



# **Project FORTE - Nuclear Thermal Hydraulics Research & Development**

## **Application of Multiphase CFD models to rod bundle boil-off**

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**SYSTEMS AND ENGINEERING TECHNOLOGY**

## An introduction to Project FORTE

The Department for Business, Energy and Industrial Strategy (BEIS) has tasked Frazer-Nash Consultancy and its partner organisations to deliver the first phase of a programme of nuclear thermal hydraulics research and development.

Phase 1 of the programme comprises two parts:

- ▶ The specification and development of innovative thermal hydraulic modelling methods and tools; and
- ▶ The specification of a new United Kingdom thermal hydraulics test facility.

The work is intended to consider all future reactor technologies including Gen III+, small modular reactors and advanced reactor technologies.

## Our project partners

The team is led by Frazer-Nash Consultancy and includes:



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University  
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## Executive Summary

Two-phase flows feature extensively in the context of nuclear thermal hydraulics and are expected to be present during both normal operation and off-design conditions. During an unexpected power loss or severe accident at a Nuclear Power Plant, a loss of primary coolant circulation may result in unwanted boiling within the fuel assemblies present in the reactor vessel. If left unmitigated, vapour generation within the rod bundles will eventually create a boiling “front” that moves downwards through the bundle as the remaining liquid boils off. This phenomena, known as rod-bundle boil-off, has the potential to compromise reactor safety, and so it is important to ensure that it can be accurately assessed and reliably predicted.

The objective of this research is to assess the current status of commercially available multiphase CFD modelling approaches in a nuclear thermal hydraulics context that are available to industrial engineers working on reactor design and problem mitigation.

The test case considered comprises a single heated rod immersed within a circular channel filled with water. The channel is open to the atmosphere at the top but is otherwise enclosed and the heated rod provides a fixed heat flux into the quiescent fluid. The problem is solved as 2D axisymmetric and unsteady. The initial temperature of the fluid is set a few degrees below saturation and the solution marched forward in time. Once the liquid begins to boil-off, the aim is to capture the liquid-vapour boiling front as it travels down the channel.

Two multiphase modelling methodologies have been investigated, the Eulerian-Eulerian and Volume of Fluid approaches, as currently implemented within the commercial CFD package ANSYS FLUENT (v19.2). These differ significantly in their approach to modelling multiple phases and in how they incorporate mass transfer (boiling) between the phases. The former utilizes an extended version of the so-called RPI model to capture the effects of nucleate boiling at the wall, whilst the second, an interface tracking method, is best suited to resolving the morphology of the liquid-vapour boiling front.

Results show that the complexity and dependence of both the multiphase approaches on experimentally derived sub-models led to numerical difficulties which prevented the full solution of the case. A number of key conclusions can be drawn from this work:

- ▶ The Eulerian-Eulerian methodology coupled with the RPI wall boiling model is the most physically complete approach and is capable of predicting the subcooled boiling present in the initial evolution of the case. However, its ability to model the vapour boiling front could not be assessed due to difficulty obtaining numerical convergence.
- ▶ The Volume of Fluid methodology is (at least in principle) best placed to capture the complex morphology of the boiling front but this could not be assessed due to difficulty obtaining numerical convergence. It is not best suited to modelling nucleate boiling in cases where the mesh sizing near the nucleating surface prevents resolution of a discernible liquid-vapour interface. Further research is required to determine whether the effect can be modelled instead, as is done with the RPI wall boiling model.
- ▶ In general, the sheer number and variety of models and sub-models used within multiphase approaches is likely to be a source of confusion for engineers who do not have significant experience or expertise in the field.
- ▶ Multiphase CFD has not yet reached levels of maturity enjoyed by its single-phase counterpart and there is a clear need for continued research and development of both approaches considered here. This should be driven by the production of openly available high-quality experimental data.

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# 1 Introduction

Two-phase flows feature extensively in the context of nuclear thermal hydraulics and are expected to be present during both normal operation and off-design conditions. During an unexpected power loss or severe accident at a Nuclear Power Plant, a loss of primary coolant circulation may result in unwanted boiling within the fuel assemblies present in the reactor vessel. If left unmitigated, vapour generation within the rod bundles will eventually create a boiling “front” that moves downwards through the bundle as the remaining liquid boils off. Once exposed, the fuel rods may experience significant surface temperature excursions which may ultimately threaten their integrity. A similar process may also be initiated in occupied spent fuel pools if coolant pumps are interrupted for an extended period of time. Since this scenario, known as **rod-bundle boil-off**, has the potential to compromise reactor safety it is important to ensure it can be accurately assessed and reliably predicted.

Whilst a number of previous studies have investigated boil-off experimentally (Aksan *et al.* 1993; Arai *et al.* 2015), only a very limited number of numerical studies are available in the open literature and most make use of ‘system codes’, the favoured modelling approach within the nuclear industry. These are typically one-dimensional and rely wholly on empirical and scale-dependent correlations obtained via experimentation. Arai *et al.* (2015) conducted a boil-off experimental study in a 5x5 full length (3.7m) heated rod bundle and found that their void fractions measurements agreed with predictions by the severe accident analysis code MAAP to only within  $\pm 30\%$ .

For more detailed modelling approaches, Computational Fluid Dynamics (CFD) is now quite widely used in many single-phase fluid problems. Multiphase CFD schemes are, however, less mature than their single-phase counterparts owing, in part, to the significantly increased physical diversity within the flow. Nevertheless, they have begun to play an important role in the prediction of nuclear thermal hydraulics phenomena, due to their potential to reduce empiricism and increase fidelity.

## 1.1 Objectives

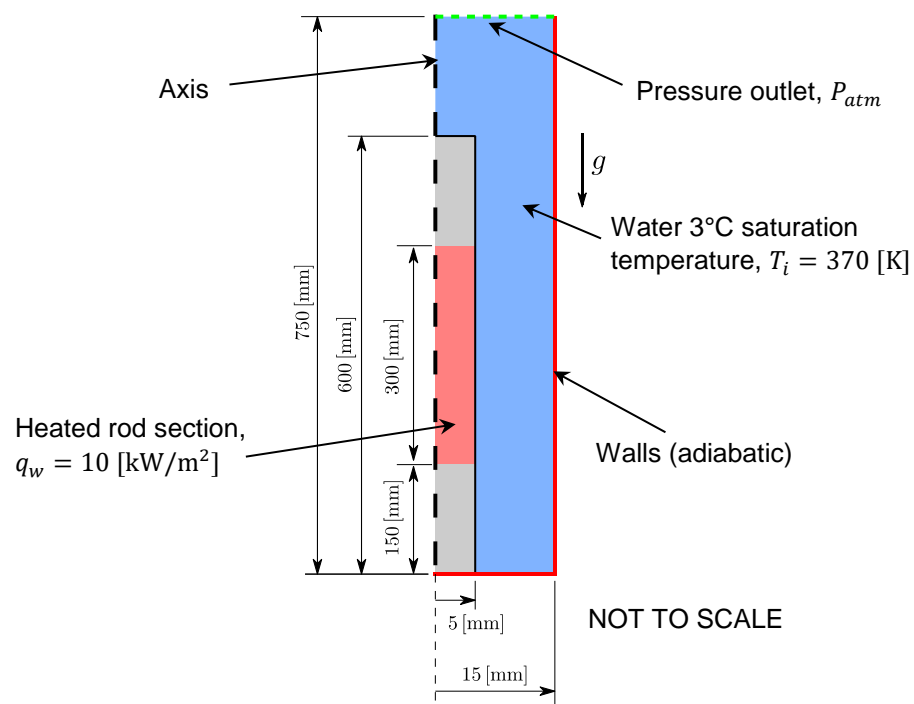
This preliminary study aims to investigate the potential of multiphase CFD approaches currently available in commercial software to numerically simulate the boiling front that develops around a single heated rod immersed within a circular channel. Two widely employed multiphase modelling approaches have been applied, the Eulerian-Eulerian ‘two-fluid’ model and the Volume of Fluid (VOF) model.

