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The development of the numerical method for simulation of metal material quenching

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Original scientific paper

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Abstract

Quenching is a general term for the rapid cooling of an austenitized hardenable steel or a solution treated aluminum alloy in liquid mediums with a boiling point lower than austenitization or annealing temperature. In this paper, an approach in development of a novel numerical method for computation of quenching of metal materials by immersion in liquids subjected to the Leidenfrost phenomenon has been described. Upon the known initial temperatures of the quenchant and the specimen, the numerical method by application of two-fluid VOF model solves the Stefan problem and the temperature distribution within the specimen in the first stage of quenching, in which the surface of the specimen is covered with the vapour film. The validation of the solution by comparison of the estimated temperature distribution with the experimental results from literature has been carried out, and the instantaneous distribution of the heat flow rate has been analyzed. The obtained results show the suitability of the suggested method for the numerical analysis of the initial phase of metal material immersion quenching.

Keywords:
Stefan problem; two-fluid VOF model; boiling flow; immersion quenching; heat transfer

1. Introduction

Sustainable development assumes the development, production and application of high quality, energetically more efficient and environmentally less harmful new products. The energy efficiency and the need for the reduction of the environmental impact are especially pronounced in the manufacturing and usage of the products that require transfer and conversion of huge amounts of energy and heat flow rates. These products are applied in power engineering, thermal- and process- engineering, metallurgy and manufacturing technologies such as casting, welding, hot deformation, heat treatment of metals, etc. In the manufacturing of such products, a series of mechanical, chemical, metallurgical and physical processes are present, that are in most cases induced by the thermodynamic processes inside the metal material and the heat and mass transfer at the surface of the material. The thermal energy that is appended to the metal material in the heating phase activates the processes of change in mechanical properties, microstructural changes, chemical reactions, diffusion processes, dissolution of the alloying elements, homogenization of the chemical compound, nucleation of new structural phases, and so on. Within the cooling phase, the heat removal from the metal material, in the majority of the technological processes, has to be carried out in a shorter period than the heating phase, while achieving the required desirable material properties and the product characteristics. The heat removal from the surface of the metal materials is determined by the thermal conductivity of the material and by the established temperature gradient from inside the material to its surface, and the heat transfer coefficient and the temperature difference between the surface and the cooling medium that is present around the object. In the description of the cooling process itself, the cooling of material at a rate higher than 1 K/s is usually termed quenching. By the application of liquids with a boiling point lower than the initial temperature of a cooled metal material, one may achieve intensive and rapid cooling, so-called quenching. The typical representatives of these liquids are water, water suspensions, quenching oils, oil-water emulsions and water solution of liquid polymers (e.g. poly-alkyl glycol, poly-vinyl propylene and similar ones). Each of the aforementioned cooling methods cool at a different cooling rate, thus giving them a characteristic cooling curve shape. How-

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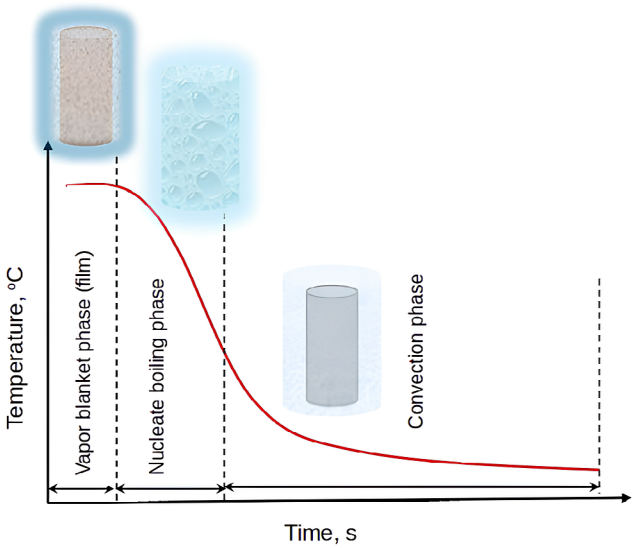

Figure 1: The schematic view of cooling characteristics for a cylinder surface in a liquid subjected to the Leidenfrost phenomenon

ever, they all have the presence of so-called Leidenfrost phenomenon in common, which consists of the vapour film phase, nucleate boiling phase and the convection cooling phase, schematically shown in **Figure 1**.

In industrial cooling processes, nucleate boiling is of significant importance for heat transfer efficiency, by means of which the highest removal of the heat flow rate is realized through the surface of a material at the relatively low difference between the surface and the cooling medium, thus resulting in high values of heat transfer coefficients. On the other hand, in the heat treatment of metals, due to extremely high heat fluxes, in the first stage of quenching a vapour blanket (film) is formed around the surface of an object, which acts as a thermal insulator and reduces the heat transfer from the surface of the object to the quenchant. Therefore, by different methods (circulation of medium, the addition of salt or nanoparticles and similar ones) one strives to shorten the vapour blanket phase and support the nucleate boiling phase. The convection phase appears after the heat flux through the specimen surface is insufficient to form bubbles and represents slow cooling without a phase change of the liquid at the contact surface with the cooled object. Due to the complexity of the mass transfer process, turbulent flow and thermodynamics and hydrodynamics processes, until now the mathematical model for a complete description of all three phases of Leidenfrost phenomenon has not been proposed.

The numerical modelling of the heat and mass transfer, within the context of the industrial application of cooling and quenching processes, implies the application of basically two types of methods for solving the multiphase flow. The first group are the so-called volume methods, such as Volume-of-Fluid (VOF) and level-set method (LSM), in which one obtains a detailed description of the phase interface, but the application of a fine resolution of the mesh in the vicinity of the interface, to adequately consider the interface in the computation. These methods are mostly applied within the fundamental numerical investigations due to the necessity of usage of high resolution meshes. The other group is formed by the averaged methods, in which through derivation of the mathematical model, the information about the interface is lost, and thus the interphase transfer is modelled via the source terms in the conservation equations. The mixture model (MM) and the Eulerian two-fluid model (TFM) are part of this group, and are applied on industrial scale domains (the applied studies) since those are less computationally demanding in the sense of the usage of the computational resources and time. A comparison of characteristics of the most commonly used multiphase flow computational models is shown in **Figure 2**.

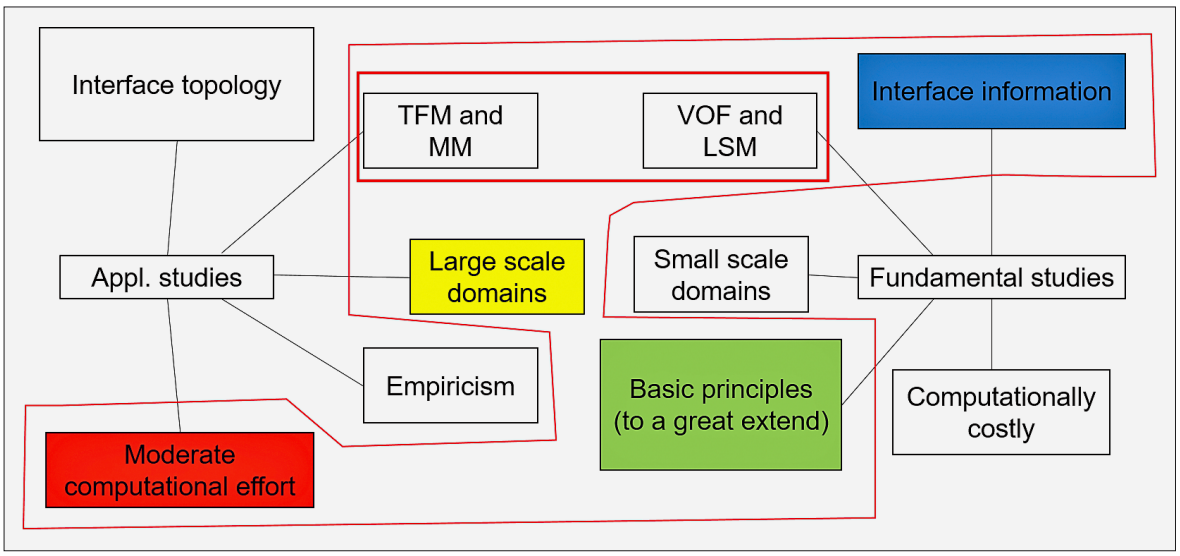

Figure 2: A comparison of characteristics of commonly used multiphase flow computational methods

