 - 0.75 \phi)^2$$ (31)

The functional dependence of the ratio $C_{di}/D_b$ on the void fraction is given in fig. 2. For transitional flow patterns, there is a rapid decrease of $C_{di}/D_b$ ratio. This could be attributed to the decrease of the two-phase flow interfacial area concentration.

According to the applied porous media approach, the control volume within the tube bundle is occupied with tubes and a free area filled with single phase or two-phase mixture. Tube bundle is represented as porous area, with the porous factor:

$$\psi = 1 - \frac{D^2}{4\pi a^2}$$ (32)

The presented models are solved with the control volume based numerical method and code presented in [16]. Details about the solving procedure are presented in [17].

*Figure 2. Ratio of interfacial friction coefficient $C_{di}$ and particle diameter $D_p$ vs. void fraction for two-phase flow across a tube bundle*
Boundary conditions

Boundary conditions include the line of symmetry, the shell wall, and the inlet flows and outlet recirculating flow. At the line of symmetry gradients of all variables are constant. Saturated liquid inflow was specified at the bottom center of the heat exchanger, simulating the feed flow in an actual kettle reboiler. The flow rate was specified using the overflow and the vaporization rate. At the outflow boundary in an actual kettle reboiler, the vapour separates from the liquid and leaves the reboiler. In the process, most of the liquid recirculates within the reboiler, but some of the liquid recirculates within the evaporator, and some of the liquid is carried over the weir. Recirculation of the liquid is simulated by defining the velocity gradient at the outflow surface. Boundary conditions are presented in fig. 3 for two fluid model velocity components \( V \) along vertical coordinate and \( W \) component along horizontal coordinate. The reduction of these boundary conditions to the mixture model is straightforward. In the mixture model the void fraction at the free surface of the two-phase mixture is equal to 1, while no change of the two-phase mixture velocity components is assumed as in case of the vapour velocity component in the two fluid model (fig. 3).

Results and discussion

Developed models of two-phase flow on the kettle reboiler shell side are applied to the numerical simulation and analyses of the experimental conditions presented in [18]. Geometric parameters required to specify the heat exchanger are shown in fig. 4 and tab. 1. Experiments were performed under atmospheric pressure.

The presented reboiler geometry is discretized with two-dimensional control volumes, fig. 5.

Results of the numerical simulations performed with two fluid model and mixture model are presented in figs. 6, 7, and 8. In those pictures total two-phase flow mass flux vectors were calculated as:

\[
\vec{G} = \alpha_f \rho_f \vec{U}_f + \alpha_g \rho_g \vec{U}_g
\]  

(34)
The results in fig. 6 clearly show the formation of one circulation centre at the boundary of the upper half of the tube bundle (the bundle is depicted with dashed line). Strong downward flow exists in the downcomer between the bundle and the shell wall. This natural circulation is governed by the density differences between the mixture in the bundle-shell downcomer (lower void fraction and higher density) and the boiling two-phase mixture in the bundle (higher void and lower density). The reference mass flux vectors of 1400 kg/m²s for two fluid model results and 1700 kg/m²s in case of mixture model indicate almost the same intensity of the overall circulation around and through the bundle. But, the mixture model predicts less intensive lateral flow from the downcomer towards the tube bundle. According to the mixture model, the two-dimensional character of the flow between the downcomer and the tube bundle is suppressed; both the bundle and downcomer flows are vertical in opposite directions.

The two-phase flow model predicts lower void fractions than the mixture model, fig. 7. This is due to the more intensive liquid downward flow in the bundle-shell downcomer and liquid penetration from the downcomer to the bundle, as presented in the corresponding left picture in fig. 7. The thick full line in both pictures in fig. 7 represents

| Table 1. Dimensions and parameters of the experimental kettle reboiler [18] |
|--------------------|--------|
| Tube diameter 2r   | 19 mm  |
| Pitch h            | 25.4 mm|
| Shell radius R     | 0.368 m|
| Weir height from the center of shell b | 0.210 m |
| Bundle center/shell radius offset a  | 0.114 m |
| Number of tubes    | 241    |
| Tubes arrangement  | In-line square |
| Working fluid      | Refrigerant R113 |

Figure 5. Meshes used for modeling

Figure 6. Mass flux vector for liquid for two fluid model (left) and mixture model (right)
the lower boundary of the region of higher void as observed in the experimental investigation. The region above the full thick line is characterized as frothy. In right side of fig. 7 a very rapid increase in void is calculated above the dividing line with void values above 0.8 at the top of the bundle. It is hardly to expect that the high values of void fraction can be achieved under considered heat flux of 20 kW/m².

Figure 8 shows the horizontal void fraction distributions at the half of tube bundle height calculated with the Schrage et al. empirical correlation as reported in [9] and predicted with here presented two fluid model and mixture model. The mixture model does not provide satisfactory agreement with the two fluid model and the referent data of Schrage, especially in the inner areas of the bundle close to the axis of symmetry. The two fluid model provides much better agreement with the referent void fraction data.

