

## BOILING HEAT TRANSFER MODELLING A Review and Future Prospectus

by

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Review paper

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*This paper reviews the current status of boiling heat transfer modelling, discusses the need for its improvement due to unresolved intriguing experimental findings and emergence of novel technical applications and outlines the directions for an advanced modelling approach. The state-of-the-art of computational boiling heat transfer studies is given for: macro-scale boiling models applied in two-fluid liquid-vapour interpenetrating media approach, micro-, meso-scale boiling computations by interface capturing methods, and nano-scale boiling simulations by molecular dynamics tools. Advantages, limitations and shortcomings of each approach, which originate from its grounding formulations, are discussed and illustrated on results obtained by the boiling model developed in our research group. Based on these issues, we stress the importance of adaptation of a multi-scale approach for development of an advanced boiling predictive methodology. A general road-map is outlined for achieving this challenging goal, which should include: improvement of existing methods for computation of boiling on different scales and development of conceptually new algorithms for linking of individual scale methods. As dramatically different time steps of integration for different boiling scales hinder the application of full multi-scale methodology on boiling problems of practical significance, we emphasise the importance of development of another algorithm for the determination of sub-domains within a macro-scale boiling region, which are relevant for conductance of small-scale simulations.*

Key words: *boiling, boiling curve, nucleation density, phase interface, micro-layer, triple line, multi-scale modelling*

### Introduction

Boiling is a phase change phenomenon characterized by a rapid liquid vaporization and creation of discrete gas-liquid interfaces under conditions in which the heating wall is maintained above the saturation temperature of the boiling medium. Unlike many other thermal-hydraulic phenomena, boiling is not often encountered in nature. Scarce examples are related to the boiling of water due to heat released by a submarine volcano eruption, by hot rocks or magma present near the earth's surface or, in an extreme case, by a meteor falling in a large volume of liquid like a sea or an ocean. Although not having many opportunities to observe this natural phenomenon, somewhere along the way, humans discovered boiling and used it for cooking food. In old civilisations the boiling was used for sophisticated technical applications,

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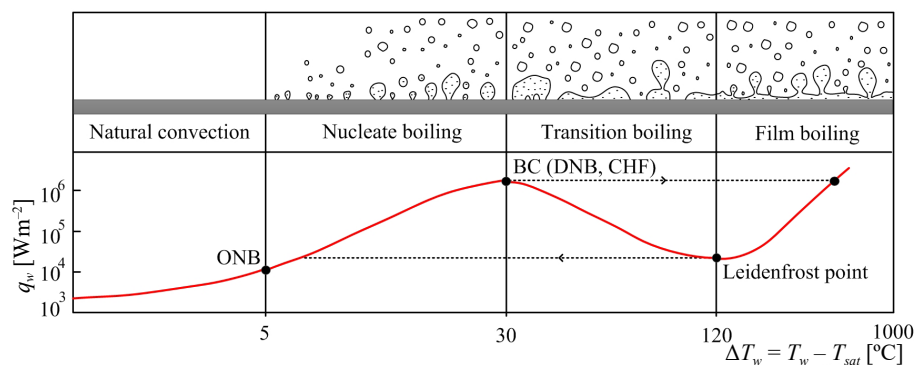
too. The oldest one is probably quenching of weapons mentioned by Homer around 800 B. C. [1]. The first precise technical record which dates to 130 A. D. notes the use of boiling to generate the steam for a turbine-like engine developed by Heron of Alexandria [2]. The commencement of vast boiling applications in industry and transportation is related to the 18<sup>th</sup> century and James Watt's invention related to the steam engine.

In modern times the boiling is due to its extraordinary thermal performance extensively utilized as a safe and reliable cooling method in various engineering applications such as power and chemical plants, industrial machinery, refrigeration systems, automotive engines, and electronic devices. Another widespread utilization of boiling is the steam generation in all kinds of the steam turbine based power plants (fossil-fired, nuclear, and solar) as well as in diverse chemical facilities involving vapour consuming technological processes. In addition, the development of compact technologies with high heat densities (such as high performance computers, hybrid vehicle power electronics, avionics, and space systems) has brought boiling anew into focus as one of the most promising candidate for an effective thermal management.

Regarding the boiling research, it is generally accepted that the only noteworthy study before the 20<sup>th</sup> century is the one reported by German medical doctor Leidenfrost in 1756 [3]. Investigating the boiling of water droplets on a hot metal surface Leidenfrost observed that the evaporation of a liquid droplet on an extremely hot surface took longer than on the surface with moderate temperature. The former case of boiling, which is now called Leidenfrost effect, is caused by creation of an insulating vapour film on the hot surface which prevents the liquid from the rapid evaporation.

A breakthrough in the studying of boiling happened in 1934 when celebrated Japanese scientist Nukiyama [4] invented the milestone of the boiling science – the boiling curve. The boiling curve, depicted in fig. 1, shows the relationship between the heat flux input and the wall superheat (defined as the difference between the wall temperature and the saturation temperature of the boiling fluid). Thorough investigations and improvements of the original work of Nukiyama showed that a slanting N-shape of the boiling curve remains alike for an assortment of boiling settings. Each leg of the boiling curve indicates one of the boiling regimes: nucleate, transition, and film boiling.

The nucleate boiling regime is peculiar for its enormous potential for transferring heat – in comparison to the single-phase flow, heat transfer is enhanced orders of magnitude enabling



**Figure 1. Boiling curve with the indication of two-phase mixture pattern over heated wall (heat flux and heated wall superheating temperature values are typical for water boiling; ONB – onset of nucleate boiling, BC – boiling crisis, DNB – departure from nucleate boiling, CHF – critical heat flux)**

small temperature differences between the heated surface and the coolant. However, after reaching the upper limit of the nucleate boiling leg, boiling crisis occurs (also known as departure from nucleate boiling or critical heat flux – CHF), and the boiling system can follow two paths. In power controlled systems any further increase of the wall heat flux leads to a sudden creation of a vapour layer over the heating surface and will cause a crossing straightaway to the third leg of N-shaped curve which represents the regime of film boiling. This jump from nucleate to film boiling regime is accompanied with a substantial increase of the wall superheat and can provoke a damage of the heating surface which is often referred to as burn-out. On the other hand, in temperature controlled systems any further increase of the wall superheat above the boiling crisis point will decrease the heat transfer rate and will lead to the transition boiling regime. The unusual negative slope of the transition boiling leg is caused by contact condition on the heating surface which changes from partial liquid film to a complete vapour layer. The point at which the transition boiling leg meets the leg of film boiling is known as Leidenfrost point.

When developing technical solutions that involve heat removal by boiling, engineers strive to reach heat flux magnitudes as high as possible, but to ultimately stay in the nucleate boiling regime. The reason for this is that everything on the boiling curve that occurs beyond the developed nucleate boiling, *i. e.* boiling crisis, transition regime and film boiling, can lead to a catastrophic event regarding the safety, reliability, and efficiency of the cooling equipment. In doing so, engineers are faced with a crucial problem regarding the absence of accurate and comprehensive predictive tools for boiling heat transfer. Therefore, although the functional dependence presented by the boiling curve and the phenomenological description of the boiling mechanisms that stand behind it are relatively simple, no universal theory or methodology for the prediction of heat transfer in different boiling regimes is reported by now.