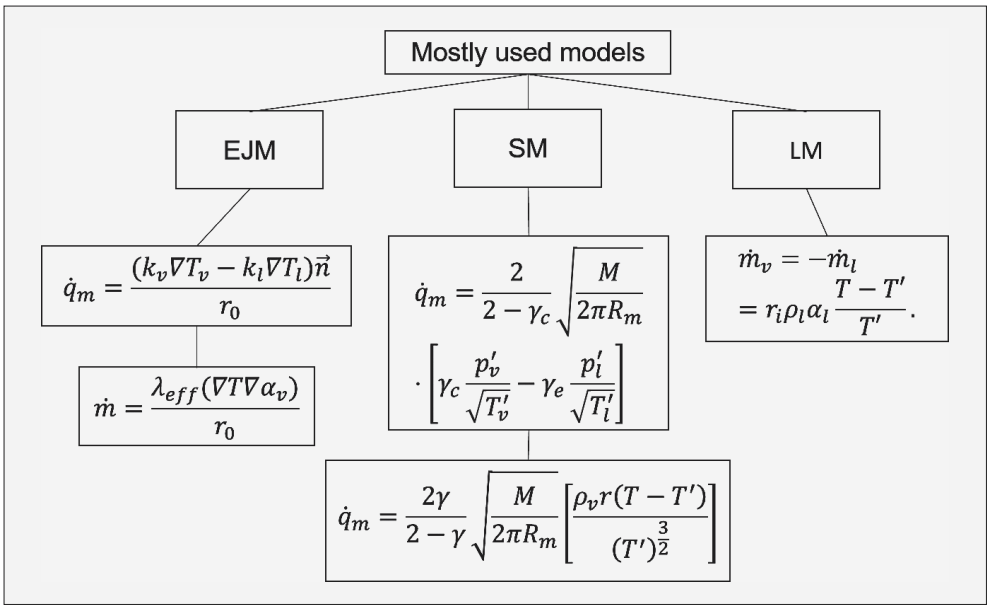

Figure 3: Most frequently used mass transfer models according to the review in **Kharangate and Mudawar (2017)**.

Since the mixture model is actually a simplified two-fluid model (the detailed description of the interphase transfer at the phase interfaces is omitted), in what follows, only the Eulerian two-fluid model would be applied for the computations in this study, in which it is necessary to involve additional correlations between two phases, the vapour and liquid phase, by means of which the interphase transfer of momentum and energy is described. In this model, the information about the interface position is lost, and this makes modelling of the boiling process difficult, e.g. in the heat treatment of the metal, i.e. the immersion quenching process of an austenitic steel in a pool or liquid bath. Therefore, within the framework of the present paper, a two-fluid formulation is combined with the VOF method. This Eulerian two-fluid VOF model combines the benefits of the VOF method in a sense that the interface is exactly described and keeps the property of the two-fluid model by allowing for the application of coarse meshes and longer time frames during the simulation.

By the review of the research studies that were carried out so far, it is evident that both types of numerical modelling of the multiphase flow were applied within the context of the immersion quenching modelling (**El Kosseifi, 2012; Srinivasan et al., 2010; Kopun et al., 2014**), while in the spray quenching, the Eulerian two-fluid model is used (**Subhash, 2017; Stark and Fritsching, 2015; Edelbauer et al., 2016**). The key role in all the multiphase flow computations is played by the mass transfer modelling at the phase interfaces. In the mass transfer modelling, the three main approaches are outlined, and are summarized in **Kharangate and Mudawar (2017)**: energy jump model (EJM); Schrage model (SM); and Lee model (LM). The graphical visualization of these models together with the equations for the computation of the mass transfer at the interface is schematically shown in **Figure 3**.

The energy jump model (EJM) shown in **Figure 3**, stems from the simple reasoning that is based on a continuum mechanics, and states that the heat flux that is transferred in a phase change process is equal to the difference of the conduction heat fluxes (Fourier's law) at both sides of the interface, that is described by the thermodynamically well-known Fourier's law. This kind of approach requires the definition of an initial vapour layer (in the boiling case) in the immediate neighbourhood of the specimen, due to the gradient of the vapour volume fraction that is present in the mass transfer equations, but it is not thereby necessary to involve in the equations the empirical coefficients or factors. On the other hand, the Schrage model (SM) shown in **Figure 3** is derived from the kinetic theory of gases and the so-called accommodation is necessary to define its application, in order to obtain accurate computational results. However, this model also requires the definition of an initial layer of a dispersed phase. The last Lee model (LM) noted in **Figure 3** by its definition does not require the definition of an initial dispersed phase layer, which makes this model suitable for phase change calculations in a bulk fluid. However, this model also requires calibration of an empirical coefficient in order to achieve satisfactory accuracy.

Hence, in this paper an approach that is the most similar to the energy jump method is applied because it phenomenologically describes the best boiling process of liquid mediums in immersion quenching. The presence of an initial vapour layer is justified by the fact that the goal of the paper is to model the film boiling in the immersion quenching process, that as a consequence causes a time shift of the results of the numerical simulations for the time required for the generation of a vapour blanket. By reviewing the research carried out so far, it has been confirmed by only a few cases, one of which has successfully resolved the advancement of an interface

using two-fluid formulation on a fundamental level. Therefore, in this paper, the development of a novel method for numerical computation of the heat transfer suitable for the mathematical modelling of the vapour blanket phase in the processes of immersion quenching of a heated steel in liquid quenchants subjected to Leidenfrost phenomenon would be described.

In contrast to a finite element method (FEM) based approach used in the simulation of quenching, presented for example in **Demirel (2009)** and **Steuer (2015)**, within the computational fluid dynamics (CFD) based technique there is no need for temperature input from the experiment, yet only the turbulence model and the initial temperatures of the solid specimen and a liquid bath are necessary to obtain a solution. Furthermore, using the CFD approach, one may gain insight in the temperature and flow fields, and the heat transfer coefficient is part of the solution, not an obtained input parameter, for example, by an inverse heat conduction analysis (IHTA).

Generally speaking, the advantage of the application of the present method is in consideration of the flow field, in particular the boiling process using the novel mass transfer model, in calculation of the temperature field in a solid specimen and, consequently, the corresponding integral quantities.

2. The method for calculation of the mass transfer due to energy jump at the phase interfaces

The successful numerical modelling of the nucleate boiling process, the same as the film boiling process, necessarily requires the efficient mass transfer modelling at the phase interfaces. In this paper, a novel method for computation of the mass transfer is suggested, based on the energy jump model, developed for a case of pure heat conduction in a vapour layer at the presence of one saturated (liquid in this case) and one unsaturated (vapour in this case) phase (e.g. saturated liquid and superheated vapour) and the thermal phase change model (TPCM), that is documented in **Ansys® Fluent (2019)**. With the suggested numerical method, an approximation is determined by the temperature gradient in the vicinity of the interface, whereby the distance from the neighbouring cell center to the interface is treated as the half width of an edge of a cuboidal control volume of a numerical mesh. This approximation is conducted via the application of the heat transfer coefficient, h_{pq}, that is available in the TPC model, as a fictitious variable by which the local cell length is included in the TCP model. The interface area density is calculated as the gradient of the phase volume fraction, by which the application of the constitutive relations at the interface is ensured. Furthermore, with this approach, one also ensures the behaviour of a two-fluid method similar to one of the single-fluid VOF formulation, i.e. the sharp distinction between the two phases, that is, the modelling of separated flow. The same behaviour of the numerical results has also been noted in the other methods, the algebraic interfacial area density (AIAD) method, that is suggested by **Höhne and Vallée (2010)**, and the large bubble method (LBM), suggested in **Denèfle et al. (2015)**. The suggested numerical method is implemented in the computational software Ansys® Fluent by using the user-defined functions (UDFs).

