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Application of Enhanced Phase-Change Model for Simulation of Film Boiling Around a Cylinder

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ABSTRACT

Phase-change modelling is crucial for accurate and universal numerical simulation of film boiling around a cylinder. In our previous studies, Lee's evaporation-condensation model has been used. The main challenge of this model is determining the value of the empirical mass transfer intensity factor. The presented work investigates the Chen's modification of Lee's model. The modification enables to calculate the mass transfer intensity factor as a function of fluid properties and mesh size. The Chen's model was tested against the benchmark problem – the one-dimensional Stefan problem. The model was realised using user-defined functions in ANSYS Fluent. Results showed key advantages over the Lee's model and a good agreement with the analitical solution.

1 INTRODUCTION

Recent life cycle analyses have identified conventional nuclear power plants as one of the cleanest energy sources. In terms of carbon emissions, even current operable NPP could be superior to renewables, such as wind and solar [1]. Furthermore, fourth-generation reactors with better fuel efficiency and nuclear safety show immense potential for clean and reliable energy production. One of the technologies of this kind is a sodium-cooled breeder reactor (SBR) [2].

Our research focuses on the interaction between melt and sodium during a hypothetical core melt accident in SBR: a rapid and intense heat transfer interaction between the molten core material and the sodium coolant may lead to vapour explosions [3]. At the forefront of the research are the phenomena and processes during vapour explosion in sodium. Experimental investigation of liquid sodium is complex, mainly due to its chemical reactivity and opaqueness [4]. Hence numerical studies could deliver valuable insight into the heat and mass transfer mechanisms. On the other hand, vapour explosions are experimentally widely investigated in water, hence these experiments provide a solid basis for the validation of numerical models [5].

Present work is focused on developing an appropriate numerical model for solving the two-phase flow around a melt particle. Our final numerical model will represent a benchmark experiment conducted in the TREPAM (CEA, France) apparatus that mimicked film boiling conditions around a melt fragment [6]. In the TREPAM apparatus, the melt fragment was represented by a heated wire moving at a constant velocity through the pressurised subcooled water [6].

In the previous studies [5], we investigated the applicability of numerical models included in the ANSYS Fluent code to simulate the film boiling conditions around the wire. The simulations of forced convection boiling were preformed using the Volume of Fluid (VOF) method with the Lee evaporation-condensation model. However, there is an empirical factor in the Lee model, named mass transfer intensity factor and is denoted as r with units [1/s]. The results showed high dependency of the solution accuracy on the value of r [5]. Thereby, other models need to be implemented to further enhance the universality and accuracy of the simulation. In this paper, the modification of Lee's model proposed by Chen et al. [7] is evaluated. The main aim of the presented work is to implement the Chen's phase-change model in the ANSYS Fluent code and to perform code verification and validation by simulating the one-dimensional Stefan problem. The implemented model can then be used in future for more complex simulations of boiling problems.

2 NUMERICAL MODEL

2.1 Modelling of two-phase flow

Our past studies have shown that interface tracking is significant when simulating two-phase flow phenomenon around a wire. Namely, the thickness of the vapour film in front of the wire has the highest impact on the wall heat flux [5]. Therefore, we selected a single fluid approach for modelling two-phase flow. In this study, the simulation is based on the VOF method developed by Hirt and Nichols [8]. In the VOF method, the phase distribution is represented by the volume fraction α. For two-phase flows, applies the equation:

$$\alpha_L + \alpha_V = 1, \tag{1}$$

where α_L and α_V represents the volume fraction of the liquid and vapour phase, respectively.

The volume fraction equations describe the advection of the interface. For the vapour phase, the equation is formulated as follows:

$$\frac{\partial}{\partial t}(\rho_V \alpha_V) + \nabla \cdot (\rho_V \alpha_V \boldsymbol{v}) = -\mathrm{S_V}, \tag{2}$$

where α_v, ρ_v, and $\boldsymbol{v}$ are the vapour volume fraction, vapour density, and the velocity field, respectively. Phase change phenomenon is modelled with mass source term S_V. The volume fraction of the liquid phase is calculated according to Eq. (1).