In relation to this, to obtain an accurate boiling curve or at least its part related to the nucleate boiling up to the CHF point it is mandatory to perform experimental investigations for every design that involves a new combination of any of the numerous (~20) influencing parameters such as: a new pair of boiling fluid and heated wall material, a new geometry, dimensions and roughness state of the heated wall surface, a new range of process pressure, a new spatial heat load distribution, *etc.* Attempting to evade this costly and time demanding effort when designing various types of boiling equipment, research teams all over the World have developed a number of empirical correlations for prediction of boiling heat transfer coefficient and CHF values. It is probably not necessary to say that these correlations are valid only for a narrow range of specific boiling regimes. The situation with currently available mechanistic models of boiling is not much better, as none of them is free of empirical parameters which need to be carefully tuned on the basis of experimental data obtained for a narrow range of the aforementioned influencing parameters.

The main reason for the absence of generality and, therefore, the poor performance of available boiling models is that they do not incorporate a convoluted interplay of multiple time, velocity and length scales. Although being aware of this multi-scale nature of boiling for a long time, the researchers have undertaken the computational predictions of boiling on different scales as recently as the beginning of this century owing to the advances in small scale experimental techniques and powerful computational resources.

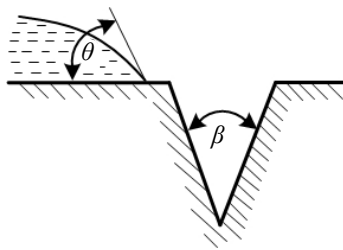
### **The most convincing arguments for performing future extensive boiling research**

This section deals with arguments for an extensive boiling research which needs to span the wide domain from the pure scientific field, in which the intriguing fundamental aspects

of boiling phenomena should be enlightened and formulated, up to the essentially practical one, in which predictive tools for engineering applications of boiling should be developed.

*Necessity for investigations of unresolved experimental findings regarding fundamental mechanisms of boiling phenomena*

For decades, it has been generally accepted that the bubble nucleation on the heated wall can be explained by the pre-existing nuclei (PEN) theory. According to the PEN theory the bubble nucleation is initiated by embryos of non-condensable gas entrapped in ridges (cavities, scratches, grooves) on the heated wall surface. Experimental evidence for this assumption was first provided by Clark *et al.* [5] and later on by numerous other researches. Theoretically, the gas entrapment in cavities on the heated wall was studied by Bankoff [6]. Bankoff considered



**Figure 2. Parameters which determine entrapment of gas in a conical cavity by an advancing liquid front: the cone angle  $\beta$  and wetting angle  $\theta$**

a liquid front with contact angle,  $\theta$ , which advances over an isolated conical cavity (defined with the cone angle,  $\beta$ ) and concluded that the gas entrapment in the cavity depends on two conditions:  $\theta > \beta$  and  $\theta < \pi - \beta$  (for notations of angles see fig. 2). When the first condition is satisfied and the second condition is not satisfied, the cavity will certainly entrap the gas. However, when both conditions are satisfied, the cavity may entrap either gas or liquid. In all other cases the gas will not be entrapped in the cavity. Activation of the gas embryos in cavities was studied by Griffitt and Wallis [7]. They derived a relation in which the wall superheat,  $\Delta T_w$ , necessary for incipient bubble nucleation depends on the physical properties of the fluid (like surface tension, specific volume change on vaporization, latent heat, saturation temperature), but also on

the radius of the cavity,  $r$ . The dependence of  $\Delta T_w$  on  $r$  is inverse – the larger cavities require lower wall superheats and *vice versa*. Based on these findings, the PEN theory was developed and further extended by Wang and Dhir [8].

The validity of the PEN theory was questioned by experimental results of Theofanous *et al.* [9], who investigated boiling of water on titanium film with root mean square (RMS) roughness of 4 nm and found the bubble incipience superheat of  $\sim 10$  °C. This value of the superheat is much lower than the corresponding one predicted by the PEN theory. The results confronting PEN theory were also reported by Qi and Klausner [10], who used ultra-smooth brass and stainless steel surfaces to induce boiling of ethanol or pentane and butane [11]. On the other hand, the same research team found that boiling of FC 72 on a nano-smooth silicon surface required much higher wall superheat of  $\sim 80$  °C [12]. Based on these results the authors assumed that the low superheats for boiling incipience are associated with metallic heating surfaces. However, the latest findings, published by Al Masri *et al.* [13] for the boiling of acetone on a smooth aluminum surface, opposed this conclusion.

Regarding the PEN theory, we note that the question about its validity is not new as one may get from the aforementioned contemporary papers. Moreover, some doubts about the validity of this theory had also been expressed in *old* papers from 1960s and 1970s. In this paper we would like to point out to the boiling investigations performed in former Yugoslavia in Boris Kidric Institute of Nuclear Sciences (now Vinca Institute of Nuclear Sciences) in Belgrade. For several decades in this Research Centre extensive, mainly experimental, boiling investigations had been conducted by an internationally recognized research team in which also number of master and Ph. D. students were involved. A comprehensive review of research activities with

historical aspects included is given by Spasojević *et al.* [14]. In the spirit of this paper, we will mention only investigations reported in international journal papers which deal with incipience of bubble. These investigations were conducted within former ambitious nuclear engineering research program.

The peculiarity of some conducted investigations is the use of ideally smooth heating surface with the goal to exclude the effects of surface roughness elements which according to the PEN theory serve as preferable nucleation sites. The ideally smooth surface was obtained heating the layer of mercury which prior to experiments was distilled to eliminate any impurities and air. Novaković and Stefanović [15] used water and ethyl alcohol at atmospheric pressure as boiling fluids and constructed corresponding boiling curves. The following low liquid superheats were measured at atmospheric pressure: for water  $\Delta T_w = 13.5\text{-}23\text{ }^\circ\text{C}$  within the heat flux range  $q_w = 29\text{-}125\text{ kW/m}^2$  and for ethyl alcohol  $\Delta T_w = 26\text{-}44\text{ }^\circ\text{C}$  for  $q_w = 5.81\text{-}69.73\text{ kW/m}^2$ . The visual and photographic study revealed that bubbles nucleated at preferred sites of the heated liquid surface similar to the situation on a rough solid surface. However, unlike the nucleation on a rough solid substrate, the bubble nucleation sites on the ideally smooth mercury surface exhibited irregular motion.

An extended study of the boiling on mercury surface was presented by Stefanović and Afgan [16] who considered four different boiling fluids: water, ethyl alcohol, benzene, and n-pentane. Similar to the results of Novaković and Stefanović [15] the superheats measured during boiling for all four fluids again did not show significant difference from those observed by boiling on surface of the solid heated wall. Based on these findings, the authors concluded that the effect of gas entrapment in surface cavities is overestimated by the PEN theory. Moreover, this effect should not be considered as predominant cause for low liquid superheats recorded by bubble nucleation on solid surfaces. Instead, the authors pointed out to the importance of violent liquid temperature and velocity fluctuations in the vicinity of the heated surface which could lead to high local superheats and initiate bubble nucleation. The importance of taking into account fluctuating and therefore statistical character of the superheat in the heated surface vicinity is widely discussed by Afgan [17].

A theoretical analysis of the aforementioned experimental results was presented by Ristić [18]. We would like to emphasise that Ristić, who founded our research group, was one of the pioneers in recognizing that the boiling phenomena needs to be analysed also from molecular dynamics (MD) point of view, especially because the MD simulations are nowadays increasingly getting on importance (see Section *Contemporary approaches for computational investigations of boiling on different scales: State-of-the-art and a critical review*).