2.1. Mathematical model, boundary conditions and the software used in calculation

2.1.1. Mathematical model

The two-fluid model stems from, according to **de Bertodano et al. (2017)**, Landau's Nobel theory on the superfluidity of Helium II, and within this model the conservation equations are defined on a per phase basis, while the interaction between the phases is established via the source terms. These source terms that appear in the conservation equations are a consequence of an averaging process that has been applied to those partial differential equations, and as a consequence of the averaging process, the information about the interface is lost. The conservation equations underlying the phenomena studied herein one may find in **Drew and Passman (1999)**, and, written for k^{th} phase involved in a multicomponent system, they read:

- conservation of mass:

$$\frac{d}{dt}\int \alpha_k \rho_k dv + \oint \alpha_k \rho_k \mathbf{v}_k \cdot \mathbf{n} ds = \int \Gamma_k dv \tag{1}$$

- conservation of linear momentum:

$$\frac{d}{dt}\int \alpha_k \rho_k \mathbf{v}_k dv + \oint \alpha_k \rho_k \mathbf{v}_k \mathbf{v}_k \cdot \mathbf{n} ds =$$

$$= \oint \alpha_k \mathbf{t}_k ds + \int \left(\alpha_k \rho_k \mathbf{b}_k + \mathbf{M}_k + \Gamma_k \mathbf{v}_{ki} \right) dv \tag{2}$$

- conservation of energy:

$$\alpha_k \rho_k \left(\frac{\partial u_k}{\partial t} + \mathbf{v}_k \cdot \nabla u_k \right) = \alpha_k \mathbf{T}_k : \nabla \mathbf{v}_k - \nabla \cdot \alpha_k \mathbf{q}_k +$$

$$+ \alpha_k \rho_k r_k + E_k + \Gamma_k \left(u_{ki} - u_k - \frac{1}{2} v_k^2 + \mathbf{v}_{ki} \cdot \mathbf{v}_k \right) \tag{3}$$

where special attention in the present work, among other quantities, is made on the terms Γ_k that refers to the mass transfer due to the phase change, and $\mathbf{M}_k$ that involves the forces that act on phase k in the interaction with other phases that are present in the flows. The former has been modelled using the mass transfer model proposed in **Cukrov et al. (2021)**, while in the latter term, that stems as a consequence of the averaging process that is used in the derivation of the model equations, only the interphase drag is considered. The modelling approach applied to this end follows the exposure in **Strubelj et**

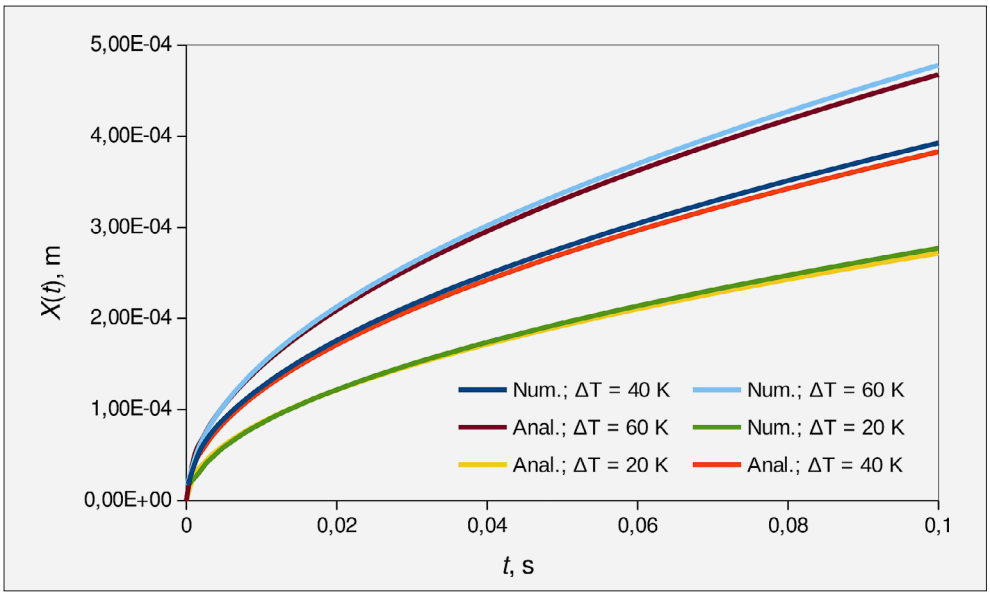

Figure 4: The interface position for different wall superheats. A comparison of numerical and analytical solutions.

al. (2009), wherein by the application of a huge value of the interphase drag, one may achieve equality of the phase velocities at the interface between the phases. Within the scope of the present work, it is done by the application of an anisotropic drag model available in the computational software Ansys® Fluent.

2.1.2. Boundary conditions

The standard Dirichlet and von Neumann boundary conditions were assigned to the boundaries of the computational domain, and are outlined in former publications (**Cukrov et al., 2021**; **Cukrov et al., 2023b**; **Cukrov et al., 2023a**). It is important to note that, due to the two conservation equations sets that are necessary to describe the two phase flow, it was mandatory to assign the boundary conditions for each phase separately, but also, for the mixture of phases where necessary. The communication between the solid and fluid part of the domain has been established using the "coupled" boundary condition available within the software Ansys® Fluent.

2.1.3. The software used in computation

The software used in the calculation performed herein is **Ansys® Fluent (2019)**, a commercial CFD code. The software has a relatively long history in the calculation of boiling phenomena. Starting from the work by **Sun et al. (2012)** different attempts were made to model the boiling processes using the mass transfer model that belongs to the EJM category of the models, that are physically the most correct since they came from the basic principles of the heat transfer applied at the interface. The real size cylindrical specimen has been, furthermore, studied in **Arévalo et al. (2014)**, using the derivative of the EJM in the film boiling simulation over a sphere. In the work by **Perez-Raya and Kandlikar (2018)** the necessity for the accurate evaluation of the temperature gradient at the interface in the software has been outlined, and a novel approach in the calculation of the distance between the so-called G-cell (gradient cell) and the interface has been proposed by the authors. Within the present study, the distance between the interface and the neighbouring cell center has been included in the model, and involved within the software via the UDF.

2.1. Method verification

The model for the estimation of the temperature distribution in a metal material on whose surface the Leidenfrost phenomenon tends to appear is verified by solving the Stefan problem, an unsteady advancement of phase interface; whereby the numerical simulation result is compared with the analytical solution of the position of the interface, $X(t)$, and the temperature distribution along the spatial x-coordinate. The computation is carried out on three different meshes: uniform quadrilateral, stretched quadrilateral and a hybrid mesh. The hybrid mesh was composed of non-uniform quadrilateral control volumes and triangular control volumes. The detailed description of the applied approach is given in the paper **Cukrov et al. (2021)**. For each of the mentioned mesh types, a mesh sensitivity study has been carried out for the obtained solutions, and the well-known assumption that by application of an Eulerian two-fluid model, the mesh resolution does not have a significant impact on the final result of the simulation. The same has been confirmed in the study conducted by **Gauss et al. (2016)**, while the irrelevance of the mesh resolution on the solution accuracy in the application of an Eulerian two-fluid model is stated in **Pointer and Liu (2017)**. The position of the interface for three different wall superheats is shown in **Figure 4**.

The obtained results using the proposed numerical method are in good agreement with the analytical solu-

tion, and reveal how an increase in the wall superheat advances the vapour layer at a higher speed. This is due to the higher temperature gradient at the vapour-liquid interface in the case of higher wall superheat.

2.2. Method validation

The Eulerian two-fluid model of an unsteady advancement of the vapour-liquid interface is validated using the experimental results available in **Momoki et al. (2007)**, that are obtained for a complete process of the cooling of silver in liquid water at the saturation temperature. The complete model validation process is given in detail in **Cukrov et al. (2023b)**, and is briefly explained as follows. In the numerical simulation conducted herein, the silver specimen is subjected to the saturated water-liquid with a thin vapour film that initially surrounds the specimen. The specimen is initially at 600°C, while the water-liquid is at 100°C. Furthermore, to induce the appropriate heat extraction from the specimen, the turbulent flow has to be considered in the domain. The calculation has been performed for approximately 10% of the total film boiling duration reported in **Momoki et al. (2007)** for the case of silver cooling in saturated water at an atmospheric pressure, that is, the total time in simulation was 15 s. During the film boiling modelling, the importance of turbulent flow modelling of the liquid around a vapour film has been noted. It was confirmed how the dispersed turbulence model, i.e. the turbulence model in which the conservation equations of the flow variables are solved only in the continuous phase, while in the dispersed phase the turbulence is modelled using correlation, adequately describes the physics of the film boiling process with conjugate heat transfer (CHT). Due to the complexity of the turbulent flow modelling for this case, the constant value of turbulent kinetic energy has been assumed in the domain, the so-called "frozen turbulence". The particular value of the turbulent kinetic energy is prescribed through the majority of the domain, with the exception of a cell layer in the vicinity of the cooled material; by which the laminar flow in the vapour film in the immediate neighbourhood of the object itself. On the basis of the conducted computations, it was confirmed that the turbulent kinetic energy value of 0.25 m^2/s^2 adequately models the conjugate heat transfer, because with this value, a satisfactory agreement of the temperature field in a solid (obtained by the numerical simulation) with the experimental results, for the first 15 s of the whole process duration is achieved. It was confirmed how by the application of a Kelvin-Helmholtz instability theory, one may obtain an adequate value of turbulent kinetic energy, using the relation derived in **Hillier et al. (2020)**, if one takes for the relative velocity, that is present in the numerator of that relation, the average flow velocity in a vapour film. The flow velocity in a vapour film is calculated from the boundary layer theory, presented in **Yamada et al. (2001)**, with an assumption of a smooth liquid-vapour interface, and that the velocity at the edge of the vapour blanket is equal to zero (no slip condition). It was noted that the turbulent viscosity coefficient, that is a flow quantity, ideally follows the course of vapour formation. This could be explained by the application of the strain rate tensor, that is present in the definition of the turbulent viscosity of the chosen turbulence model.