The simplified nature of the geometry, when compared with the larger rod bundle type geometries (i.e. full fuel assemblies) typically found within a light water reactor, reduces computational complexity whilst retaining the correct core boiling phenomenology.

## 2 Case description

A schematic of the geometry considered, along with the imposed boundary conditions, is presented in Figure 1. The problem is modelled as 2D axisymmetric, where the symmetry axis is concentric with the circular rod which itself only rises part way up the channel. The channel is sealed at the bottom but contains an outlet at the top, maintained at a fixed (atmospheric) pressure, to enable generated vapour to leave the domain.

All walls are adiabatic except a subset of the rod surface, as indicated in Figure 1, where a constant heat flux of  $q_w = 10 \text{ [kW/m}^2\text{]}$  is applied. The working fluid is water, with variable (temperature dependent) properties computed as per IAPWS-IF97<sup>1</sup> (IAPWS 1997; Wagner *et al.* 2000). The initial temperature is set as 3°C below saturation ( $T_i = 370 \text{ [K]}$ ), to allow initial subcooled boiling to be captured.



**Figure 1: Schematic of geometry with boundary conditions. Only the fluid domain, in blue, is modelled**

<sup>1</sup> The International Association for the Properties of Water and Steam (IAPWS) is an international non-profit association which provides internationally accepted formulations for the properties of water. IAPWS-IF97 represents “Industrial Formulation 97”, which is recommended for the calculation of thermodynamic properties of ordinary water in its fluid phases. See <http://www.iapws.org/index.html> and Wagner *et al.* (2000) for further details.

## 3 Numerical modelling

### 3.1 Methodology

As detailed further in the thermal hydraulic modelling critical review (Laurence *et al.* 2019), the increased physical diversity exhibited by two-phase flows has led to a much broader range of modelling methodologies than that developed for single-phase flows. Two of the most widely used approaches, the Eulerian-Eulerian ‘two-fluid’ model (Section 3.1.1) and the Volume of Fluid (VOF) model (Section 3.1.2), have been utilized in this work. Each methodology handles boiling differently and is discussed in more detail in the following sections.

The transient simulations are computed using ANSYS FLUENT version 19.2. The imposed heat flux at the rod surface was linearly ramped up from  $q = 0$  [kW/m<sup>2</sup>] to  $q_w = 10$  [kW/m<sup>2</sup>] over the period of  $0 < t$  [s]  $< 2$  to aid numerical stability following issues experienced with the Eulerian-Eulerian approach. Following sensitivity studies a timestep of  $\Delta t = 0.001$  seconds was adopted for both approaches.

#### 3.1.1 Eulerian-Eulerian ‘two-fluid’ model

The Eulerian-Eulerian multiphase model treats both phases as continuous and interpenetrating, solving separate continuity, momentum and energy equations for each phase which are valid throughout the entire domain. The continuity equation for phase  $q$  can be written as:

$$\frac{\partial(\alpha_q \rho_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \vec{U}_q) = \sum_{p=1}^n (\dot{m}_{pq} - \dot{m}_{qp}) \quad 1$$

where  $\vec{U}_q$  is the velocity of phase  $q$  and  $\dot{m}_{pq}$  denotes the mass transfer from phase  $p$  to phase  $q$ . The volume fraction of phase  $q$ ,  $\alpha_q$ , is defined via:

$$V_q = \int_V \alpha_q dV, \quad \sum_{q=1}^n \alpha_q = 1 \quad 2$$

where  $V_q$  is the volume of phase  $q$ . The momentum equation, as solved by FLUENT, is:

$$\begin{aligned} \frac{\partial(\alpha_q \rho_q \vec{U}_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \vec{U}_q \vec{U}_q) \\ = -\alpha_q \nabla P + \nabla \cdot \bar{\tau}_q + \alpha_q \rho_q \vec{g} \\ + \sum_{p=1}^n (R_{pq}(\vec{U}_p - \vec{U}_q) + \dot{m}_{pq} \vec{U}_{pq} - \dot{m}_{qp} \vec{U}_{qp}) \\ + (\vec{F}_q^l + \vec{F}_q^{wl} + \vec{F}_q^{td}) \end{aligned} \quad 3$$

where  $\bar{\tau}_q$  is the stress-strain tensor of the  $q^{\text{th}}$  phase,  $R_{pq}$  is the interaction drag between phases,  $\dot{m}_{pq} \vec{U}_{pq}$  represents momentum transfer and  $\vec{F}_q^l$ ,  $\vec{F}_q^{wl}$  and  $\vec{F}_q^{td}$  represent forces due to lift, wall lubrication and turbulent dispersion respectively. The energy equation is written as:

$$\begin{aligned} \frac{\partial(\alpha_q \rho_q H_q)}{\partial t} + \nabla \cdot (\alpha_q \rho_q \vec{U}_q H_q) \\ = -\alpha_q \frac{\partial P}{\partial t} + \bar{\tau}_q : \nabla \vec{U}_q - \nabla \cdot \vec{q}_q \\ + \sum_{p=1}^n (Q_{pq} + \dot{m}_{pq} H_{pq} - \dot{m}_{qp} H_{qp}) \end{aligned} \quad 4$$

where  $H_q$  is the specific enthalpy of the  $q^{\text{th}}$  phase,  $\vec{q}_q$  is the heat flux,  $Q_{pq}$  is the volumetric rate of energy transfer between the phases, and  $H_{pq}$  is the inter-phase enthalpy.

Interfacial interactions between the phases are incorporated through the prescription of various source terms which, together with the volume fraction, couple the phased equations together. These terms require modelling and a wide variety of formulations have been presented in the literature (see, for example, Chuang & Hibiki 2017), varying in both complexity and applicability; many contain sub-models which utilize empirical correlations. Most require the interfacial area  $A_i$  to be determined, and this is also provided by a sub-model.

Those used within this study, which were chosen based on guidance provided with the solver (ANSYS Inc. 2018b), together with details provided in the literature accompanying the models are presented in Table 1.