Therefore, in [18] the liquid is supposed to be made of molecule clusters. A cluster is composed of individual molecules. When colliding with each other or with a solid body, the clusters reach an excited internal state. A sufficiently high excitation can cause a partial destruction (splitting), or a total destruction (vaporization) of the cluster structure. The theoretical analysis of bubble nucleation due to cluster interactions is based on the energy conservation laws during critical excitation (excitation sufficient to convert a unit of liquid mass into a vapour bubble). Two forms of energy balance equation are considered – the macro form and the molecular form. On the macro-level the supplied energy is used for a change in enthalpy and for increase of liquid superheat,  $\Delta T$ . On the micro-level this energy is transformed into a change of bond energy due to transition from liquid to vapour clusters, work done by vapour expansion and bubble surface energy. Assuming that only a miniature bubble of spherical shape can survive the interaction with surrounding liquid and serve as a nucleus and equating the two forms of energy balance, the limiting metastable liquid superheat is expressed in terms of surface en-

ergy,  $\sigma$ , change of bond energy,  $\varepsilon$ , and change of internal energy,  $u$ . Further,  $\sigma$  and  $\varepsilon$  are related by:  $\sigma = n_s \varepsilon$  where  $n_s = N_s/A_c$  is expressed through the number of molecules  $N_s$  in the liquid-layer around the nucleus of critical surface area  $A_c$ . The unknown  $N_s$  is assumed to be related to the total number of molecules within the nucleus  $v_c$  as:  $N_s = x v_c$ , where the variable  $x$  is function of fluid kind and temperature. The range of  $x$  values is estimated either from geometrical reasoning or by considering the limiting case in which the liquid superheat is zero. For water the following values are found:  $x = 1.4-4$  in the temperature range  $T/T_c=0.422-0.55$  ( $T_c$  is the temperature of critical point). Making use of the aforementioned relations, the author comes to the following expression for the liquid superheat  $\Delta T_w$  in the case of boiling on a heating surface:  $c\Delta T_w = cq/\alpha = (36\pi)^{1/3} \sigma(v''/mv_c)^{1/3} (1 - 1/x) - (u'' - u')$ , where  $c$  represents the specific heat,  $m$  – the mass of elementary particle, and  $v$  – the specific volume, while the states of saturated water and saturated vapour are indicated in the common way. It is noted that the liquid superheat  $\Delta T_w$  in the above expression represents temperature difference between the heating surface and the thin liquid-layer above the surface. In relation to this, the author notes that the temperature bulk has no effect on the bubble nucleation, *i. e.*  $\Delta T_w$  is not dependent on whether saturated or sub-cooled boiling takes place. The results for the liquid superheat evaluated by the above relation are compared with measured data published in the aforementioned paper of Stefanović and Afgan [16] as well as with data from other experimental groups (for references see the author's paper). An excellent agreement is reported.

Finally, we would like to shortly note that besides the aforementioned, another group of experimental evidence, which seeks for further investigation, is the role of nano-bubbles in the activation of the nucleation sites on polished surfaces. As an example we cite the work of Tyrrell and Attard [19] who observed that closely packed nanobubbles occur at the hydrophobic glass surface with 0.5 nm RMS roughness when it is submerged in water.

Therefore, summarizing the experimental findings presented above it is evident that the PEN theory is not complete because besides gas trapping some additional, currently unrevealed, bubble nucleation mechanisms exist which seem to be in close connection with micro scale mechanisms in the boiling fluid as well as with the nanoscale interaction between the boiling liquid and the heating surface.

#### *Urgency for more accurate modelling of boiling heat transfer due to development of novel technical applications*

An accurate modelling of boiling phenomenon is necessary for all situations in which boiling is dominant heat transfer mode. However, what makes the thorough boiling investigations absolutely essential at the moment is the recent global tendency in developing technical applications with high heat flux density for which boiling cooling systems are being considered as a replacement for the less efficient single-phase ones.

An example of the novel boiling applications are the compact heat exchangers with flow boiling in mini- and micro-channels which have been regarded as an outstanding heat removal solution in the wide field of technical applications such as computer and IT electronics, laser diodes, miniature refrigeration systems, insulated gate bipolar transistors (applied amongst others in ecologically friendly electric vehicles and wind turbines), fuel cells and hydrogen storage systems. The use of such heat exchangers could result in enormous energy savings. For instance, the energy consumption of large data centres in the USA in 2010 was estimated to be 82 billion kWh that is about 2% of the total electricity production [20]. The potential for an increase of energy efficiency in these centres by use of boiling based removal of hardware generated heat is evident when one takes into account that currently non-efficient chilled air

cooling technique consumes half of the aforementioned electricity amount [21]. Another novel technical utilization of boiling is related to the water-cooled fusion reactors in which the cooling components are exposed to plasma and, therefore, to one-sided heating with extremely high heat flux rates (*e. g.* in ITER\*, that is just an experimental device, heat loads as high as 5 MW/m<sup>2</sup> are expected according to [22]). Further, the understanding of new aspects of boiling phenomena in conditions of low gravity is indispensable for the design of cooling systems in powerful electronic packages for space applications [23]. Finally, we would like to emphasise that extensive boiling research will also have a positive impact on the scientific efforts directed to designing of techniques for boiling heat transfer enhancement and CHF delay as it will provide a basis for the assessment of the existing methods (*e. g.* use of micro/nano-structured surfaces, increase of surface wettability, addition of nanoparticles) and establish guidelines for the development of conceptually new ones.

### **Contemporary approaches for computational investigations of boiling on different scales: State-of-the-art and a critical review**

This section presents approaches currently used for computational investigations of boiling: macro-scale boiling models implemented in two-fluid approach with interpenetrating liquid-vapour phases, micro-/meso-scale boiling simulations by use of interface capturing methods, and nanoscale boiling simulations with MD methods.

#### *Macro-scale boiling models implemented in two-fluid approach*

The macro-scale boiling models focus on wall heat flux as this term plays a crucial role in the evaluation of the source term for vapour void. In contemporary CFD codes the wall heat flux is modelled applying the so-called partitioning approach. This approach is based on investigations of Bowring [24] who was the first to point out that different heat transfer mechanisms are involved within a complex boiling process: latent heat content of bubbles, liquid convection caused by bubble agitation, condensation at the top of the growing bubble and transient heat conduction during liquid flooding of the heating wall at locations previously occupied by growing bubbles. This observation led to the development of various boiling models which consider individual heat transfer mechanisms and on that basis partition the total wall heat flux in different components. In the following the most relevant approaches are presented.

Kurul and Podowski [25] formulated a scheme for partitioning wall heat flux that was the first one to be implemented in a CFD code. In boiling modelling community this approach, often referred to as RPI model, has been extensively used to compute either the pool or flow boiling situations in simple as well as in complex geometrical configurations. In relation to this, different variants of RPI model can be found in the literature: the original RPI based models and the modified RPI models. In line with the goal of this paper, we do not present details of all the published models, but only highlight the fundamental model formulations.

As a contemporary example of an original RPI based model we cite the paper of Gu *et al.* [26]. In this model the total heat flux from the wall to the boiling fluid is partitioned into three components: the evaporative, the convective and the quenching heat flux,  $q_w = q_c + q_q + q_e$ , while the heated wall surface area is fractioned into the one covered by bubbles,  $A_b$ , and the other one covered by the liquid phase  $A_l = 1 - A_b$ . The heat flux components describe the following physical phenomena. The convective heat flux,  $q_c$ , accounts for the heat transfer by forced convection between the wall and the liquid phase on the liquid covered wall surface. The

\* International Thermonuclear Experimental Reactor

quenching component,  $q_q$ , represents heat transfer occurring during liquid refill of the space previously occupied by bubble which detached from the heated wall. The evaporative heat flux,  $q_e$ , takes into account the latent heat for evaporation of the liquid phase *i. e.* for bubble nucleation and growth.