Both fluids share a single momentum equation and velocity field $\boldsymbol{v}$. The momentum equation is:

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \nabla \cdot (\rho \boldsymbol{v}\boldsymbol{v}) = -\nabla p + \nabla \cdot [\mu(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)] + \rho \boldsymbol{g} + \boldsymbol{F}_s, \tag{3}$$

where ρ, k, μ and p are the mixture density, thermal conductivity, viscosity and pressure field, respectively. Mixture properties are calculated as volume-fraction weighted averages of individual phases. Term $\boldsymbol{g}$ represents the gravitational acceleration vector. The surface tension effects at the interface are modelled by source term $\boldsymbol{F}_s$, which is calculated by the continuum surface force (CSF) model proposed by Brackbill et al. [9].

Similarly, the energy equation is also shared for both fluids. It is defined as:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot [\boldsymbol{v}(\rho E + p)] = \nabla \cdot [k \nabla T] + S_h, \tag{4}$$

where S_h is the volumetric energy source, E is sensible enthalpy calculated with:

$$E = C_p(T - T_{\text{sat}}), \tag{5}$$

where T_{sat} is the saturation temperature, and C_p is the mixture specific heat capacity. The specific heat capacity is defined as:

$$C_p = \frac{\rho_V \alpha_V C_{p,V} + \rho_L \alpha_L C_{p,L}}{\rho_V \alpha_V + \rho_L \alpha_L}, \tag{6}$$

where $C_{p,V}$, $C_{p,L}$ are the specific heat capacity for the vapour and liquid phases, respectively.

For the interface reconstruction we applied the High-Resolution Interface Capturing (HRIC) scheme that is included in the ANSYS Fluent code [10]. The HRIC scheme is based on the donor-acceptor method. The interface position is then determined by spatial interpolation. Based on a composite Normalised Variable Diminishing (NVD) scheme consisting of a nonlinear blend of upwind and downwind differencing. It can be used with explicit and implicit formulation of VOF [10]. It should be noted that for the 2D problems use of a more precise scheme, such as the Geometric reconstruction scheme, needs to be considered, but in the presented work the HRIC scheme is sufficient.

2.2 Modelling of phase change

Lee's evaporation-condensation model [11] is widely adopted as phase-change model in the single-fluid multiphase approach. It is the simplest to implement with computational fluid dynamics (CFD) software. It is also the only available model in commercial CFD code ANSYS Fluent.

The model assumes that the mass transfer rate is proportional to the deviation of the cell temperature from the saturation temperature. The rate is determined based on the interfacial cell temperature and phase volume fraction. Lee's model allows the phase change to occur at the existing interface or within the saturated phase without an interface. Thus, it allows the simulations of the boiling process without a predetermined phase interface and subcooled boiling. Convergence of simulation is ensured by empirical factor r, called as mass transfer intensity factor with unit [s^{-1}] [11].

For the boiling problem, the mass source term of the vapour volume fraction equation (Eq. (2)) is:

$$S_V = r\ \alpha_L\ \rho_L \frac{T - T_{\text{sat}}}{T_{\text{sat}}}; \qquad T > T_{\text{sat}}. \tag{7}$$

The energy source term in the energy equation (Eq. 4)) corresponds to the heat exchanged during the interphase change and is defined as:

$$S_h = -S_V\ h_{LV}, \tag{8}$$

where h_{LV} represents specific latent heat.

Several previous studies performed by different researchers [7], as well as our own [5], demonstrated that the value of r significantly affects the accuracy of the simulation. Accordingly, the simulation result accuracy is unclear without experimental data validation. As shown in our previous work [5], the simulations with an inadequate value of r can even forecast completely different flow regimes. Furthermore, in all simulation practices, the factor r is used as a constant throughout the computational domain, which is not valid, especially when dealing with large temperature gradients [7].

To overcome the issues with the empirical factor r, Chen et al. (2020) [7] suggested an enhanced evaporation-condensation model. It is based on the Lee's model but follows explicit formulation for empirical factor r. The Chen's model is derived from two assumptions:

i. There is a liquid cell neighbour to the interfacial cell, and the temperature of the liquid cell equals the saturation temperature during the phase change process.
ii. The conductive heat flux from the interfacial cell to the neighbour liquid cell is the driving force of the phase change process.

A hypothetical example that corresponds to the above assumptions is shown in Fig. 1a. The belonging temperature profile of discretised domain is shown in Fig. 1b. It should be noted that in actual numerical simulation, the temperature of cell i+1 may be larger than the saturation temperature [7].