Model	Solver code	Reference
Interfacial area, $A_i$	ia-symmetric	ANSYS Inc. (2018a)
Interfacial momentum transfer terms		
Drag, $\vec{R}_{pq}$	ishii-zuber	Ishii & Zuber (1979)
Lift, $\vec{F}_q^l$	tomiyama	Tomiyama (1998)
Wall lubrication, $\vec{F}_q^{wl}$	antal-el-al	Antal <i>et al.</i> (1991)
Turbulent dispersion, $\vec{F}_q^{td}$	lopez-de-bertodano	Lopez de Bertodano (1992)
Interfacial heat transfer terms		
Heat transfer (to vapour), $\vec{Q}_{lv}$ via $\vec{h}_{sl}$	ranz-marshall	Ranz and Marshall (1952)
Heat transfer (to liquid), $\vec{Q}_{vl}$	lavieville-et-al	Lavieville <i>et al.</i> (2005)

**Table 1: Interfacial area, momentum and heat transfer sub-models used within this study. Formulations as implemented in the solver can be found in the FLUENT Theory Guide (ANSYS Inc. 2018a)**

Wall boiling is modelled using an extended version of the Rensselaer Polytechnic Institute (RPI) wall heat flux partitioning model of Kurul and Podowski (Kurul & Podowski 1991), which can account for departure from the nucleate boiling regime. The RPI model is a mechanistic model which partitions the imposed wall heat flux according to the various physical mechanisms involved in the ebullition cycle:

- ▶ Vapour generation during bubble nucleation and growth;
- ▶ Wall-liquid transient heat conduction as cooler liquid replaces departing bubbles (quenching);
- ▶ Single-phase wall-liquid conduction at locations without bubbles; and
- ▶ Single-phase wall-vapour conduction.

In the baseline model, the temperature of the vapour is not calculated, but is fixed at the saturation temperature. Thus, in order to be able to model boiling up to the critical heat flux and post dry-out it is necessary to include the vapour temperature in the solution process. These mechanisms also require closing with sub-models, which themselves are based on varying levels of modelling. Table 2 details the sub-models used in this work.

Interfacial mass transfer (evaporation/condensation away from the walls) is directly dependent on the interfacial heat transfer and it is assumed that all of the heat transferred to the interface is used in mass transfer. A brief mathematical description of the extended RPI model is provided in Appendix A1.

Model	Solver code	Reference
Area of influence, $A_b$	delvalle-kenning	Del Valle and Kenning (1985):
Frequency of bubble departure, $f$	cole	Cole (1967)
Nucleate site density, $N_w$	kocamustafaogullari-ishii	Kocamustafaogullari and Ishii (1995)
Bubble departure diameter, $D_w$	kocamustafaogullari-ishii	Kocamustafaogullari and Ishii (1983)

**Table 2: Sub-models used within the RPI wall boiling model, see Appendix A.1.1.4 and the FLUENT Theory Guide (ANSYS Inc. 2018a) for more details**

### 3.1.2 Volume of Fluid (VOF) model

In contrast to the Eulerian-Eulerian model, the VOF model solves a single set of momentum equations within the domain and tracks the interface between the phases by solving an equation for the volume fraction. The phase present at any given location depends on the value of the volume fraction, and material properties are varied within the domain accordingly. For the liquid-vapour two-phase system under consideration here, the vapour volume fraction equation solved by FLUENT can be written as:

$$\frac{1}{\rho_v} \left[ \frac{\partial(\alpha_v \rho_v)}{\partial t} + \nabla \cdot (\alpha_v \rho_v \vec{U}_v) \right] = \dot{m}_{lv} - \dot{m}_{vl} \quad 5$$

where subscripts  $l$  and  $v$  denote the liquid and vapour phases respectively and  $\dot{m}_{lv}$  is the mass transfer from the liquid phase to the vapour phase (vice-versa for  $\dot{m}_{vl}$ ). The volume fraction is not solved for the primary phase (liquid phase) and is instead computed from the constraint:

$$\alpha_v + \alpha_l = 1 \quad 6$$

Material properties within the energy and momentum equations are determined by the presence of the component phases within each control volume. The density, for example, is computed as:

$$\rho = \alpha_v \rho_v + (1 - \alpha_v) \rho_l \quad 7$$

The momentum and energy equations take the same form as those used for single-phase flow; the reader is referred to the FLUENT Theory guide for more details (ANSYS Inc. 2018a).

Interphase mass transfer is handled through the Lee (2013) evaporation-condensation model. This is a mechanistic model which calculates the mass transfer rate ( $\dot{m}_{lv}$ ,  $\dot{m}_{vl}$ ) as a function of the difference between the local temperature and the saturation temperature.

If  $T_l > T_{sat}$  (evaporation), then:

$$\dot{m}_{lv} = \eta_E \alpha_l \rho_l \frac{T_l - T_{sat}}{T_{sat}} \quad 8$$

and if  $T_v < T_{sat}$  (condensation), then

$$\dot{m}_{vl} = \eta_C \alpha_v \rho_v \frac{T_{sat} - T_v}{T_{sat}} \quad 9$$

where  $\eta_E$  and  $\eta_C$  are coefficients that can be interpreted as a relaxation time and should be fine-tuned to match experimental data relevant to the case being considered. Since experimental data is not available for the case considered here, the default values suggested by FLUENT,  $\eta_E = 0.1$  and  $\eta_C = 0.1$ , are used.

It is important to note that the Lee (2013) model does not model wall boiling per se, it models evaporation/condensation at the liquid-vapour interface rather than nucleate boiling at the liquid-wall interface, as the RPI model does. The VOF model however, as primarily an interface tracking method, is more suited to resolving the morphology of the boiling front as it develops and travels down the rod. If the rate of mass transfer between the two phases can be correctly accounted for (in the first near-wall cell, and into the bulk fluid as the bulk temperature reaches saturation) then the method should, at least in principle, be able to reproduce the correct movement of the vapour front. It is included here to investigate how it performs as implemented currently in the FLUENT solver and to identify any potential routes for improvement.

### 3.1.3 Turbulence and near-wall modelling

Modelling turbulence within multiphase flows is considerably more complex than with single-phase flows owing primarily to the large number of modelled source terms within the multiphase momentum equations. Within the Eulerian-Eulerian framework ANSYS FLUENT provides several options for modelling turbulence in multiphase flows, including applying a turbulence model to the mixture as a whole, to just the dispersed phase, or to each phase separately. The former route is adopted within this work, utilizing the 'standard' high- $Re$   $k$ - $\varepsilon$  model of Jones & Launder (1972). This solves a single set of equations for the turbulent kinetic energy  $k$ , and its dissipation  $\varepsilon$ , using the mixture properties.