3. Numerical simulation of metal material quenching by immersion in a liquid

In this work, a computation of immersion quenching of a cylinder made from Inconel 600 superalloy is carried out, whereby the quenchant medium and the initial cylinder temperatures are known. A detailed description of the numerical procedure is available in **Cukrov et al. (2023a)**, and is briefly tackled herein. The two-fluid VOF method applied on a hybrid computational mesh that is composed of the quadrilateral and triangular cells required a change from the cell based to a node based interpolation, after the initialisation of the dependent variables in the domain has been made. In the studied case, the subcooled liquid at the temperature 60°C is considered, and it is, for the sake of simplicity, assumed the same temperature for the surrounding medium inside which is the specimen prior to immersion. It is important to note that, for the sake of simplicity, the material chosen as the surrounding medium above the free surface of the liquid has the properties of the water-vapour, and that its temperature is 60°C. This way the mathematical model is simplified because it is not necessary to involve an additional set of the equations for modelling the heat transfer to the surrounding air. Otherwise, another set of conservation equations for air would be needed, that would further slow down the computation. This assumption is justified due to significantly low values of the heat transfer coefficients from the heated solid (temperatures higher than 800°C) to the surrounding medium. Furthermore, in this way in the numerical method applied herein, a temperature uniformity is established through the computational domain and, hence, the mass transfer across the large scale liquid-surrounding medium interface cannot be induced by the temperature gradient because the bath and the surrounding medium are at the same temperature

The cylinder made from Inconel 600 is initially at the temperature 855°C, that is in agreement with the ISO 9950 standard, that prescribes the conditions under which this experiment should be carried out. Together with the already mentioned values, the initial temperatures of the quenchant and the specimen, the turbulent kinetic energy value 0.1 m^2/s^2 is also prescribed, upon the basis of the former investigations. The two zones, with respect to the flow regime (turbulent or laminar) were defined in the domain. The first is interface zone 1, that surrounds the surface of the specimen and is only one cell layer in the vicinity of the specimen. Inside this

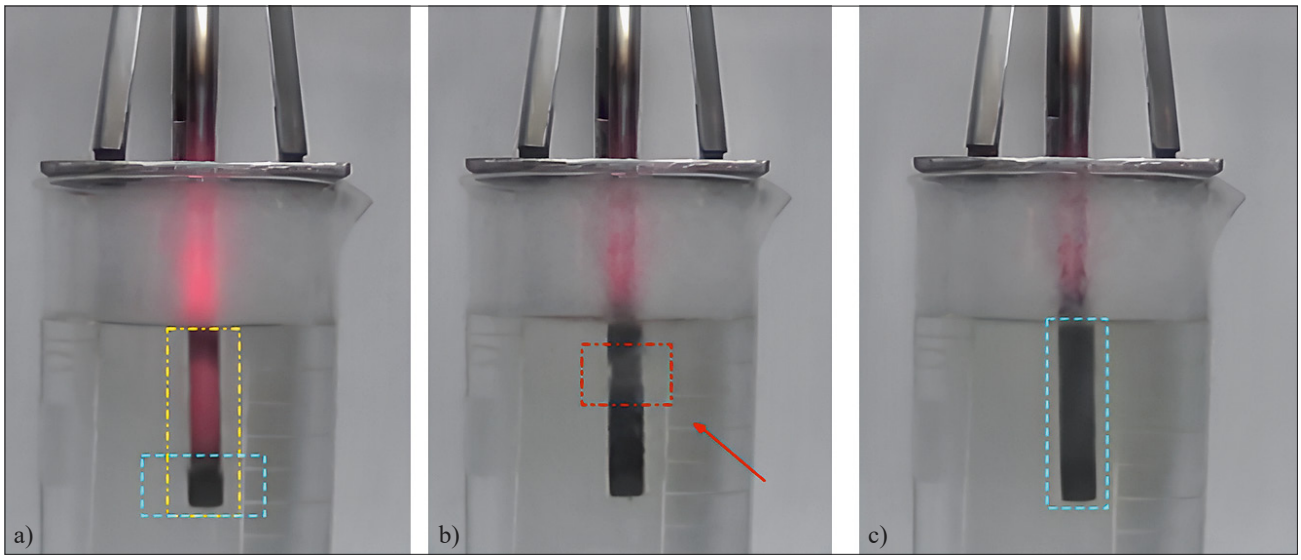

Figure 5: The advancement of a rewetting front during quenching of Inconel 600 alloy in liquid water of an approximate temperature of 52°C.

zone, the laminar flow is assumed, i.e. the turbulent kinetic energy tends to its zero value.

The other zone embraces the area in the immediate neighbourhood of an object itself, but not zone 1, and inside it the already mentioned values of turbulent kinetic energy are defined. In the remainder of the domain, the laminar flow is assumed, in the same way as described for the interphase zone 1. Also, the moving mesh method with the topological change has been applied, that is, during the mesh motion (of the object) the new cells are generated and some existing ones are being erased, while the results are being interpolated from the old mesh to a new one. The specimen is immersed at a constant speed of 0.13 m/s. For the motion of the specimen in the numerical simulation, an arbitrary Lagrangian-Eulerian approach has been used, in which inside of each computational domains, an Eulerian set of equations is being solved (tracking changes inside a control volume), while the boundary between the two domains is described with the Lagrangian formulation (tracking the motion of the material volume). A special feature of Inconel 600 nickel superalloy is that the change of the physical properties, the thermal conductivity, λ_s, and the specific heat capacity, c_s, is well reproducible with respect to the specimen's temperature; that has to be taken into consideration in the calculation. The material is of significantly high thermal effusivity, and hence, during the immersion quenching, all the Leidenfrost evaporation regimes are present (e.g. film and nucleate boiling, and the convection heat transfer).

For the purposes of the qualitative analysis of the temperature field inside the material and the behaviour of the vapour blanket, an experiment with an approximate temperature of liquid water at 52°C has been carried out. Thus, the behaviour of the vapour blanket is shown in **Figure 5**.

Hence, in **Figure 5a** one may note the presence of spatial temperature gradients inside the material due to the non-uniform temperature distributions, i.e. the presence of the zones with the higher temperature (outlined red colour of the material) and dark zones with the lower temperatures (denoted with the yellow dash-dot line). This implies the case $Bi \rightarrow +\infty$, when the temperature gradients with respect to space are significant in the solid. Furthermore, **Figure 5a** (blue dashed rectangle) reveals the incipience of the wetting front at the bottom side of a specimen. By the advancement of the rewetting front, as shown in **Figure 5b**, one may note its existence at both sides of a specimen. Finally, film boiling has finished when the wetting fronts meet each other, as in **Figure 5c**. Since these photographs were made at the bath temperature of 52°C, these observations are qualitative in nature. For a rigorous comparison of the numerical method capabilities in estimation of the transient temperature distribution in the center of the specimen, the experimental results obtained for the water-liquid at 60°C, that are available in **Landek et al. (2014)**, have been chosen within the scope of the present research.

4. Results

In contrast to the study **Cukrov et al. (2023a)**, in which the temperature from the center of the specimen was obtained with numerical simulation, compared with the results available in **Landek et al. (2014)**, in this research an additional comparison with the measurement data available in **Cremonini (2014)** has been carried out. The results in **Cremonini (2014)** were also obtained with the liquid water at the temperature 60°C, but in that investigation a distilled water was used. The unsteady temperature distribution in the center of the specimen is shown in **Figure 6**.