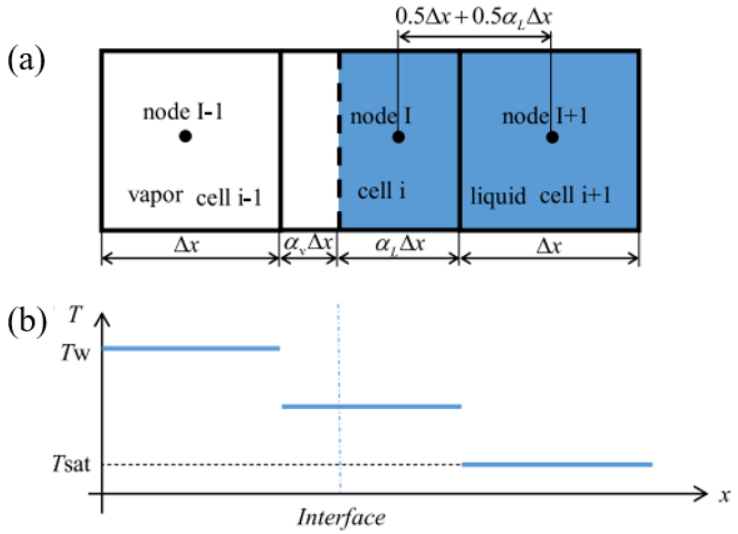

Figure 1: Graphical representation of assumptions in Chen's model (a) and belonging temperature profiles in discretised domain (b) [7]

The main idea of the model is that all the heat transferred through the liquid subdomain of the cell i and i+1 is used for phase change. Hence, the mass source of the volume fraction equation can be formulated as (for boiling):

$$S_V = k_L \frac{T-T_{\text{sat}}}{h_{LV}(0.5+0.5\alpha_L)\Delta x}\frac{A_{\text{int}}}{V}, \tag{12}$$

where k_L represents thermal conductivity of liquid phase and $\frac{A_{\text{int}}}{V}$ is the ratio of the interfacial area to the cell volume, this ratio can be evaluated according to the following expression:

$$\frac{A_{\text{int}}}{V} = |\nabla\alpha_V|. \tag{11}$$

The Chen's phase change model was realised in ANSYS Fluent by user defined functions (UDF) [10]. In presented work we applied the simplification $\frac{A_{\text{int}}}{V} = \frac{1}{\Delta x}$, which is valid for 1D problems. Additionally, we applied two conditions to assure that phase-change only occurs in the interfacial cells:

i. for evaporation: $\alpha_L > 0,\ T > T_{\text{sat}}$
ii. for condensation: $\alpha_V > 0,\ T < T_{\text{sat}}$

For better stability of the simulation, the conditions were relaxed to $\alpha_L > 10^{-6}$ and $\alpha_V > 10^{-6}$.

3 VALIDATION OF PHASE-CHANGE MODEL

3.1 Computational setup

The computational setup is a representation of the one-dimensional Stefan problem. The problem describes the time evolution of the boundary between two phases undergoing a phase change. In this case, we observed the movement of the free boundary between saturated liquid and overheated vapour. This case was chosen because it has an analytical solution, that served as a basis for validation. The solution for the interface position $x(t)$ is given by [12]:

$$x(t) = 2\,\beta\sqrt{\frac{k_V\,t}{\rho_V\,C_{p,V}}}, \tag{12}$$

where β is the solution of the transcendental equation:

$$\beta\,\exp(\beta^2)\mathrm{erf}(\beta) = \frac{C_{p,V}\,(T_{\mathrm{wall}}-T_{\mathrm{sat}})}{h_{LV}\,\sqrt{\pi}}. \tag{13}$$

The problem was simulated with the ANSYS Fluent code in a 2D domain. Free-slip and adiabatic conditions were applied at the top and bottom boundaries. Thus, no gradients existed along the y-axis, which guaranteed the comparability between the simulation results and the one-dimensional analytical solution. The computational domain is shown in Fig 2.