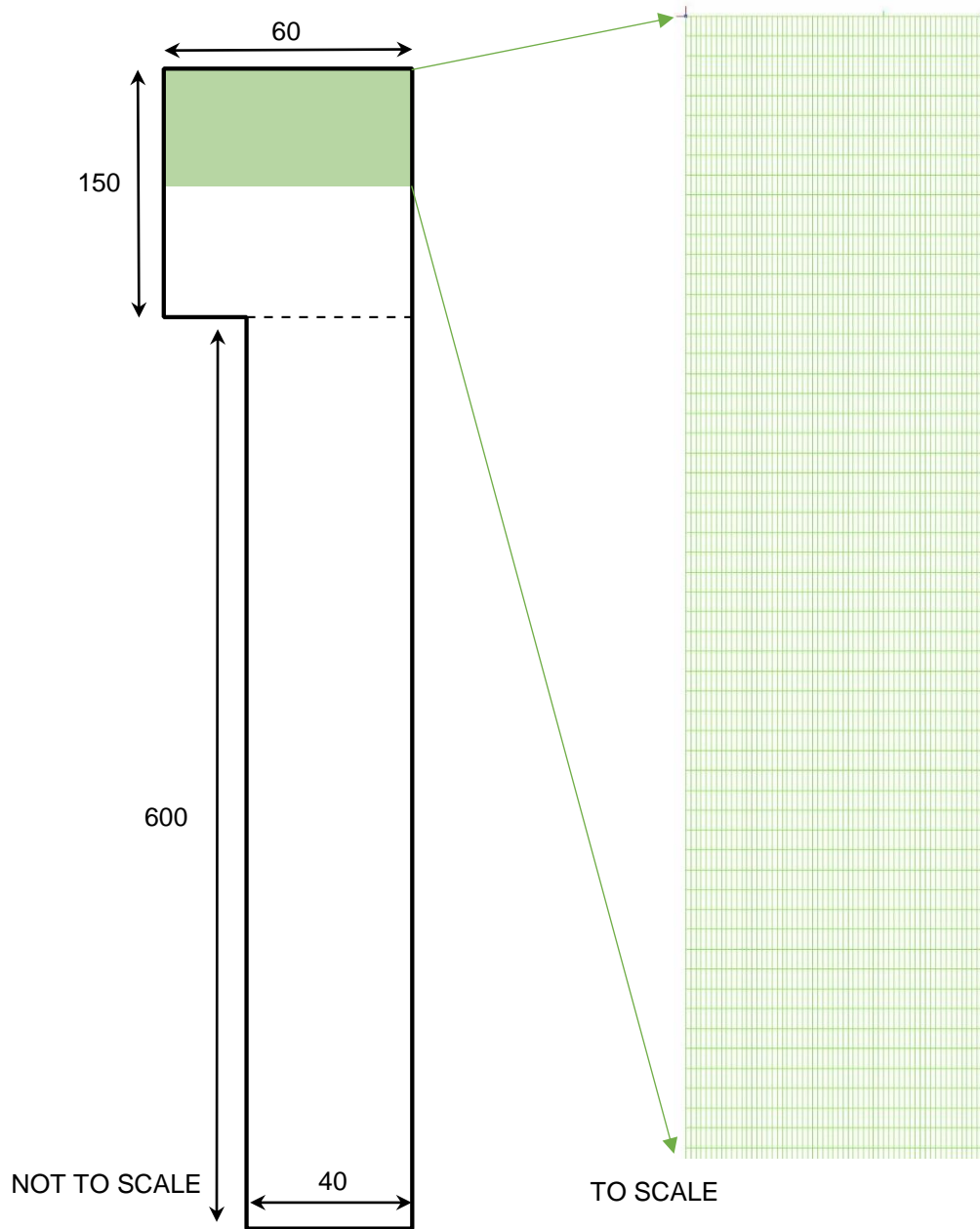
Within the VOF framework, the same turbulence model is adopted and a single set of turbulence equations is solved. Fluid properties are determined by the presence of the component phases within each control volume, as per Equation 7. Turbulent interactions between the phases are accounted for through a modification to the turbulent viscosity proposed by Sato and Sekoguchi (1975).

In the case considered, the flow is not driven externally and motion is only expected to arise from buoyancy. The density differences which cause this can arise both within a phase, due to single-phase natural convection, and between phases, owing to the significant density ratio between liquid water and its vapour. To account for the wide range of near-wall flow conditions this may create, so-called "scalable wall functions" (ANSYS Inc. 2018a) are employed which aim to avoid the deterioration of the standard wall function approach when the near-wall cell  $y^* < 11$  through introduction of a limiter in the calculation of  $y^*$ .

## 3.2 Mesh

A block structured mesh comprising 33,000 quadrilateral cells was created using ANSYS ICEM CFD v19.2. Owing to the large aspect ratio of the geometry, a significant number of cells was required in the wall-parallel direction to avoid the generation of large aspect ratio cells. The maximum aspect ratio in the final mesh was 4.05.

A schematic indicating the number of nodes, along with representative images of the resultant mesh, are shown in Figure 2. Uniform node spacing was employed.



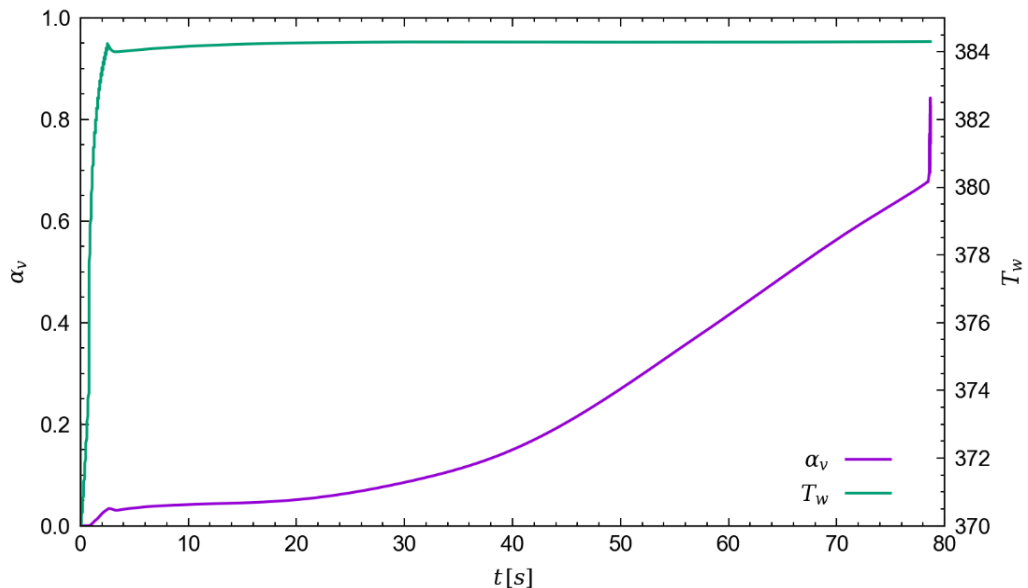
**Figure 2: Schematic of geometry with node counts (left) and blow-up of a section of the resulting mesh (right)**

## 4 Results

### 4.1 Eulerian-Eulerian approach

Figure 3 plots the time-history of the maximum vapour volume fraction and maximum wall temperature along the heated rod section up to  $t = 80$  [s]. Since the initial fluid temperature is a few degrees below the saturation temperature ( $T_i = 370$  [K]  $<$   $T_{sat} = 373.15$  [K]), there is initially no vapour generation. As the imposed wall heat flux increases to its nominal value over the first 2 [s] of solution time, the maximum wall temperature increases significantly, reaching a maximum of  $T_w \approx 384$  [K].