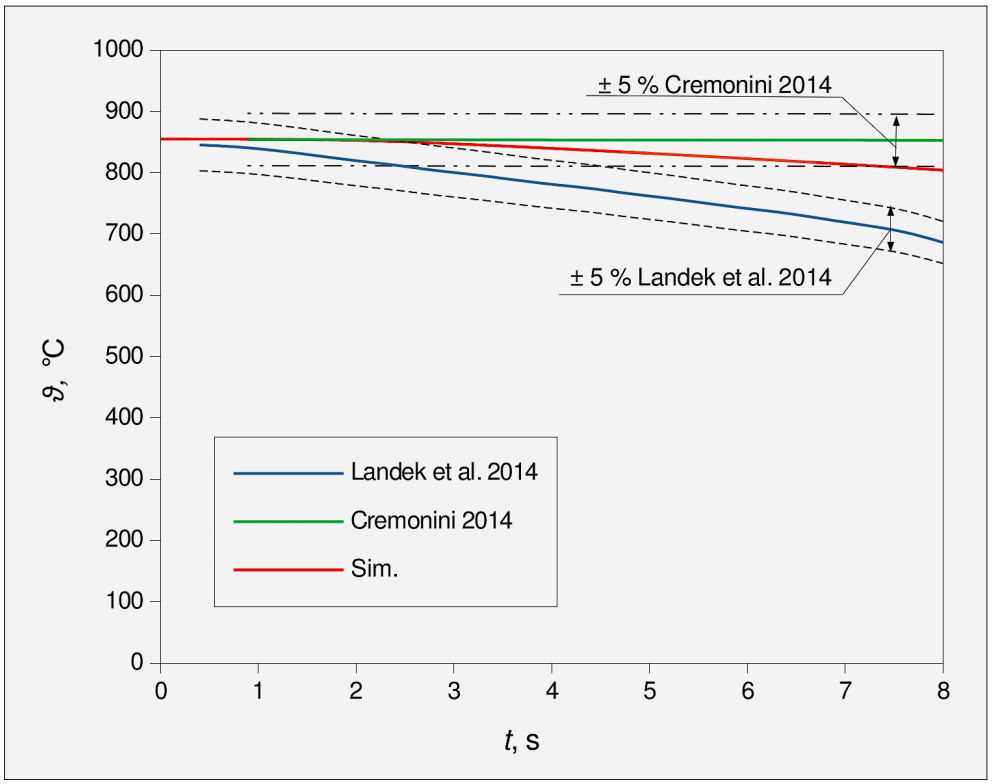

Figure 6: A comparison of the computational results with the experimental data available in **Landek et al. (2014)** and **Cremonini (2014)**. The experimental results were extracted using **Rohatgi (2021)**.

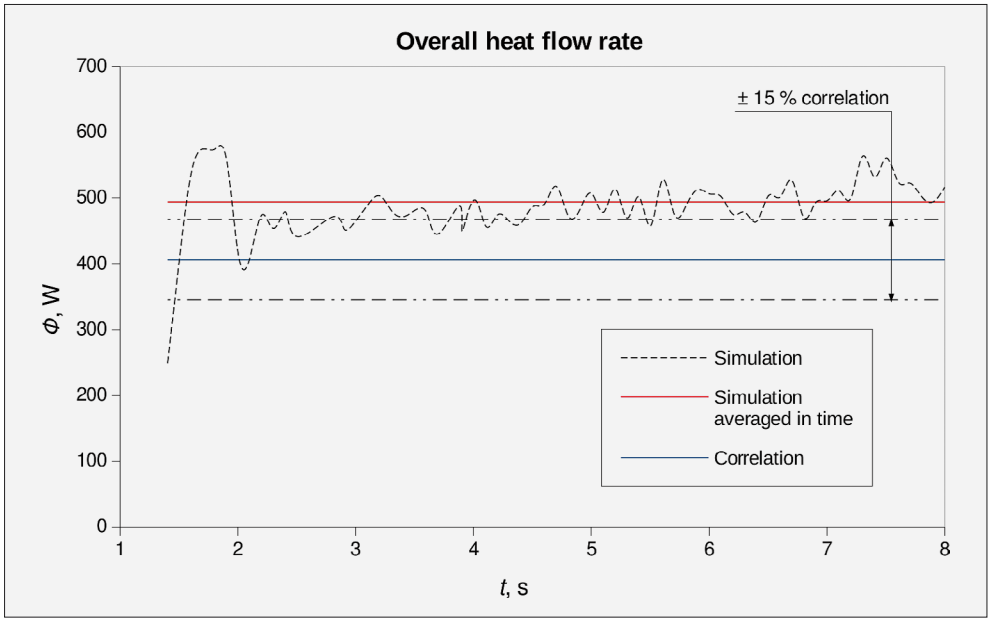

Figure 7: The total heat flow rate transferred from the specimen surface to the surrounding medium during the first 8 s of the quenching by immersion in a liquid. The comparison with the results obtained using correlations in **Momoki et al. (2007)**.

From the obtained results, one may note that by an application of the method suggested herein, one may achieve satisfactorily accurate solutions of the temperature distribution in the specimen's center. Further work on turbulence modelling, of course, would yield even better agreement with the experimental results. However, the goal of this work is to avoid any fine-tuning of the results, yet by the application of the basic principles to arrive at a satisfactorily accurate solution for an engineering application. The method is limited to the area of film boiling, and the further work is aimed at finding out a way to model the breakup of the vapour blanket. The accuracy of the proposed method is visible via the prescribed ± 5 % error band on the available experimental data. It is obvious that the mild turbulence level, noted in **Cremonini (2014)**, wherein the experiment is carried with distilled water with temperature 60°C, better suits the obtained numerical solution using a turbulent kinetic energy value of 0.1 m^2/s^2. On the other hand, in the experiment by **Landek et al. (2014)** the turbulence is

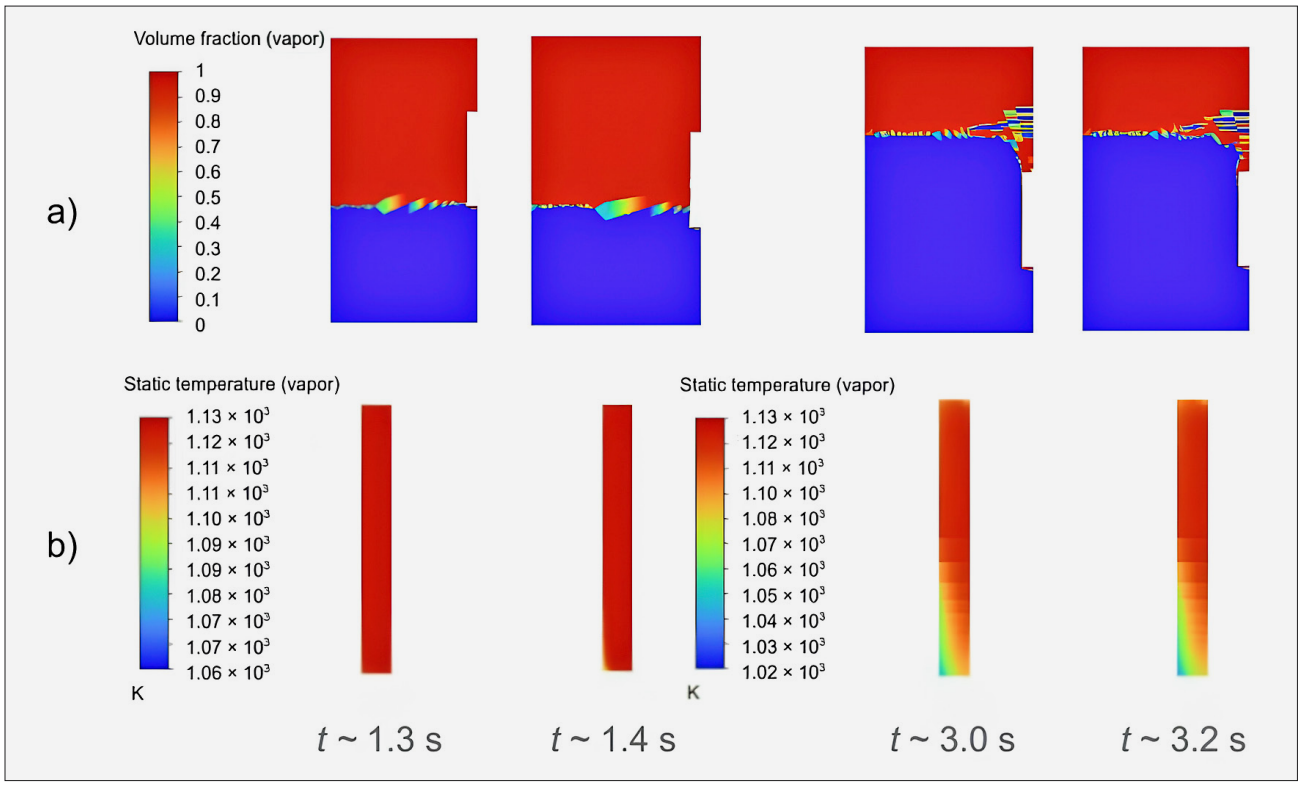

Figure 8: The results of the numerical simulation of the immersion quenching: a) vapour volume fraction field; b) the temperature field inside the solid; both, during the immersion and after the material is immersed in liquid bath.

stronger, and the numerical solution obtained with the present method fits the prescribed error band only within the first ca. 2.5 s of the total simulation time herein.