The heat flux components are formulated in the following way. The convective heat flux is expressed using common formulation  $q_c = h_c(T_w - T_l)A_l$  with single phase heat transfer coefficient,  $h_c$ , and the difference between wall and liquid temperature,  $T_w - T_l$ . Two-phase effects in this component are implemented through,  $A_l$ , which is formulated via bubble nucleation site density,  $n$ , bubble departure diameter,  $D_d$ , and an empirical constant which takes into account liquid sub-cooling as well as physical properties of boiling fluid. The quenching heat flux  $q_q = h_q(T_w - T_l)A_b$  is evaluated using the heat transfer coefficient,  $h_q$ , which depends on bubble detachment frequency,  $f$ , and physical properties of the liquid phase. Finally, the evaporative heat flux  $q_e = \rho_v V h_v$  is expressed as the product of vapour volume generated at the unit wall surface area and in unit time,  $V$ , vapour density,  $\rho_v$ , and latent heat,  $h_v$ . Note that  $V$  is formulated in terms of  $D_d$ ,  $n$ , and  $f$ . For clarity reasons, the aforementioned forms of heat flux components will hereafter be referred to as *standard*.

A modified version of RPI model is reported by Gilman and Baglietto [27] for the case of sub-cooled flow boiling. In this model an additional heat flux component,  $q_{sc}$ , is introduced, which accounts for bubbles sliding along the heated wall. The effects of sliding bubbles are multiple. First, a sliding bubble leads to disruptions of the thermal boundary-layer in which colder liquid penetrates and causes transient conduction in the wall. It is assumed that the component  $q_{sc}$  contributes to the total wall heat flux only during the time interval,  $t^*$ , when the thermal boundary-layer is disrupted. The determination of  $t^*$  is based on the use of Fourier and Biot numbers. The heat flux component,  $q_{sc}$ , is formulated through averaging of 1-D transient heat conduction in a semi-infinite medium over time interval,  $t^*$ . The relation for heat flux,  $q_{sc}$ , obtained in this way depends on nucleation site density,  $n$ , and bubble frequency,  $f$ , while the area affected by the sliding bubble is determined by using empirical relations for bubble diameter and sliding distance. During time intervals when the thermal boundary-layer is re-established, sliding bubble enhances forced convection. This effect is taken into account by splitting the forced convection component into two parts: the single-phase forced convection on the wall surface without sliding bubbles and the modified convection on the surface covered by bubbles sliding on re-established thermal-layer. In both parts the same heat transfer coefficient is used, which is evaluated considering bubbles on the wall surface as elements of surface roughness. Another effect of a sliding bubble is the intensification of evaporation due to the thinning of underlying liquid-layer. This effect is accounted for by introducing an additional term in the standard RPI evaporation component. The additional term is formulated in a similar way as the evaporation component due to bubble growth, but the volume of micro-layer below the sliding bubble is adopted to be relevant. The volume of the liquid-layer below the bubble is evaluated assuming its shape and thickness. Finally, the original RPI quenching heat flux component is replaced with a new formulation in which the *dry spot* in the heated wall below the bubble base plays the central role. This quenching component is defined as the function of temperature difference between heater material in dry spot region and the wall bulk region and the volume of the dry spot region. Both of the mentioned quantities are defined empirically.

Sateesh *et al.* [28] presented a wall heat flux model for the case of pool boiling on non-horizontal surfaces. To determine relevant heat flux components, the authors consider the effects of bubble mutual interactions using the parameter,  $R$ , which is defined as the ratio of area available per nucleation site and the projected area of a departing bubble. When  $R > 1$  the total



wall heat flux consists of natural convection term,  $q_{nc}$ , as well as of evaporative and transient conduction terms for both, the non-sliding bubble case ( $q_{me}$  and  $q_{tc}$ ) and the case with sliding bubbles ( $q_{mes}$  and  $q_{tcs}$ ). However, when  $R \leq 1$ , bubbles on the wall are closely packed, so that there is no space for bubble sliding and the bubble – bubble interaction takes place. In this case, heat flux components  $q_{mes}$  and  $q_{tcs}$  are neglected, while the sum of  $q_{me}$  and  $q_{tc}$  is weighted with a parameter which depends only on  $R(\text{water})$  or on  $R$  and reduced pressure (for propane and R113a). In a non-sliding bubble situation the evaporative component,  $q_{me}$ , and the transient conduction,  $q_{tc}$ , are formulated in the standard way. In the sliding bubble case the evaporative component,  $q_{mes}$ , is evaluated taking into account the volume increase of the sliding bubble due to micro-layer evaporation (which causes the increase of bubble diameter from the departure  $D_d$  up to the lift-off  $D_l$  value). Finally, the transient conduction during bubble sliding has the standard form in which the surface area available for heat transfer (expressed in terms of bubble diameter and bubble velocity) is determined by numerical integration during time period from bubble detachment up to bubble lift off. It is noted that evolution of bubble diameter and bubble velocity with time has been expressed by use of corresponding correlations.

In their wall heat flux model Hoang *et al.* [29] assumed that bubble dynamics mechanisms play a crucial role for a proper formulation of the evaporative as well as quenching component. In relation to this, the evaporative component consists of the following contributions: evaporation of the liquid micro-layer between the wall and the base of the growing bubble,  $q_{ev,st}$ , evaporation of additional micro-layer during bubble sliding,  $q_{ev,sl}$ , and evaporation of superheated liquid-layer surrounding the bubble,  $q_{ev,sl}$ . The quenching component accounts for transient conduction due to the standard liquid rewetting of the wall after bubble departure,  $q_{tc,rw}$ , and transient conduction in wakes of sliding and/or merging bubbles,  $q_{tc}$ . As the formulation of each of these individual contributions would introduce a lot of additional empirical parameters, all the evaporative terms and the quenching component,  $q_{tc,rw}$ , have been grouped and considered as the latent heat crossing the bubble surface,  $q_{lat}$ . The component  $q_{lat}$  takes into account the standard latent heat for evaporation, but also accounts for the condensation on the bubble cap once it comes into sub-cooled liquid domain. The heat transfer coefficient necessary for the evaluation of the latter term is obtained through recasting of available correlations and expressed as the power function of bubble diameter with a multiplier that depends on fluid properties as well as on bubble and liquid velocity. The fraction of heat transfer area available for condensation is derived from the averaged energy balance on the bubble interface exposed to the sub-cooled liquid. The transient conduction term,  $q_{tc}$ , is defined using the standard form as basis and taking into account that this heat transfer mode can be caused in different ways. Therefore, the transient conduction due to a sliding bubble starts after bubble detachment, while in the merger case it occurs right after the bubble growth phase. Comparing the maximum bubble diameter,  $D_m$ , with the spacing between active nucleation sites  $s = 1/n^{1/2}$  the sliding bubbles ( $D_m < s$ ) are distinguished from the merging ones ( $D_m \geq s$ ). Based on these considerations a factor which takes into account the influence area and the characteristic time periods of sliding / merging bubbles is formulated and implemented in the expression for the transient conduction heat flux component. Finally, the forced convection component is formulated in the standard way.

Different to other authors, who simply added different wall heat components, Chu and You [30] formulated the total heat flux as:  $q_w = (q_e \tau_g + q_q \tau_w) / (\tau_g + \tau_w) + q_c$  where the components associated with bubble generation and detachment (evaporation,  $q_e$ , and quenching,  $q_q$ , respectively) are weighted with relevant times (bubble growth,  $\tau_g$ , and bubble waiting,  $\tau_w$ , time). As pool boiling is considered, the heat flux component,  $q_c$ , is evaluated as natural convection. The starting form of all three heat flux components corresponds to the standard ones.