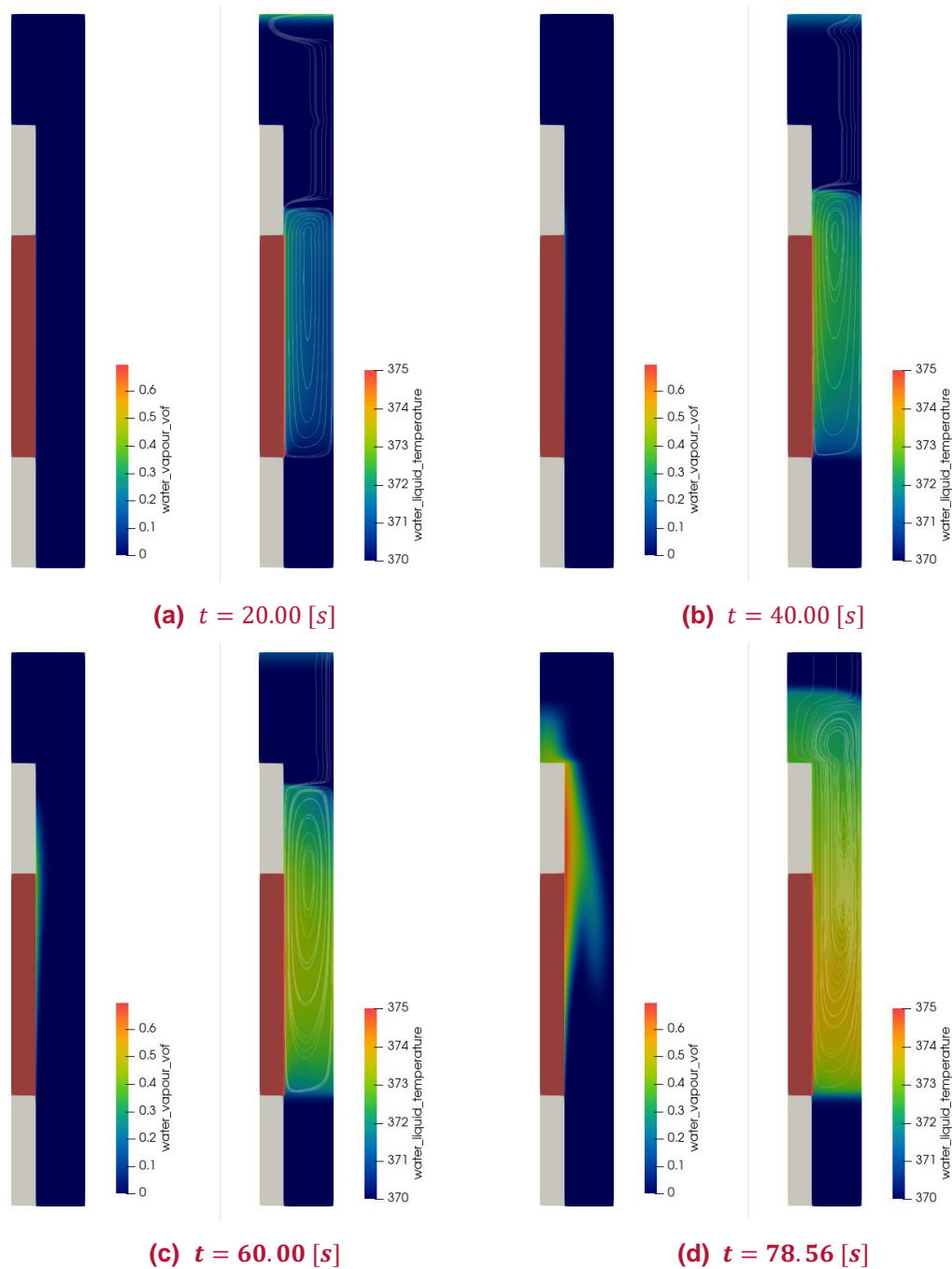
The vapour volume fraction time-history indicates that wall boiling commences after approximately 1 [s] of solution time, after which it slowly increases until  $t = 40$  [s] where it then appears to linearly increase until just before  $t = 80$  [s]. As the maximum wall temperature remains relatively constant during this period it indicates the vapour generation is due to nucleate boiling.



**Figure 3: Time-history showing maximum vapour volume fraction ( $\alpha_v$ ) and wall temperature ( $T_w$ ) along the heated section of the rod surface**

A large spike is observed in the vapour volume fraction at the end of the time period considered in Figure 3. Unfortunately, significant numerical instabilities were observed in the solution process at this point and prevented further solution of the case. Upon investigation, the instabilities appeared to arise whenever the vapour volume fraction at the heated surface became greater than 0.8; spurious values of vapour velocity were then observed which caused the solution to diverge.

Such high near-wall values of volume fraction typically indicate that vapour generation is predicted to be sufficient enough to start to prevent the wall surface from being completely wetted, and this would suggest a transition away from nucleate boiling. Whilst the extension to the RPI wall boiling model used in this work should, in principle, be able to account for this, the model still ultimately relies on the applicability and stability of the various sub-models, and the corresponding experimentally derived correlations, used within it (see Table 2). Further investigation, including a parametric exploration of the various sub-models, would be required to identify the precise reason for the instabilities.



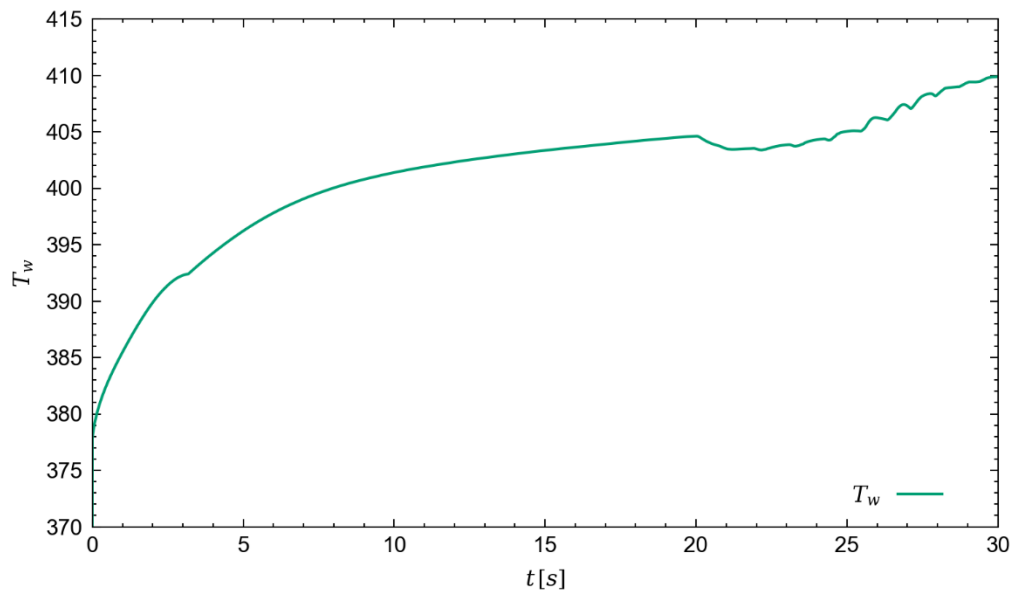
**Figure 4: Snapshots of vapour volume fraction (left) and liquid temperature (right), with liquid velocity streamlines superimposed, at selected time values for the Eulerian-Eulerian approach. Solid red to the left of the domain represents the heated rod and the vertical direction has been scaled by 0.15.**