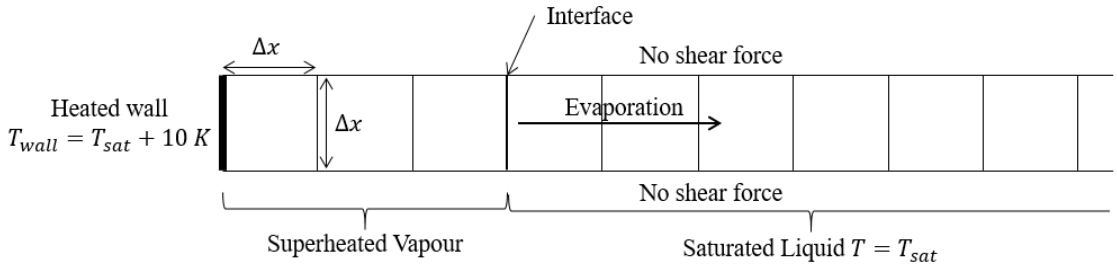

Figure 2: Graphical representation of computational setup

The domain length was 1 mm. To evaluate mesh sensitivity of Chen's model realised with our UDF, the simulations were conducted on three mesh configurations with uniform sizes of 2 μm, 5 μm and 10 μm. On the left and right boundaries, a no-slip condition and a given pressure condition were provided, respectively. Additionally, an isothermal condition $T_{\mathrm{wall}} = T_{\mathrm{sat}} + 10$ K was applied to the left boundary. In order to meet the interfacial cell conditions required by Chen's model, vapour film was initially applied to the first computational cell next to the wall.

The system pressure of 101.3 kPa was assumed in the simulation. The properties of the liquid water and vapour are listed in Table 1.

Table 1: Thermodynamic properties of fluids

	Density	Viscosity	Specific heat capacity	Thermal conductivity	Latent heat of vapourisation	Surface tension coef.
	$[kg/m^3]$	$[kg/(m\ s)]$	$[J/(kg\ K)]$	$[W/(m\ K)]$	$[J/kg]$	$[N/m]$
Vapour	0.597	1.26×10^{-5}	2030	0.025	2.26×10^{6}	0.059
Liquid	958.4	2.8×10^{-4}	4216	0.679		

The buoyancy effects and gravity were neglected due to the domain size and dimension. Laminar flow conditions were assumed on account of domain dimension and low velocities.

3.2 Results

The comparison between the simulation results and the analytical solution of the Stefan problem is shown in Fig. 3. Simulations with the Chen's phase-change model agree well with the analytical solution; we estimated the error of Chen's model at 2.5 % (for 2 μm). The results clearly show the advantages of Chen's over Lee's model, as with the latter the magnitude of the interface movement and the trend's shape (especially with low r) are mispredicted.

Mesh analysis was performed based on the results from cell size of 2 μm, 5μm, 10 μm. Discretisation error was assessed using the Richardson extrapolation scheme [13]. The extrapolation was based on interface position at several time steps. We evaluated the discretisation error to 2.70 %, 0.24 % and 0.04 % for meshes of size 10 μm, 5μm, 2 μm, respectively.

The final aim of our study is an accurate and universal simulation of film boiling around a cylinder in a subcooled flow, so evaporation and condensation need to be modelled. That is why we also performed several simulations with both phenomena modelled. The results confirmed the adequacy even in such formulation.