However, the authors further developed the model by using the fractal theory of porous media to characterise the distribution of nucleation sites on boiling surfaces. In this context, in all heat flux components the fractal distribution of bubble nucleation sites is implemented. This fractal distribution depends on the active cavity diameter as well as on fractal dimension of nucleation sites, which in turn are functions of wall superheat, the total number of nucleation sites, the minimum and maximum diameter of active cavities, the contact angle and physical properties of fluid. Developed in this way, the model does not need the correlation for nucleation site density,  $n$ . However, the correlations for bubble departure diameter,  $D_d$ , as well as for the bubble growth time,  $\tau_g$ , and for bubble waiting time,  $\tau_w$ , are necessary.

Finally, we outline the model for pool boiling on the horizontal heating surface developed in our research group. The model was established by Stosic and Stevanovic [31] and improved by Pezo and Stevanovic [32] and Stojanovic *et al.* [33]. Different to the aforementioned approaches, which using empirical correlations for nucleation site density,  $n$ , determine the integral vapour generation per unit surface and unit time, in our approach the locations of individual nucleation sites are specified by use of the following algorithm. First, the surface of the heated wall is divided into a distinct number of equally sized square zones and then the width of a zone  $b$  is derived from the geometric condition that one square meter is covered with  $n$  nucleation sites, *i. e.*  $b = 1/n^{1/2}$ . Further, each zone is divided into the finite number of control volumes, but the bubble can be generated only within one cell. This cell is chosen in a random way (by use of the generator of random numbers). The wall heat flux in our model is computed in the following way. The evaporative heat flux is evaluated at each bubble location as  $\dot{q}_e = \pi D_d^3 \rho_v h_v / (6\tau_g)$ , where the expression for bubble growth time,  $\tau_g$ , is derived combining empirical correlations of Fritz for bubble growth [34] and of Isachenko [35] for bubble detachment diameter. Obtained in this way  $\tau_g$  depends on contact angle,  $\theta$ , Jacob number, physical properties of boiling fluid and some empirical constants. The heat transfer from the wall to the adjacent liquid film in control volumes which do not contain an active bubble nucleation site is assumed to take place by thermal conduction. We would like to note that in cases of engineering applications with large boiling configurations, the present version of this model is applied at several discrete areas, since the zone width  $b$  must be small and the modelling domain could not cover the whole heated surface due to huge number of required computational cells. Values of the heat transfer coefficient on the surface outside the areas of boiling simulation are estimated by the interpolation of the computed values. We would also like to emphasise that from the research point of view, this model is peculiar as it represents a *bridge* between boiling scales. Therefore, our model represents a deeper version of a common macro-scale model as the positions of bubble nucleation sites and local evolution of void fraction can be observed. On the other side, this model is a *smearred* version of a micro-/meso-scale model (to be presented in Section *Micro-/Meso-scale simulations of boiling based on interface capturing methods.*) as evolution of the phase interface is not resolved.

Based on the aforementioned text, the status of macro-scale boiling models can be summarized as follows. Significant progress has been made in the development of macro-scale boiling models with formulations which are successfully implemented in computer codes for computations of boiling equipment from the real engineering praxis. Nevertheless, further efforts are necessary to develop improved versions of these models in order to overcome serious limitations associated with their accuracy, generality and reliability. In relation to this, current research activities are related to replacement of numerous empirically based relations for bubble departure diameter, nucleation site density, contact angle, bubble release frequency, *etc.*, as well as various empirical parameters with formulations derived from mechanical principles.

### *Micro-/Meso-scale simulations of boiling based on interface capturing methods*

The micro-/meso-scale simulations of boiling phenomena comprise splitting the flow domain into two regions: a micro-layer region which involves a thin fluid film between the bubble base and the heating surface and a meso-scale region in which the dynamics of one or more dispersed bubbles enclosed in the continuous phase is figured out by use of interface capturing methods. The micro- and the meso-scale regions are coupled by matching the heat and mass fluxes, temperatures and pressures at the outer edge of the micro-layer.

The first boiling computations by use of interface capturing methods were developed by Son *et al.* [36] for conditions of pool boiling in a 2-D domain with the constant temperature of the heating surface and saturated vapour phase. The meso-scale region is numerically solved by the Level Set (LS) method in which the phase interface is captured as a zero LS of a continuous function which is defined as a signed distance function. The formulation of the phase change model in meso-scale domain is based on the energy transfer across the interface (energy jump model) which accounts for the heat conduction only on the liquid side. The micro-region is divided into the adsorbed-layer, an extremely thin non-evaporative liquid film in the central part of the bubble base, and an evaporative layer with increasing thickness in the peripheral part of the bubble base. The model for micro-layer is formulated using the lubrication theory to set-up governing equations for mass, momentum and energy, Clausius-Clapeyron equation for the evaporative heat flux at the outer edge of the liquid film and capillary, disjoining and vapour recoil pressure to define the force balance at the phase interface. This approach gives a fourth-order ODE for the evolution of micro-layer thickness with bubble radius. The model was applied to simulate nucleate boiling of saturated water on a hot silicon surface and investigate the growth and dynamics of a single bubble by Son *et al.* [36], vertical merging of two bubbles subsequently generated at the same nucleation site by Son *et al.* [37] and lateral merging of 2 or 3 bubbles being attached to the heating surface by Mukherjee and Dhir [38]. The model was extended to three dimensions by Abarajith *et al.* [39] and applied to simulate bubble merging in high performance fluid PF5060 under low gravity conditions. Lee *et al.* [40] modified the model presented in [36] introducing an additional LS function, which represents a signed distance from the fluid–solid interface, and in that way replaced the original micro-layer model with a simplified version in which the constant slope of the liquid film thickness depends only on the apparent contact angle. The model was used to simulate the dynamics of a bubble nucleated in a small cavity. The final improvement of the model presented in [36] was made by Aktinol and Dhir [41] who implemented the conjugate heat transfer and incorporated the energy equation for the vapour phase.

The Volume-of-Fluid (VOF) method, in which the phase interface is identified as a sharp transition of the liquid volume fraction and reconstructed in a geometrical way, was first used by Kunkelmann and Stephan [42] for multi-scale boiling simulations. The model of the macro-region solves energy equations for both phases and includes the conjugate heat transfer. The phase change mass transfer is evaluated by the model of Tanasawa [43] in which the evaporative mass flux linearly depends on the difference between the interface temperature and the saturation temperature. The deviation of the interfacial temperature from the saturation one is expressed by the law proposed by Hardt and Wondra [44] which takes into account the evaporative coefficient (the portion of the molecules which leave the interface during evaporation) and distance from the heated wall. The micro-region was handled by the model of Stephan and Busse [45] which is formulated in a similar way as the one in [36], except that the vapour recoil pressure was neglected. This VOF based multi-scale simulation tool was utilised to compute

the growth and detachment of a single bubble in the refrigerant HFE-7100 on a steel heating foil. The model was significantly modified by Kunkelman and Stephan [46] who applied the commonly used energy jump model to account for the phase change at the interface and combined VOF and LS methods to provide a more precise interface reconstruction. This model was used to investigate nucleate boiling of the refrigerant HFE-7100. However, Herbert *et al.* [47] returned to the micro-layer model presented in [45] and extended it to account for the contact line motion during the impingement of a refrigerant F 72 droplet on a hot chromium surface. This version of the model was used by Sielaff *et al.* [48] to investigate horizontal merging of bubbles from two artificially controlled nucleation sites during boiling of refrigerant FC 72 on a stainless steel foil. A model very similar to the one presented in [42] was reported by Jia *et al.* [49]. The authors introduced a modified height function in the VOF method in order to improve the evaluation of interface normal vector and decrease spurious currents. The model was used for 2-D simulations of saturated nucleate boiling of the refrigerant R113 on the heating surface with constant temperature. Ling *et al.* [50] coupled VOF and LS methods to simulate 2-D boiling configurations with a single bubble, two isolated bubbles and bubble merger on a surface with constant temperature. To simulate the micro-region, the model of Ma *et al.* [51] was applied. In this model besides the evaporation, the liquid-flow into the thin film bordering on the adsorbed-layer is accounted for by steady Navier-Stokes equations in which the advection term is neglected. Using the order analysis the model is simplified to a system of five ODE which could be solved numerically.