As it is presented with the results of the numerical simulation, the mixture model is less suitable for the simulation and analyses of the kettle reboiler shell side thermal-hydraulics. This is attributed to the fact that the mixture model is inherently not suitable for the modelling of vapour and liquid phase separation in the large two-phase volumes with liquid phase recirculation, especially at the two-phase mixture free-surface (so called swell level).
Conclusions

The mixture and two fluid models are applied to the simulation of the kettle reboiler shell side thermal-hydraulics. Results obtained with the mixture, based on the two-phase mixture continuity and momentum equation and corresponding semi-empirical closure laws for the vapor and liquid phase slip velocity, does not provide reliable results of the kettle reboiler shell side thermal-hydraulics. The lateral two-phase flow from the downcomer to the tube bundle is suppressed and too high values of the void fraction are obtained. On the other hand, more complex two fluid model, based on the mass and momentum balance equations for each phase and corresponding closure laws for the interface momentum exchange due to the interface friction, provides much better agreement with the referent results of the void fraction distribution. Also, two fluid model provides more plausible results of the two-phase flow structure on the kettle reboiler shell side than the mixture model. The inability of the mixture model to predict correctly the shell side thermal-hydraulics is due to the solving of one momentum equation for the two-phase mixture, and corresponding limitations in modelling the vapour and liquid phase separation within the large volume of the kettle reboiler shell side with liquid phase circulation.

Nomenclature

\begin{itemize}
  \item \( A \) – area of tube bundle cell, [m]
  \item \( \dot{a} \) – mixture acceleration, [ms\(^{-2}\)]
  \item \( a_{wo} \) – specific area of tube bundle cell, [m\(^{-1}\)]
  \item \( C_{\text{di}} \) – interfacial drag coefficient, [-]
  \item \( c_p \) – specific heat at constant pressure, [kJkg\(^{-1}\)K\(^{-1}\)]
  \item \( D \) – tube diameter, [m]
  \item \( D_b \) – diameter bubble, [m]
  \item \( D_{hy} \) – hydraulic equivalent diameter, [m]
  \item \( d_g \) – bubble diameter, [m]
  \item \( \hat{e} \) – unit vector in the direction of the Cartesian coordinate axis, [-]
  \item \( \Delta e \) – width of the computational cell in y or z direction, [m]
  \item \( \mathcal{F} \) – source term, [Nm\(^{-1}\)]
  \item \( F_{\text{wm}} \) – volumetric force of tube bundle resistance to two-phase mixture, [kgm\(^{-2}\)s\(^{-2}\)]
  \item \( f_{\text{drag}} \) – drag coefficient, [-]
  \item \( G \) – mass flux, [kgm\(^{-2}\)s\(^{-1}\)]
  \item \( g \) – gravitationnal acceleration, [ms\(^{-2}\)]
  \item \( h \) – heat transfer coefficient, [Wm\(^{-2}\)K\(^{-1}\)]
  \item \( k \) – thermal conductivity, [kWm\(^{-1}\)K\(^{-1}\)]
  \item \( Pr \) – Prandtl number, (\(=\mu c_p/k\)) [-]
  \item \( p \) – pressure, [Pa]
  \item \( q \) – heat flux, [Wm\(^{-2}\)]
  \item \( \text{Re} \) – Reynolds number, (\(=\rho U D_b/\mu\)), [-]
  \item \( T \) – temperature, [K]
  \item \( t \) – time, [s]
  \item \( U \) – velocity of the phase \( (U_{ky} = V_k, U_{kz} = W_k) \), [ms\(^{-1}\)]
\end{itemize}
\( v \) – velocity, \([\text{ms}^{-1}]\)
\( \psi_\phi \) – drift velocity, \([\text{ms}^{-1}]\)
\( \psi_m \) – mass-averaged velocity, \([\text{ms}^{-1}]\)
\( \psi_f \) – relative velocity, \([\text{ms}^{-1}]\)
\( X \) – flow quality, [-]
\( X_{TT} \) – Martinelli parameter, [-]

**Greek letters**

\( \alpha \) – volume fraction in the control volume, [-]
\( \Gamma_\varepsilon \) – evaporation rate, [-]
\( \zeta \) – pressure loss coefficient, \([\text{Nm}^{-1}]\)
\( \sigma \) – surface tension, \([\text{Nm}^{-1}]\)
\( \mu \) – viscosity, \([\text{Pas}]\)
\( \rho \) – density, \([\text{kgm}^{-3}]\)
\( \varphi \) – vapour volume fraction (void) in two-phase flow, [-]
\( \psi \) – porosity, [-]

**Subscripts**

\( \text{conv} \) – convection
\( \varepsilon \) – \( \varepsilon \) direction
\( \text{f} \) – liquid
\( \text{g} \) – gas
\( i \) – interface parameter
\( \text{in} \) – inlet
\( \text{k} \) – phase
\( \text{m} \) – mixture
\( \text{nb} \) – neigbour cell
\( \text{p} \) – particle
\( \text{sat} \) – saturation
\( \text{tp} \) – tube bundle
\( \text{w} \) – wall
\( y \) – pertain to y direction
\( z \) – pertain to z direction

**References**

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