To illustrate the behaviour of the flow during this period of nucleate boiling, Figure 4 presents snapshots of the vapour volume fraction and liquid temperature, with liquid velocity streamlines superimposed, at selected time values up to just before  $t = 80$  [s]. At the start of the simulation, the heat entering the domain leads to the establishment of a natural convection cell which extends from the bottom to just above the top of the heated rod section. This grows vertically upwards as the solution progresses, almost reaching the top of the rod section by  $t = 60$  [s].

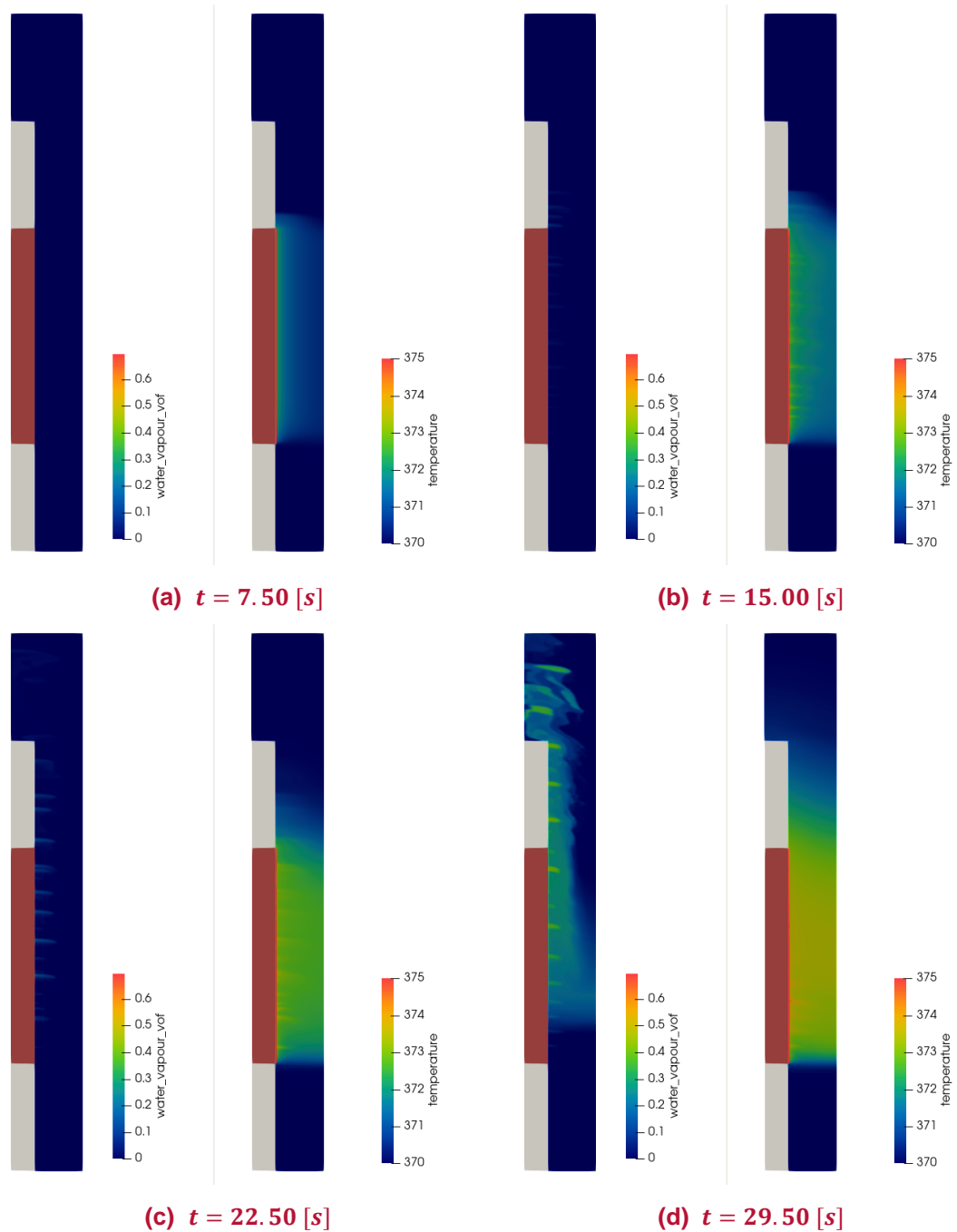
The cold plug at the bottom, beneath the heated section of the rod, remains unaffected. Solution playback (from which the snapshots in Figure 4 were taken) indicate that the RPI boiling model employed initially generates a number of small, but separated, regions of vapour very close to the rod surface. These slide up the rod but condense once sufficiently above the heated surface due to the still subcooled nature of the bulk liquid. As the near-wall liquid heats up, these vapour regions begin to merge to form a more contiguous region which eventually reaches the top of the rod section (Figure 4(d)). Vapour has not reached the top of the domain at the end of the simulated period (when the previously mentioned numerical instabilities occur) and thus the boiling front could not be captured.

## 4.2 Volume of Fluid approach

Figure 5 plots the time-history of the maximum wall temperature along the heated rod section and Figure 6 presents selected snapshots of vapour volume fraction and fluid temperature. The Volume of Fluid method, in contrast to the Eulerian-Eulerian approach, appears to produce finger like vapour regions which grow outwards into the fluid and move rapidly up the rod wall (Figure 6(c) and (d)). Vapour generation and condensation proceed at notably different rates between the two approaches, something which is partly attributed to the relatively un-tuned relaxation coefficients in the mass transfer terms present in the VOF model (previously discussed in Section 3.1.2). This is also apparent in the bulk of the domain, near the heated rod surface, where the volume fraction extends much further out from the rod in the VOF approach despite a lower liquid temperature.



**Figure 5: Time-history showing maximum wall temperature ( $T_w$ ) along the heated section of the rod surface**



**Figure 6: Snapshots of volume fraction (left) and temperature (right) at selected time values obtained with the Volume of Fluid approach. Solid red to the left of the domain represents the heated rod and the vertical direction has been scaled by 0.15**

Maximum wall temperatures, as shown by Figure 5, are also predicted to be significantly higher than those predicted by the Eulerian-Eulerian approach. This is believed to be due to the absence of a specific wall boiling model. In the RPI model used with the Eulerian-Eulerian approach the partitioning of the wall heat flux ensured it was consumed by the distinct physical processes known to occur during the nucleate boiling ebullition cycle.