The most recent method for micro-, meso-scale boiling simulations was reported by Sato and Niceno [52] and implemented in their own interface capturing method in which a colour function (CF) was used to identify the interfacial cells and a sharpening algorithm was applied to reconstruct the phase interface. The micro-region was simulated by the model of Stephan and Busse [45]. The model was used to compute a single bubble growth in initially quiescent saturated water. Lal *et al.* [53] also applied this model to compute nucleate boiling in the laminar water-flow along the heated wall with constant temperature. The model was modified by Sato and Niceno [54] who implemented conjugate heat transfer and introduced a new model for the micro-layer region. Therefore, arguing the validity of the micro-region model presented in [36], which results in an effective heat transfer only along the triple line, the authors developed a model in which heat transfer from the solid occurs across a definite area of the liquid film. The thickness of the film is determined taking into account only the evaporation mass transfer. The initial micro-layer thickness was assumed to linearly increase with the distance from the nucleation site, while the proportionality coefficient needs to be specified as an external parameter. Although the micro-layer can dry-out, for numerical reasons its minimal thickness of the molecular size order is prescribed. An advanced version of the model reported by Sato and Niceno [55] enables bubble nucleation from multiple sites by use of non-biased random number generator and turbulence modelling by use of Smagorinsky-based large eddy simulation model. The model was applied to simulate boiling regimes in which vapour bubbles are either discrete or coalesce to create vapour mushrooms. In their latest journal publication Sato and Niceno [56] used this model to perform a series of pool boiling simulations which span the range from nucleate to film boiling regime and include CHF occurrence.

The previous text shows that CFD simulations of boiling on micro-/meso-scales have made a great advance. This advance is, however, uneven – the development of efficient numerical schemes reached a mature level, but in the domain of physical phenomena the generally acceptable models have been developed neither for meso-scales nor for micro-scales. After a careful analysis we could identify the following problematic points:

- The immense problem of all micro-/meso-scale based boiling models is related to the bubble nucleation which does not occur due to physical reasons, but is a priori prescribed by placing a small *seed* bubble at an externally specified nucleation site. Moreover, the activation of the nucleation site is also done by specifying a priori the value of surface temperature which triggers bubble incipience.
- The models of micro-layer region also have serious drawbacks. The models based on lubrication theory assume unrealistic conditions of a steady-state, axisymmetric configuration and require the value of Hamaker constant to be specified as an external parameter. Besides the dependence on external parameters, the problematic issue with the simplified micro-layer models is that they are essentially empirical and in that sense do not have a potential for eventual extension regarding various boiling parameters and configurations.
- Another concerning point is the treatment of the mass transfer at the phase interface in the framework of meso-scale modelling. In most published papers the interface is assumed to be at idealised saturation temperature and the energy jump model is used to evaluate the evaporative mass flux. The only attempt to model phase change taking into account the heat resistance of the vapour-liquid interface was published by Kunkelmann and Stephan [42], which, unfortunately, was abandoned in the authors' later publications.
- The reported simulations of bubble merger process are associated with at least the following two problematic issues: bubble coalescence is modelled only numerically with no hint of physics - the merging of bubbles takes place as soon as the liquid-vapour interfaces shared the same numerical cell and when merging of the bubbles growing on the wall is considered, the micro-layer model developed for the single bubble is adopted in its original form without taking into account any complexity of liquid film which arises beneath the coalescing bubbles.
- Finally, turbulence effects are ignored in almost all reported models. In fact, only in the recent publications of Sato and Niceno [55, 56] turbulence is taken into account by use of large eddy simulation approach with Smagorinsky subgrid-scale model. As this model is originally developed for single-phase flows, it is questionable whether it is valid for the considered case of pool boiling. The reason for this doubt is the following. The rising bubbles cause specific fluctuations of liquid phase quantities even in adiabatic systems and when the liquid is originally stagnant. These fluctuations, named bubble-induced turbulence, are in many aspects quite different from the common single-phase turbulence. In the case of boiling it is to expect that fluctuations of fluid quantities are even more peculiar and of great importance as discussed in the Section *Necessity for investigations of unresolved experimental findings regarding fundamental mechanisms of boiling phenomena*.

#### *Molecular dynamics simulations of boiling*

Molecular dynamics simulations as a powerful tool for boiling investigations have emerged in past years and is increasingly getting on popularity in the USA, Japan, and China, but do not seem to have been spread to Europe to that extent.

Probably the most important advantage of this method is that the bubble nucleation site can be detected for different geometrical configurations and wettability conditions of the heated surface. Therefore, Yamamoto and Matsumoto [57] conducted MD simulations of water boiling on a smooth Cu wall and concluded that bubble nucleation occurs easier on a hydrophilic than on a hydrophobic surface. The results of Novak *et al.* [58] for the boiling of liquid argon on hot nanostructured surfaces show that bubble nucleation is not affected by defects smaller than the critical nucleus size ( $1-2 \text{ nm}^3$ ), but increases two orders of magnitude for larger indentations.

Another important nanoscale boiling distinctiveness which MD simulations can elucidate is related to the non-evaporating adsorbed liquid-layer. In this regard, Maroo and Chung [59] noted a large temperature gradient (9.64 K/nm) across the argon layer adsorbed to the superheated platinum wall, what makes it act as insulation. In their later paper Maroo and Chung [60] reported that the heat flux rate from the hot platinum wall before the creation of non-evaporating film ( $\sim 258 \text{ MW/m}^2$ ) is two orders of magnitude higher than those at the micro-scale, but is only sustained for a time period of ns order. The MD simulations of Ji and Yan [61] for the case of completely wetting argon on ideally smooth platinum surface show that the thickness of the adsorbed-layer decreases with the increase of wall temperature – from 2 nm for the temperature of 110 K to only one layer of densely packed molecules for the temperature of 210 K, while for the wall temperature of 600 K a deteriorated adsorbed-layer and argon molecules sparsely distributed among dry spots could be observed on the solid wall.

Explosive boiling of argon liquid films was investigated by Wang *et al.* [62] on a hot hydrophobic aluminum surface with and without nanoposts and by Diaz and Guo [63] on a Cu wall with different surface wettability, while the Leidenfrost-like phenomenon of rapid water boiling on Cu wall was investigated by Mao and Zhang [64] for a smooth and by Fu *et al.* [65] for a nanostructured wall surface. The results show a vapour blanket above the hot wall on which the water film levitates and a layer of non-evaporating water molecules being adsorbed to the heating plate no matter how long the heating process lasts.

Reconstruction of the boiling curve by MD simulations was conducted by Inaoka and Ito [66] for the boiling of liquid argon on a smooth wall and by Wang *et al.* [67] for boiling of water on the Cu wall with smooth and nanostructured surfaces. The MD evaluated nucleate and film boiling regimes for smooth surfaces capture typical heat flux trends, but the negative slope in the transition boiling regime could not be retrieved.