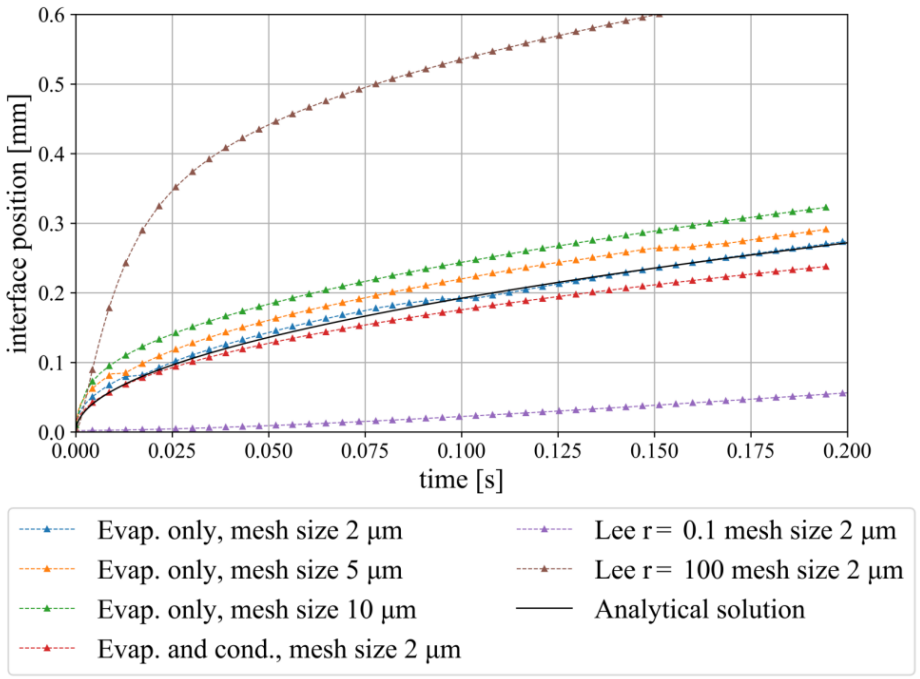

Figure 3: Theoretical and numerical interface positions as a function of time

Our past studies have shown that maintaining a sharp interface is significant when simulating film boiling in fluid flow [5, 14]. Due to the concept of interface cells, the Chen's model allows boiling only on the interface, so there is no smearing. Consequently, the model correctly predicts the shape of the temperature profile and allows for sharp gradient jumps. Comparison between the Chen's and Lee's model is shown in Fig. 4.

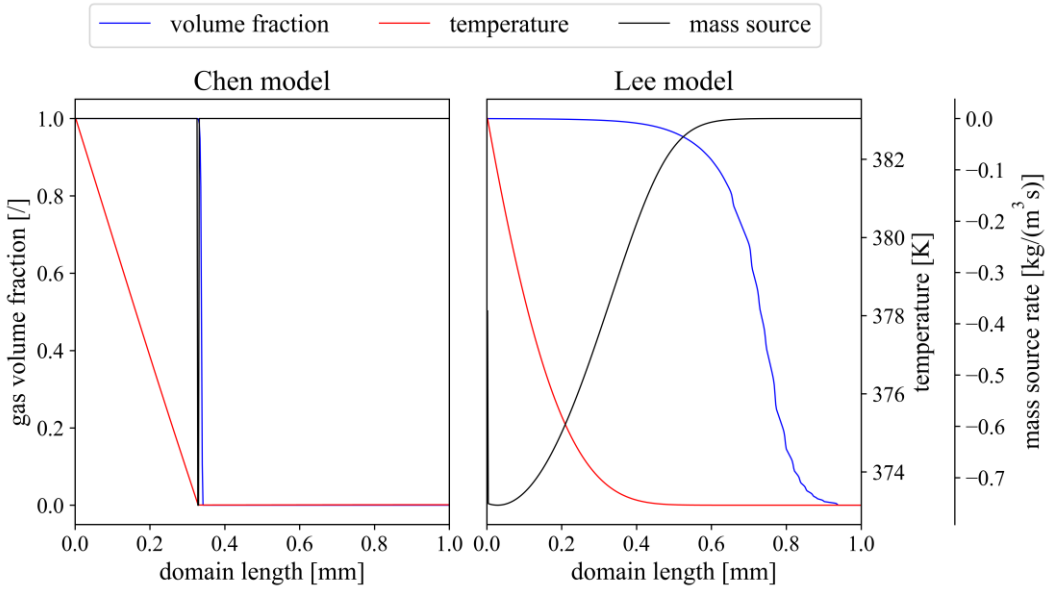

Figure 4: Comparison of different profiles between phase-change models

4 CONCLUSION

The applicability of the enhanced phase-change model (Chen et al., 2020 [7]) for the simulation of film boiling around a cylinder in subcooled flow is under investigation. The Chen's modification of Lee's model provides a way to calculate the mass transfer intensity factor as a function of fluid properties and mesh size without calibration. The model was realised in ANSYS Fluent code using the user-defined functions (UDF). The accuracy of the model has been tested against the benchmark problem – the one-dimensional Stefan problem. The results have shown the crucial advantages of Chen's model over Lee's. The model has predicted the interface evolution with an error of 2.5 %. Another crucial advantage of Chen's model is the ability to maintain a sharp interface.

The findings presented in this work, show the great potential of Chen's model for simulations of boiling-condensation problems. Furthermore, the model realised with the UDF functions is validated and can now be used for more complex simulations. In the future, our work will focus on simulations of film boiling around a cylinder in a subcooled flow with the implemented phase-change model.

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