Furthermore, analyzing the heat flow rate, instantaneous and time averaged over the complete surface of the cylinder, it is confirmed in agreement with the calculation by using the correlations available in **Momoki et al. (2007)**, as shown in **Figure 7**. One may note, from the viewpoint of the solution accuracy and the model efficiency, that the correlation data has been overestimated slightly above 15%, as visible from the prescribed error band, chosen according to the prescribed error band in **Momoki et al. (2007)** that was, however, imposed on the estimated heat transfer coefficient values in their study on film boiling. The instantaneous heat flow rate values match the prescribed error band every here and then, as shown in **Figure 7**. Those unsteady oscillations are due to the oscillatory presence of the dry spots during the boiling process, and a more fundamental treatise on this subject one may find in a recent study by **Tecchio et al. (2024)**.

From the obtained results it is also noticeable that many details related to the immersion process itself were covered with the simulation. Hence, the sudden increase of heat flow rate is obvious after the specimen reaches the free surface of the quenchant medium.

By inspection of the vapour volume fraction field (see **Figure 8a**) one may note the vapour explosion that takes place after the material reaches the free surface of the liquid bath via the change in the vapour volume fraction field. This leads to the aforementioned sharp increase in the heat flow rate shown in **Figure 7**. Due to non-orthogonal mesh that is used within the present study, as is to be expected in the real industrial application that the mesh could not always be perfectly aligned with the coordinate axes, in conjunction with continuum surface force (CSF) surface tension model by **Brackbill et al. (1992)**, the evolution of the vapour phase after immersion in the liquid bath exhibits a kind of erroneous distribution. It is believed that this could be overcome by application of the continuum surface stress (CSS) model, briefly explained in **Kharangate and Mudawar (2017)**, but still more research needs to be carried out to this end.

From the temperature distribution inside the solid (see **Figure 8b**), one may note the success of the method in estimation of the temperature distribution inside the material during quenching by immersion in a liquid medium, especially after the material has been immersed for some time in the liquid bath. This bottom-up advancement of the decrease in temperature could be, at least qualitatively and to some extent, compared to distributions in **Demirel (2009)**, that are obtained using the FEM modelling approach.

5. Conclusions

In the conducted research, a novel mass transfer model at the phase interfaces has been developed, based on the heat balance at the phase interface, in which the heat

transfer coefficient is used as the fictitious variable in the way that, using this quantity, the distance from the neighbouring cell's center to the interface is approximated, and also by the involvement of the thermal conductivity in the approximate relation for the calculation of the heat flux at the interface. The results of the conducted computations confirm the following:

- The conducted solving of the Stefan problem at higher wall superheats shows good agreement with the analytical solution.
- The faster motion of the liquid-vapour interface has been observed at the higher wall superheats due to the higher temperature gradient at the vapour side (the liquid phase is at the saturation temperature, and hence there is no temperature gradient in it).
- The relatively flat temperature distribution obtained in the numerical simulation, has been also confirmed by the experimental data found in literature, and denotes the mild turbulence in the bulk fluid during the film boiling regime.
- Tracking the distribution of the heat flow rate in time, its jump increase has been observed immediately after the material reaches the free surface of the quenchant. The average heat flow rate obtained by numerical simulation is 494.3 W.
- With the analysis of the fields of physical quantities, the vapour volume fraction and the temperature field in the solid, the relevance of the suggested numerical method has been confirmed for numerical modelling of the film boiling during quenching of a metal material by immersion in a liquid medium.

This implies that the developed numerical approach could be doubtlessly applied in the industrial computations of the film boiling during the immersion quenching process. It is necessary to provide flow conditions, together with the initial temperatures of quenchant and specimen, and the turbulent kinetic energy value. One should thereby take note whether it is mathematical modelling of the pool or forced convection boiling.

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6. References

Ansys® Fluent, 2019. ANSYS Fluent Theory Guide, Release 19.2, Help System. ANSYS, Inc.

Arévalo, R., Antúnez, D., Rebollo, L., Abánades, A., 2014. Estimation of radiation coupling factors in film boiling around spheres by mean of Computational Fluid Dynamics (CFD) tools. International Journal of Heat and Mass Transfer 78, 84–89. https://doi.org/10.1016/j.ijheatmasstransfer.2014.06.063

Brackbill, J.U., Kothe, D.B., Zemach, C., 1992. A continuum method for modeling surface tension. Journal of Computational Physics 100, 335–354. https://doi.org/10.1016/0021-9991(92)90240-Y

Cremonini, G.E.S. de O., 2014. Aplicação do método inverso de condução de calor na avaliação de fluidos de resfriamento para têmpera.

Cukrov, A., Landek, D., Sato, Y., Boras, I., Ničeno, B., 2023a. Water Entry of a Heated Axisymmetric Vertical Cylinder. Energies 16. https://doi.org/10.3390/en16247926

Cukrov, A., Sato, Y., Boras, I., Ničeno, B., 2023b. Film Boiling around a Finite Size Cylindrical Specimen – A Transient Conjugate Heat Transfer Approach. Applied Sciences 13. https://doi.org/10.3390/app13169144

Cukrov, A., Sato, Y., Boras, I., Ničeno, B., 2021. A solution to Stefan problem using Eulerian two-fluid VOF model. Brodogradnja : Teorija i praksa brodogradnje i pomorske tehnike 72, 141–164. https://doi.org/10.21278/brod72408

de Bertodano, M.L., Fullmer, W., Clausse, A., Ransom, V.H., 2017. Introduction, in: Bertodano, M.L. de, Fullmer, W., Clausse, A., Ransom, V.H. (Eds.), Two-Fluid Model Stability, Simulation and Chaos. Springer International Publishing, Cham, pp. 1–8. https://doi.org/10.1007/978-3-319-44968-5_1

Demirel, C., 2009. Experimentelle Untersuchung und Simulation des Abschreckprozesses von bauteilähnlichen Geometrien aus G-AlSi7Mg.

Denèfle, R., Mimouni, S., Caltagirone, J.-P., Vincent, S., 2015. Multifield hybrid approach for two-phase flow modeling – Part 1: Adiabatic flows. Computers & Fluids 113, 106–111. https://doi.org/10.1016/j.compfluid.2014.07.018

Drew, D.A., Passman, S.L., 1999. Continuum Balance Equations for Multicomponent Fluids, in: Theory of Multicomponent Fluids. Springer New York, New York, NY, pp. 65–80. https://doi.org/10.1007/0-387-22637-0_7

Edelbauer, W., Zhang, D., Kopun, R., Stauder, B., 2016. Numerical and experimental investigation of the spray quenching process with an Euler-Eulerian multi-fluid model. Applied Thermal Engineering 100, 1259–1273. https://doi.org/10.1016/j.applthermaleng.2016.02.131

El Kosseifi, N., 2012. Numerical simulation of boiling for industrial quenching processes, Simulation numérique de l'ébullition pour les procédés de trempe industrielle. Ecole Nationale Supérieure des Mines de Paris.

Gauss, F., Lucas, D., Krepper, E., 2016. Grid studies for the simulation of resolved structures in an Eulerian two-fluid framework. Nuclear Engineering and Design 305, 371–377. https://doi.org/10.1016/j.nucengdes.2016.06.009

Hillier, A., Doorsselaere, T.V., Karampelas, K., 2020. Estimating the Energy Dissipation from Kelvin–Helmholtz Instability Induced Turbulence in Oscillating Coronal Loops. ApJL 897, L13. https://doi.org/10.3847/2041-8213/ab9ca3

Höhne, T., Vallée, C., 2010. Experiments and Numerical Simulations of Horizontal Two-Phase Flow Regimes Using an Interfacial Area Density Model. The Journal of Computational Multiphase Flows 2, 131–143. https://doi.org/10.1260/1757-482X.2.3.131

Kharangate, C.R., Mudawar, I., 2017. Review of computational studies on boiling and condensation. International Journal of Heat and Mass Transfer 108, 1164–1196. https://doi.org/10.1016/j.ijheatmasstransfer.2016.12.065

Kopun, R., Škerget, L., Hriberšek, M., Zhang, D., Edelbauer, W., 2014. Numerical Investigations of Quenching Cooling Processes for Different Cast Aluminum Parts. Strojniški vestnik - Journal of Mechanical Engineering.

Landek, D., Župan, J., Filetin, T., 2014. A Prediction of Quenching Parameters Using Inverse Analysis. Matls. Perf. Charact. 3, 229–241. https://doi.org/10.1520/MPC20130109

Momoki, S., Yamada, T., Shigechi, T., Kanemaru, K., Yamaguchi, T., 2007. Film Boiling Around a Vertical Cylinder With Top and Bottom Horizontal Surfaces, in: HT2007. ASME/JSME 2007 Thermal Engineering Heat Transfer Summer Conference, Volume 2, pp. 611–619. https://doi.org/10.1115/HT2007-32733

Perez-Raya, I., Kandlikar, S.G., 2018. Discretization and implementation of a sharp interface model for interfacial heat and mass transfer during bubble growth. International Journal of Heat and Mass Transfer 116, 30–49. https://doi.org/10.1016/j.ijheatmasstransfer.2017.08.106

Pointer, W.D., Liu, Y., 2017. Eulerian two-fluid RANS-based CFD simulation of a helical coil steam generator boiling tube, in: Proc. 17th International Topical Meeting on Nuclear Reactor Thermal Hydraulics. Xi'an, China, p. 19.