With the VOF approach here, all of the heat imparted by the wall enters the near-wall cell and will initially serve to increase the fluid temperature. Once the cell temperature reaches the

saturation temperature, the mass transfer terms will then activate and the vapour volume fraction will increase to reflect this. However, the mass transfer terms, as discussed previously, contain a relaxation coefficient ( $\eta_C$  and  $\eta_E$  in Equation 8 and 9 respectively) which appears not to be adequately tuned for the case studied. Further study and experimentation would be required to compute suitable values of this coefficient. To properly account for vapour growth at the actual wall surface (i.e. at nucleation sites), additional user-defined models of this process would be required.

A further aspect of the VOF approach which hinders its applicability to the case considered here is its inherent design as an interface tracking method. This makes it ideal for capturing large well-defined interfaces between phases (such as the vapour boiling front which is predicted to occur as part of the case considered) but the individual vapour bubbles generated as part of the nucleate wall boiling process are far too small to be adequately reproduced with the mesh resolutions employed here. Use of a mesh with sufficient resolution would likely be computationally prohibitive for routine industrial computations.

Unfortunately, numerical difficulties were also observed during the solution process with the VOF approach, leading to divergence shortly after a solution time of  $t = 29.50$  [s] was reached (the final snapshot in Figure 6(c)). In this case, instabilities in the volume fraction equation (Equation 5) led to sudden divergence. Stabilizing techniques, including a reduction of time-step, reduction of under-relaxation parameters and a change in discretization method were not sufficient to enable further solution of the case. However, for the reasons outlined earlier, the distribution of the vapour volume fraction in the domain does not appear to be very realistic (Figure 6(c), for example) and it is feasible that some, or all, of the numerical instabilities could be related to this.

## 5 Conclusions

This report presents transient multiphase CFD simulations of a single heated rod immersed within a circular channel. The problem is solved as 2D axisymmetric using two multiphase modelling methodologies, the Eulerian-Eulerian and Volume of Fluid (VOF) approaches.

The two methods, as currently implemented within the commercial CFD package ANSYS FLUENT (v19.2), differ significantly in their approach to modelling multiple phases within the numerical domain and in how they incorporate mass transfer between the phases.

Both approaches predicted significant differences in both the spatial and temporal evolution of the vapour volume fraction once vapour generation (boiling) had commenced, but suffered from numerical instabilities which prevented a full solution from being achieved.

- ▶ With the Eulerian-Eulerian approach, the extended RPI wall-boiling model was initially able to capture subcooled nucleate boiling, predicting localized areas of vapour growing from the heated rod section before sliding up the rod surface and condensing once reaching the cooler bulk fluid. As the solution time progressed, the maximum vapour volume fraction at the wall increased, indicating the natural convection initiated by the heating was not sufficient to maintain steady vapour generation. Once the maximum vapour volume fraction reached around 60%, a sudden (unphysical) rise in vapour volume fraction, accompanied by spurious vapour velocity values, caused the solution to diverge.
- ▶ The VOF approach as implemented in FLUENT does not contain a specific wall-boiling model and instead uses an evaporation/condensation model to model mass transfer at the liquid-vapour interface. This led to both a distinct difference in the evolution of the vapour volume fraction, which extended much further away from the heated surface and into the bulk of the fluid, and significantly higher wall temperatures, as all of the imposed wall heat flux enters the near-wall cell fluid (as opposed to being partly consumed by nucleate wall vapour generation as per the RPI model). The resulting volume fraction did not appear in agreement with physical intuition and it is believed that this contributed to subsequent numerical instabilities which prevented further solution of the case.

Overall, a number of conclusions and recommendations can be drawn from this preliminary investigation:

- ▶ The Eulerian-Eulerian methodology coupled with the RPI wall boiling model is the most physically complete approach and is capable of predicting the subcooled boiling present in the initial evolution of the case. However, its ability to model the vapour boiling front could not be assessed due to difficulty obtaining numerical convergence.
- ▶ The Volume of Fluid methodology is (at least in principle) best placed to capture the complex morphology of the boiling front but this could not be assessed due to difficulty obtaining numerical convergence. It is not best suited to modelling nucleate boiling in cases where the mesh sizing prevents resolution of a discernible liquid-vapour interface. Further research is required to determine whether the effect can be modelled instead, as is done with the RPI wall boiling model.
- ▶ In general, the sheer number and variety of models and sub-models used within multiphase approaches is likely to be a source of confusion for engineers who do not have significant experience or expertise in the field.
- ▶ Multiphase CFD has not yet reached levels of maturity enjoyed by its single-phase counterpart and there is a clear need for continued research and development of both approaches considered here. This should be driven by the production of openly available high-quality experimental data.

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## ANNEX A - NUMERICAL MODELS

## A1 Eulerian wall boiling models

### A.1.1 Basic RPI model

The most well-known multi-fluid boiling model was developed by Kurul & Podowski (1991) from the Rensselaer Polytechnic Institute (RPI). It is a mechanistic model which supposes that the total heat flux from the wall is split according to the various physical mechanisms involved in the ebullition cycle:

- ▶ Vapour generation during bubble nucleation and growth;
- ▶ Wall-liquid transient heat conduction as cooler liquid replaces departing bubbles (quenching); and
- ▶ Single-phase wall-liquid conduction at locations without bubbles.

In the baseline model, the temperature of the vapour is not calculated, but is fixed at the saturation temperature. The wall heat flux is partitioned as:

$$q_w = q_C + q_Q + q_E \quad 10$$

where  $q_C$ ,  $q_Q$  and  $q_E$  are the liquid-phase convective heat flux, quenching heat flux and evaporative heat flux respectively. Models are required for each of these elements and they are considered in more detail below.

#### A.1.1.1 Convective heat flux

The convective heat flux,  $q_C$ , is modelled as:

$$q_C = h_C(T_w - T_l)(1 - A_b) \quad 11$$

where  $h_C$  is the single phase heat transfer coefficient, and  $T_w$  and  $T_l$  are the wall and liquid temperatures respectively. The heated wall surface is split into area  $A_b$ , which is covered by nucleating bubbles, and  $(1 - A_b)$ , which is covered by the fluid.  $A_b$  is referred to as the *area of influence*.

#### A.1.1.2 Quenching heat flux

The quenching heat flux,  $q_Q$ , is modelled as:

$$q_Q = \frac{2k_l}{\sqrt{\pi\lambda_l/f}}(T_w - T_l) \quad 12$$

where  $k_l$  is the thermal conductivity of the liquid phase,  $f$  is the frequency of bubble departure, and  $\lambda_l = k_l/\rho_l C_{p,l}$  is the thermal diffusivity.

#### A.1.1.3 Evaporative heat flux

The evaporative heat flux is modelled as:

$$q_E = V_d N_w \rho_v h_{fv} f \quad 13$$

where  $V_d$  is the volume of the bubble based on the bubble departure diameter  $D_w$ ,  $N_w$  is the active nucleate site density,  $\rho_v$  is the vapour density and  $h_{fv}$  is the latent heat of evaporation.