The MD simulations of flow boiling revealed an important phenomenon at the wall – fluid interface: a thermal slip (fluid temperature jump) observed by Toghraie Semiromi and Azimian [68] for the situation of argon flow boiling on a hot platinum wall and velocity slip reported by Nagayama *et al.* [69] for the case of non-thermal bubble nucleation in argon.

Another valuable information obtained by MD simulations regards the phase interface and is obtained by Dong *et al.* [70] who investigated the annular flow of Freon R141b between two solid silicon walls, the lower one being heated. The authors report violent fluctuations in temperature and surface tension interfacial profiles and the density profiles with the continuous transition from the liquid to the vapour zone. Analysing the density profiles the thickness of the phase-interface was found to get thicker with an increase in saturation temperature.

Although MD simulations can reveal distinct aspects of the smallest scale boiling mechanisms which are stumbling blocks for the CFD continuum boiling modelling (and remain elusive for currently available experimental techniques, too), they are not trouble-free. The most problematic issue is related to the computational domain size which extends from several nm to few dozens of nm. The only MD simulation which tackled a domain with a dimension of the micrometre order was reported by Inaoka and Ito [66], who applied strikingly powerful computational resources. Another problematic point in MD simulations is a reliable formulation of the potential function: for the real fluids like water or cryogenes where interatomic potential of a single molecule has to be formulated in addition to the complicated intermolecular force field, for the solid substrate especially for materials with the metallic bonding, and for modelling of intermolecular forces between the solid and fluid.

### Outline of future boiling research activities illustrated on an example of boiling modelling

The previous section shows that the current status of boiling heat transfer modelling is not satisfactory and that extensive boiling research activities need to be undertaken in the future in order to develop an advanced boiling predictive methodology. In our opinion, the most promising approach to reach this goal is the development of a complex methodology of a *universal* character which would be able to reflect the multi-scale nature of boiling mechanisms in various regimes.

Figure 3 schematically illustrates boiling mechanisms associated with different length scales which currently can be treated by scale specific computational methods. To develop an advanced boiling predictive methodology these methods need to be further improved and then linked to each other using a top-down approach regarding the scale size. In this approach the macroscopic two-fluid model would serve as a general framework in which numerous empirically based closure laws describing mechanisms from bubble nucleation up to phase-interface transfer processes, should be replaced with results obtained from boiling simulations on smaller length scales or relevant quantities derived from these results. The text below shows which information can be obtained from these simulations.

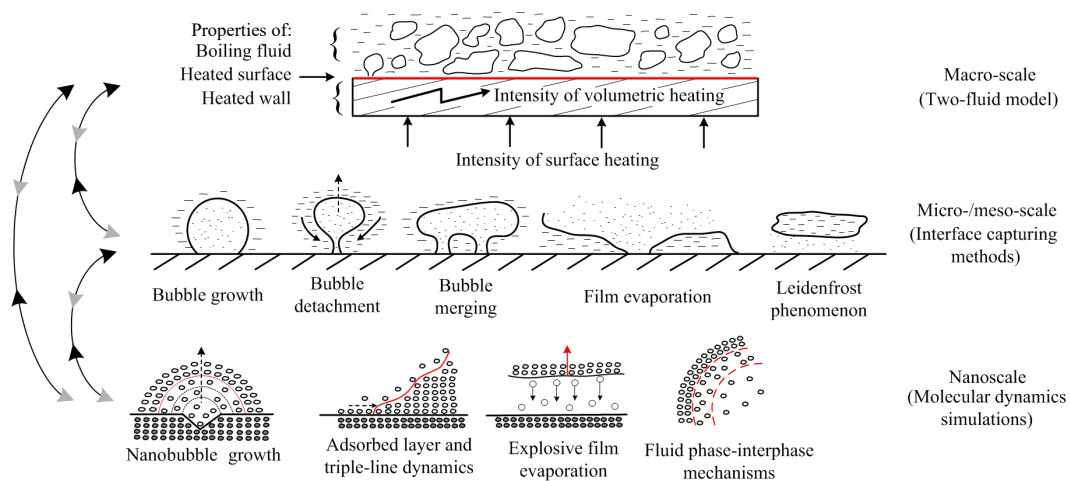


Figure 3. Illustration of boiling length scales and mechanisms associated with each of them

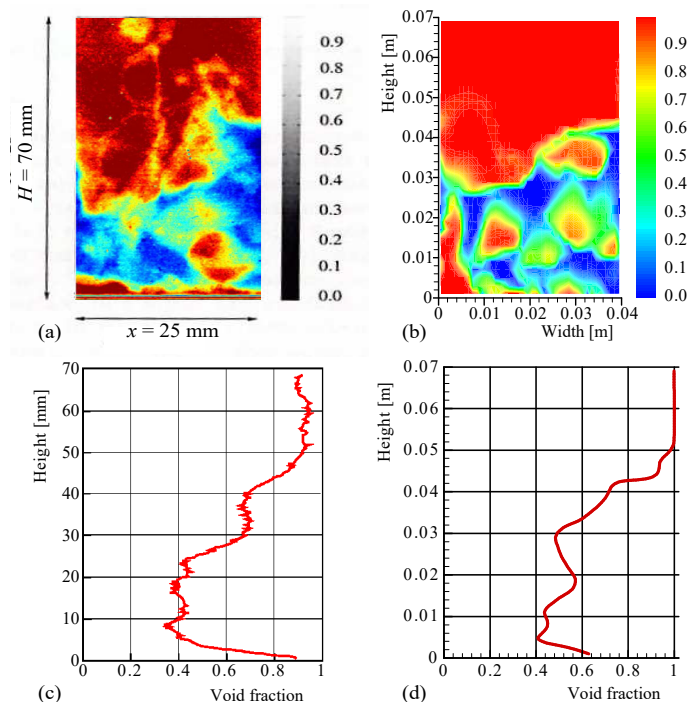
The MD simulations can provide insight into nanoboiling phenomena such as: activation of nano-bubble nucleation sites, nanobubble growth, liquid film dynamics in conditions of normal and explosive evaporation, motion of triple liquid-vapour-solid line and thermal properties of the liquid-layer adsorbed to the solid wall, evaporation of the liquid meniscus between bubble base and heated wall surface, stability of physical properties at the evaporating liquid-vapour interfaces as well as *thickness* of the phase interface and jump changes of thermal-hydraulic quantities across it. The information obtained by nanoscale simulations is particularly valuable because they cannot be retrieved by current experimental techniques.

The micro-/meso-scale simulations can deliver parameters which are related to the bubble growth and waiting time, the bubble departure diameter, the presence of liquid film patches at the wall, the impact of liquid lumps on the wall and the occurrence of Leidenfrost evaporation regime. The accuracy of micro-scale models can significantly be improved

by transferring the information obtained by nanoscale simulations. The most important improvements due to these data transfer should be visible in better formulation of conditions for activation of bubble nucleation sites, better modelling of the dynamics of micro-layer beneath the bubble base and better prediction of exchange mechanisms at the phase interface.

To emphasise the importance of the development of the aforementioned methodology, we highlight the stumbling blocks of current boiling modelling approaches. As example, we present computational results obtained by the model developed in our research group (see Section *Macro-scale boiling models implemented in two-fluid approach* for the model outline). The computations are set-up using experimental data reported by Theofanous *et al.* [71] for pool boiling on the horizontal heated wall. The boiling fluid is saturated water at atmospheric pressure. Computed and experimentally obtained results are compared in figs. 4 and 5.