Rohatgi, A., 2021. Webplotdigitizer: Version 4.5.

Srinivasan, V., Moon, K.-M., Greif, D., Wang, D.M., Kim, M., 2010. Numerical simulation of immersion quench cooling process using an Eulerian multi-fluid approach. Applied Thermal Engineering 30, 499–509. https://doi.org/10.1016/j.applthermaleng.2009.10.012

Stark, P., Fritsching, U., 2015. Simulation of the impinging liquid jet cooling process of a flat plate. International Journal of Numerical Methods for Heat & Fluid Flow 25, 153–170. https://doi.org/10.1108/HFF-04-2013-0151

Steuer, R., 2015. Ultraschallunterstütztes Flüssigkeitsabschrecken bei der Wärmebehandlung metallischer Werkstoffe, Forschungsberichte des Lehrstuhls für Werkstofftechnik der Universität Rostock. Shaker Verlag, Aachen.

Štrubelj, L., Tiselj, I., Mavko, B., 2009. Simulations of free surface flows with implementation of surface tension and interface sharpening in the two-fluid model. International Journal of Heat and Fluid Flow 30, 741–750. https://doi.org/10.1016/j.ijheatfluidflow.2009.02.009

Subhash, M., 2017. Computational modelling of liquid jet impingement onto heated surface (Ph.D. Thesis). Technische Universität, Darmstadt.

Sun, D.-L., Xu, J.-L., Wang, L., 2012. Development of a vapor–liquid phase change model for volume-of-fluid method in FLUENT. International Communications in Heat and Mass Transfer 39, 1101–1106. https://doi.org/10.1016/j.icheatmasstransfer.2012.07.020

Tecchio, C., Cariteau, B., Houedec, C.L., Bois, G., Saikali, E., Zalczer, G., Vassant, S., Roca i Cabarrocas, P., Bulkin, P., Charliac, J., Nikolayev, V.S., 2024. Microlayer evaporation during bubble growth in nucleate boiling. International Journal of Heat and Mass Transfer 231, 125860. https://doi.org/10.1016/j.ijheatmasstransfer.2024.125860

Yamada, T., Shigechi, T., Momoki, S., Kanemaru, K., 2001. An Analysis of Film Boiling around a Vertical Finite-Length Cylinder. Reports of the Faculty of Engineering, Nagasaki University 31, 1–11.

Author's contribution

Alen Cukrov (senior assistant, PhD, mechanical engineering) provided the paper conceptualization, contributed to research methodology, validation of the results, formal analysis, investigation, original draft preparation, and presentation of the results. **Darko Landek** (full professor, PhD, materials science) provided conceptualisation, contributed to the validation and formal analysis, took part in the investigation, provided the resources for the experiments to be carried out, data curation, review and editing of the initial draft, visualisation of the experiment, and supervised the research. **Yohei Sato** (senior scientist, PhD, nuclear engineering) contributed to the application of computational methodology for carrying out the research, reviewed the work, and supervised the research. **Ivanka Boras** (full professor tenure, PhD, mechanical engineering) provided the software, formal analysis, resources, supervised the project, and contributed to funding acquisition. **Bojan Ničeno** (research group leader, PhD, applied physics) contributed to project administration and the funding acquisition.

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Razvoj numeričke metode za simulaciju gašenja metalnih materijala

Rudarsko-geološko-naftni zbornik
(The Mining-Geology-Petroleum Engineering Bulletin)

Izvorni znanstveni rad

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Sažetak

Gašenje je općeniti naziv za brzo hlađenje austenitiziranoga zakaljivog čelika ili rastvorno žarene aluminijeve legure u kapljevitim medijima s vrelištem nižim od temperature austenitizacije ili žarenja. U radu je opisan postupak razvoja nove numeričke metode za proračun gašenja metalnih materijala uranjanjem u kapljevine podložne Leidenfrostovu fenomenu. Na temelju zadane početne temperature predmeta i medija za gašenje, numerička metoda primjenom dvofluidnoga VOF modela rješava Štefanov problem i raspodjelu temperature u predmetu u prvoj fazi gašenja, u kojoj je površina predmeta pokrivena filmom pare. Provedena je validacija rješenja usporedbom predviđene temperaturne distribucije s eksperimentalnim rezultatima iz literature te je analizirana vremenski promjenjiva raspodjela toplinskoga toka. Dobiveni rezultati pokazuju prikladnost predložene metode za numeričku analizu početne faze gašenja metalnih materijala uranjanjem.

Ključne riječi:

Štefanov problem, dvofluidni VOF model, strujanje s isparivanjem, gašenje uranjanjem, prijenos topline

1. Uvod

Održivi razvoj pretpostavlja razvoj, proizvodnju i primjenu kvalitetnih, energijski učinkovitih i za okoliš manje utjecajnih novih proizvoda. Energijska učinkovitost i potreba za smanjenjem utjecaja na okoliš posebno se ističu u izradi i upotrebi proizvoda koji zahtijevaju prijenos i pretvorbu velikih količina energije i toplinskih tokova. Takvi proizvodi primjenjuju se u energetici, termotehnici i procesnoj tehnici, metalurgiji te proizvodnim tehnologijama kao što su lijevanje, zavarivanje, obrada deformacijom u toplome stanju, toplinska obrada i dr. U izradi navedenih proizvoda prisutan je niz mehaničkih, kemijskih, metalurških i fizičkih procesa koji su u velikome broju obrada potaknuti termodinamičkim procesima u metalnome materijalu te prijenosom topline i mase na površini materijala. Toplinska energija dovedena metalnom materijalu u fazi zagrijavanja aktivira procese promjene mehaničkih svojstava, promjene mikrostrukture, kemijske reakcije, difuzijske procese, otapanje legirnih elemenata, homogenizaciju kemijskoga sastava, nukleaciju novih strukturnih faza i dr. U fazi ohlađivanja odvođenje topline iz metalnoga materijala u većini tehnoloških procesa treba provesti u kraćem trajanju od faze zagrijavanja, uz postizanje traženih uporabnih svojstava materijala i karakteristika proizvoda. Odvođenje topline kroz površinu metalnih materijala određeno je toplinskom vodljivošću materijala i uspostavljenim temperaturnim gradijentom iz unutrašnjosti prema površini materijala te koeficijentom prijelaza topline i razlikom temperature površine i medija za ohlađivanje prisutnoga oko predmeta. U opisu procesa ohlađivanja, hlađenje materijala brže od 1 K/s uobičajeno se naziva gašenjem. Primjenom kapljevina s vrelištem nižim od početne temperature ohlađenoga metalnog materijala može se postići intenzivno i brzo ohlađivanje, tzv. gašenje. Tipični predstavnici ovih kapljevina jesu voda, vodene suspenzije, ulja za kaljenje, emulzije ulja i vode te vodene otopine kapljevitih polimera (npr. polialkilglikola, polivinil-propilena i sl.). Svako od navedenih sredstava za ohlađivanje djeluje s drugačijim rasponom vrijednosti brzina ohlađivanja i karakterističnim oblikom krivulje gašenja. Međutim svima je zajednička pojava tzv. Leidenfrostova fenomena, koji se sastoji od faze parnoga filma, mjehurastoga vrenja i faze ohlađivanja konvencijom, shematski prikazanih na **slici 1**.