To close the above equations, models are required for the bubble departure diameter,  $D_w$ , the active nucleate site density,  $N_w$ , the frequency of bubble departure,  $f$ , and the area of influence,  $A_b$ .

#### A.1.1.4 Closure models

##### *Area of Influence*

This is expressed in terms of the bubble departure diameter and the nucleate site density, with a limiter to ensure numerical stability:

$$A_b = \min\left(1, K \frac{N_w \pi D_w^2}{4}\right) \quad 14$$

where the empirical constant  $K$  is based on the value proposed by Del Valle and Kenning (1985):

$$K = 4.8 \exp\left(-\frac{Ja_{sub}}{80}\right) \quad 15$$

and  $Ja_{sub}$  is the subcooled Jacob number:

$$Ja_{sub} = \frac{\rho_l C_{p,l} (T_{sat} - T_l)}{\rho_v h_{fv}} \quad 16$$

##### *Frequency of Bubble Departure*

This is calculated using the model by Cole (1967), which is based on inertial controlled growth:

$$f = \sqrt{\frac{4g(\rho_l - \rho_v)}{3\rho_l D_w}} \quad 17$$

##### *Nucleate site density*

The nucleate site density is usually represented by a correlation based on the wall superheat. The FLUENT solver suggests the model proposed by Lemmert and Chawla (1977), but this was found to cause numerical instabilities. Instead, the formulation by Kocamustafaogullari and Ishii (1995) is used, which was developed using existing pool boiling data.

$$N_w^* = f(\rho^*) (r_c^*)^{-4.4} \quad 18$$

where

$$N_w^* = N_w D_w^2 \quad 19$$

$$r_c^* = \frac{2\sigma T_{sat}}{\rho_v h_{fv} \Delta T_w} \quad 20$$

$$\rho^* = \frac{(\rho_l - \rho_v)}{\rho_v} \quad 21$$

and the density function  $f(\rho^*)$  is defined as:

$$f(\rho^*) = 2.157 \times 10^{-6} (\rho^*)^{-3.2} (1 + 0.0049\rho^*)^{4.13} \quad 22$$

##### *Bubble departure diameter*

The default bubble departure diameter model in FLUENT is that by Tolubinsky and Kostanchuk (1970), but this is based on a correlation determined from a subcooled flow boiling experiment. Instead, and consistent with the model for the nucleate site density, the formulation by Kocamustafaogullari and Ishii (1983) is used:

$$D_w = 0.0012 (\rho^*)^{0.9} D_{w,f} \quad 23$$

where  $D_{w,f}$  is the bubble departure diameter calculated with the correlation provided by Fritz (1935):

$$D_{w,f} = 0.208\phi \sqrt{\frac{\sigma}{g(\rho_l - \rho_v)}} \quad 24$$

Here,  $\phi$  is the contact angle in degrees and  $\sigma$  is the surface tension.

## A.1.2 Non-equilibrium and Critical Heat Flux RPI extension

In the basic RPI model, see Appendix A.1.1, the temperature of the vapour is not computed but fixed at the saturation temperature. To extend applicability beyond the subcooled boiling regime up to the critical heat flux and into post dry-out conditions the vapour temperature is included in the solution process. The heat flux partitioning, Equation 10, is extended to include heat transfer directly to the vapour phase:

$$q_w = (q_C + q_Q + q_E)f(\alpha_l) + (1 - f(\alpha_l))q_V \quad 25$$

where  $q_V$  represents the convective heat flux of the vapour phase and the function  $f(\alpha_l)$  depends on the local liquid volume fraction.

The vapour convective heat flux is computed as:

$$q_V = h_V(T_w - T_v) \quad 26$$

where the convective heat transfer coefficient  $h_V$  is computed based on the turbulent wall function employed.

The function  $f(\alpha_l)$  depends on the local liquid volume fraction and is computed in FLUENT with the formulation proposed by Tentner *et al.* (2005):

$$f(\alpha_v) = 1 - f(\alpha_l) = \begin{cases} 0, & \alpha_v < \alpha_{v,1} \\ \frac{1}{2} \left[ 1 - \cos \left( \pi \frac{\alpha_v - \alpha_{v,1}}{\alpha_{v,2} - \alpha_{v,1}} \right) \right], & \alpha_{v,1} \leq \alpha_v \leq \alpha_{v,2} \\ 1, & \alpha_v > \alpha_{v,2} \end{cases} \quad 27$$

where  $\alpha_{v,1} = 0.9$  and  $\alpha_{v,2} = 0.95$ .

## A.1.3 Interfacial Heat Transfer

Interfacial heat transfer is handled by considering heat transfer from the interface to the liquid and from the interface to the vapour separately.

### A.1.3.1 Interface to Liquid Heat Transfer

As vapour bubbles depart from the wall and move towards the subcooled region, heat is transferred from the bubble interface into the (cooler) liquid. This is computed as:

$$q_{lt} = A_i h_{sl} (T_{sat} - T_l) \quad 28$$

where  $A_i$  is the interfacial area and  $h_{sl}$  is the volumetric heat transfer coefficient. The latter is computed using the correlation of Ranz and Marshall (1952):

$$h_{sl} = \frac{k_l}{D_w} (2 + 0.6 Re_p^{0.5} Pr^{1/3}) \quad 29$$

where  $Re_p$  is the relative Reynolds number based on the bubble diameter and the relative velocity  $\vec{U}_l - \vec{U}_v$  and  $Pr$  is the Prandtl number of the vapour phase.

### A.1.3.2 Interface to Vapour Heat Transfer

FLUENT computes the interface to vapour heat transfer using the *constant time scale return to saturation method* of Lavieville *et al.* (2005). In this, it is assumed that the vapour retains the saturation temperature by rapid evaporation or condensation:

$$q_{vt} = \frac{\alpha_v \rho_v C_{p,v}}{\delta t} (T_{sat} - T_v) \quad 30$$

where  $C_{p,v}$  is the isobaric heat capacity and  $\delta t$  is the time scale set to a default value of  $\delta t = 0.05$ .

### A.1.4 Mass transfer

Vapour growth at the wall is applied at the cell near the wall and is determined by the evaporative heat flux,  $q_E$  (Equation 13). The rate of evaporative mass transfer is then:

$$\dot{m}_E = \frac{q_E}{h_{fv} + C_{p,l}(T_{sat} - T_l)} \quad 31$$

Interfacial mass transfer (away from the walls) depends directly on the interfacial heat transfer. Assuming that all of the heat transferred to the interface is used in mass transfer (i.e. evaporation or condensation), the interfacial mass transfer rate can be written as:

$$\dot{m}_{lv} = \dot{m}_{lt} + \dot{m}_{vt} = \frac{q_{lt} + q_{vt}}{h_{fv}} \quad 32$$

where  $q_{lt}$  and  $q_{vt}$  are defined as per Equation 28 and 30 respectively.

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