In fig. 4 experimentally recorded data for vapour void distribution are compared with the computational results which are obtained specifying wall heat flux of  $1 \text{ MW/m}^2$  and nucleation site density  $n = 20 \cdot 10^4 \text{ sites/m}^2$  in accordance to the corresponding experimental evidence. Figure 4 shows that the model satisfactory retrieves the structure of two-phase mixture observed experimental-



**Figure 4. Radiographic image of void fraction [71] (a) and computed values [32] (b) and area averaged void fractions along the pool height (measured – (c), computed – (d))**

ly: qualitatively in the form of correct predictions of flow structure characterized with vapour blanket formation on the heater surface with vapour plumes rising upwards and highly distorted swell level and quantitatively in the form of acceptable profiles of mean vapour void fraction along the pool height.

Therefore, it is to conclude that we could fairly well predict nucleate boiling regime for a pool boiling configuration when the bubble nucleation site density,  $n$ , is correctly specified. But the crucial question is: How can we predict the bubble nucleation site density for an arbitrary boiling configuration regarding liquid – wall material combination, topology of heated wall surface and magnitude of applied heat flux?

The question seems dramatic as it asks for extremely complex information. However, to predict the boiling curve in general, particularly in conditions of occurrence of boiling crisis even more complex information on active vapour generation sites is necessary as explained in the following. Therefore, besides the bubble nucleation, significant contribution to the vapour



generation at the heated wall is due to intensive evaporation at triple lines of liquid patches that locally wet the heated surface. These liquid patches develop on the heated surface under conditions of high heat flux and high vapour void fraction when: an originally continuous liquid film comes apart and disperses into numerous liquid patches or when liquid droplets or liquid lumps from the core region of two-phase flow deposit onto the heated wall surface which originally has been dried out. The allocation of sites at which this evaporation mechanism takes place together with the distribution of bubble nucleation locations provides the total density of sites with active vapour generation.

From the aforementioned discussion it might be concluded that one of the main objectives of an advanced boiling predictive methodology comprises substantially new research activities for development of models that can predict the total density of sites with active vapour generation. In our opinion, these activities should be conducted within the framework of long-term projects. First, academic pool boiling situation with well-defined topology of heating surface and clean boiling medium should be considered and then in each subsequent step a degree of complexity should be added with the final goal to approach realistic configuration of boiling equipment.

Figure 5 presents boiling curves computed for the wide range of heat fluxes for two different heater configurations. In accordance with [71] these cases are denoted with A3 and A4. For the case of heater configuration A4 we performed computational analyses in which the contact angle,  $\theta$ , is considered as the parameter. It is noted that experimental data in [71] are obtained for the value of contact angle being in the range 60-75° as reported in [9]. Figure 5 shows that there is discrepancy between computational and experimental results for this  $\theta$  range and that this discrepancy increases with the decrease of  $\theta$ . However, increasing  $\theta$  to 90° leads to an excellent agreement between computed and measured data. Moreover, for the case  $\theta = 90^\circ$  the experimental results could accurately be retrieved in a wide range of heat flux values (up to 1.6 MW/m<sup>2</sup>) and for both heater configurations (A3 and A4). Assuming that the reported range of measured  $\theta$  values is correct, it is to conclude that the effects of contact angle  $\theta$  in the expression for bubble growth time are not formulated in a sufficiently precise way (for the corresponding relation see [32]). This situation is only one of examples which points out that mechanisms related to the bubble dynamics need to be put into focus of future research. The necessity for the formulation of these, as well as mechanisms governing mutual interactions of growing bubbles and their interaction with surrounding liquid, stresses the importance models of boiling on micro-/meso-scale for development of future advanced boiling predictive methodology.

However, there are more difficult issues in developing of an advanced multi-scale boiling predictive methodology. The main difficulty is related to the coupling of domains with different boiling scales because the development of appropriate coupling algorithms is at the

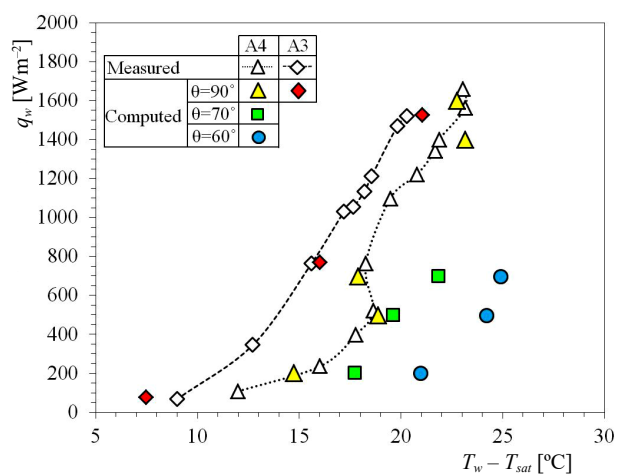


Figure 5. Computed boiling curves in comparison to the experimentally obtained ones reported in [71]

very beginning. In fact, the first attempts to couple MD simulations with continuum dynamics methods have been reported recently. The coupling is done by the introduction of a hybrid solution interface (HS interface) which matches the atomistic domain adjacent to the solid wall to the bordering continuum domain. In the paper of Mao *et al.* [72] HS interface is located at a fixed distance from the wall. In this way, the incipience and the initial stage of bubble growth are computed by MD simulations. As soon as the growing bubble penetrates HS interface, the VOF method switches on. Another path is followed by Zhang *et al.* [73] who accommodate the position of HS interface according to the location of the phase-change interface. In this way, the entire bubble growth is computed by MD simulations, while CFD is applied to compute liquid-flow containing larger length scales. Regarding the meso- and macro-scales, the authors are not aware of any publication in which the relevant computational methods are coupled for boiling case. However, the general approach reported by Weinan *et al.* [74] represents a basis for future developing of such methods.

Finally, we would like to emphasise that another difficult issue needs to be resolved if a multi-scale boiling methodology is intended to be applied for non-academic boiling configurations. This issue is related to the fact that the aforementioned length scales have drastically different time scales and, therefore, different time steps of integration. This means that micro- and especially nano-scale simulations are computationally extremely demanding and can be conducted only for the limited number of subdomains within the considered macro-scale boiling region. In relation to this, a tremendous effort is needed to develop a physically based algorithm for determination of the optimal spatial distribution of these small-scale subdomains.

## Conclusions

The review of the current status of computational boiling investigations shows that significant progress has been made in last years. This progress is mainly seen in improvement of closure relations for boiling heat transfer in macro-scale two-fluid approach, in developing models for micro-, meso-scale boiling simulations by use of interface tracking methods and in the application of MD simulations for investigations on nano-scale boiling mechanisms. Nevertheless, due to the complexity of the boiling phenomenon, all the aforementioned approaches have serious deficiencies and cannot provide reliable and accurate computational predictions of boiling heat transfer. For that reason, future research in this domain should be directed to development of an advanced boiling predictive methodology in the framework of a broad modelling approach, which takes into account the need for an accurate modelling of realistic boiling heat transfer situations in both, classical and emerging, technologies. In our opinion the advanced boiling predictive methodology should be based on a multi-scale modelling approach. In this approach, the computational domain should be divided into three regions: the region far away from the wall where the two-fluid model is applied to compute macro-scale boiling effects in liquid-vapour interpenetrating media; the region in heated wall vicinity where the continuum dynamics models are used to compute micro-/meso-scale effects of bubble dynamics; and the region at solid-fluid interface where the MD is applied to simulate nano-scale thermal-hydraulic as well as physical-chemical processes at the heated wall surface. The answer to the question how these scales should be coupled to each other is still not definite. Another issue which requires extreme research efforts is related to the development of algorithms for distribution of relevant small-scale sub-domains within a macro-scale region. The development of these methods is in its infancy and tremendous efforts should be made to achieve a robust and accurate boiling predictive methodology of a universal character.

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