U industrijskim procesima hlađenja za učinkovitost prijenosa topline iznimno je važno mjehurasto ispariva-

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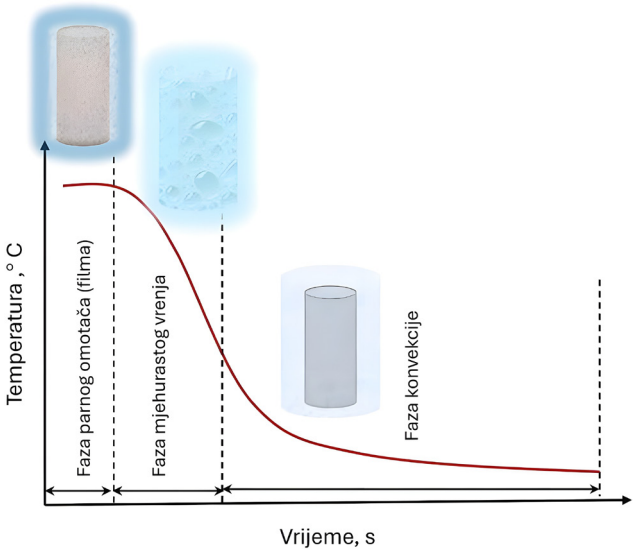
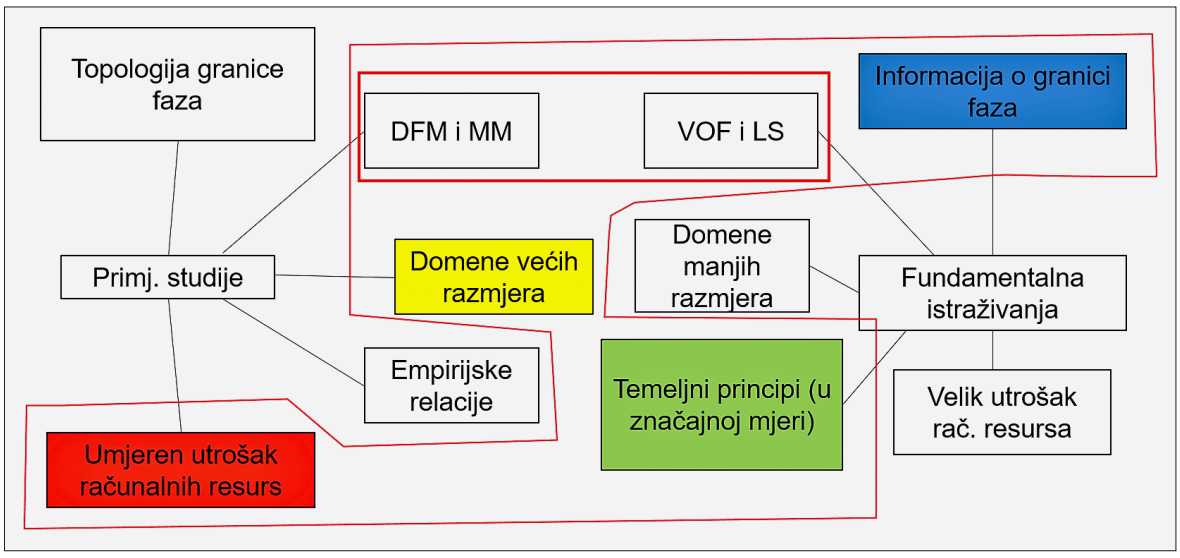


Slika 1: Shematski prikaz temperaturne krivulje površine valjka u kapljevini podložnoj Leidenfrostovu fenomenu

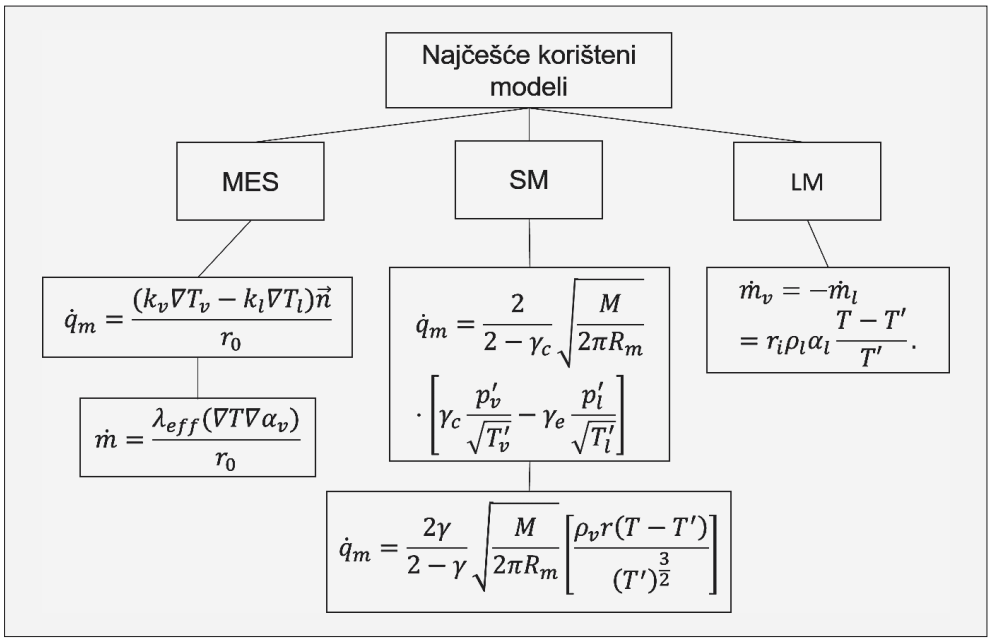
nje (vrenje) kojim se ostvaruje najintenzivnije odvođenje toplinskoga toka kroz površinu materijala uz relativno male razlike temperatura između površine i sredstva za hlađenje, što rezultira velikim iznosima koeficijenata prijelaza topline. S druge strane, u toplinskoj obradi metala, uslijed iznimno velikih gustoća toplinskoga toka, oko površine predmeta u prvoj fazi gašenja formira se parni omotač (film) koji djeluje kao toplinski izolator i reducira se prijenos topline s površine predmeta u sredstvo za gašenje. Zbog toga se različitim metodama (cirkulacijom medija, dodatcima soli ili nanočestica i sl.) nastoji vremenski skratiti faza parnoga omotača i poboljšati razvoj faze mjehurastoga vrenja. Faza konvekcije pojavljuje se kad je gustoća toplinskoga toka kroz površinu predmeta nedovoljna za formiranje mjehurića i predstavlja polagano ohlađivanje bez promjene agregatnoga stanja kapljevine na kontaktnoj površini s ohlađivanim predmetom. Zbog složenosti procesa prijenosa mase, turbulentnoga strujanja te termodinamičkih i hidrodinamičkih procesa do sada još nije predložen matematički model za cjeloviti opis svih triju faza Leidenfrostova fenomena.

Numeričko modeliranje prijenosa topline i mase, u kontekstu industrijske primjene procesa ohlađivanja i gašenja, podrazumijeva primjenu načelno dvaju tipova metoda za rješavanje višefaznoga strujanja (engl. *multiphase flow*). Prva su skupina tzv. volumne metode, poput metode volumnoga udjela fluida (engl. *Volume-of-Fluid*, VOF) te metoda razina (engl. *level-set method*, LSM), kod kojih se dobiva detaljan opis granice faza (engl. *interface*), ali se iziskuje primjena fine rezolucije mreže uz samu granicu faza kako bi se granica faza mogla adekvatno obuhvatiti u proračunu. Ove metode primjenjuju se najčešće u fundamentalnim numeričkim istraživanjima zbog nužne upotrebe mreža visoke rezolucije. Drugu skupinu čine osrednjene (engl. *averaged*) metode, kod kojih se u postupku izvođenja matematičkoga modela gubi informacija o položaju granice faza, pa se međufazni prijenos modelira putem izvorskih članova u jednadžbama očuvanja. Ovoj skupini metoda pripadaju model mješavine (engl. *mixture model*, MM) i Eulerov dvofluidni model (engl. *two-fluid model*, TFM) koji se primjenjuju u domenama industrijskih razmjera (primijenjene studije) zbog svoje manje zahtjevnosti u pogledu korištenja računalnih resursa i vremena. Usporedba odlika najčešće korištenih modela proračuna višefaznoga strujanja prikazana je na **slici 2**.

S obzirom na to da je model mješavine zapravo pojednostavnjeni dvofluidni model (eliminira se detaljan opis međufaznoga prijenosa na granicama faza), u nastavku ovoga rada za proračune će se primijeniti samo Eulerov dvofluidni model, u kojemu je potrebno uvesti dodatne korelacije između dviju faza, parne i kapljevite, kojima se opisuje međufazni prijenos količine gibanja i



Slika 2: Usporedba odlika često korištenih metoda proračuna višefaznoga strujanja



Slika 3: Najčešće korišteni modeli prijenosa mase prema Kharangate and Mudawar (**Kharangate and Mudawar, 2017**)

energije. U ovome modelu gubi se informacija o položaju granice faza, što predstavlja poteškoću pri modeliranju procesa s isparivanjem u kapljeviti medij, npr. u toplinskoj obradi metala, odnosno procesu gašenja uranjanjem austenitiziranoga čelika u bazen ili kupku za ohlađivanje. Zato se u okviru ovoga rada primjenjuje dvofluidna formulacija kombinirana s VOF metodom. Ovaj Eulerov dvofluidni model kombinira prednosti VOF metode, u smislu da je granica faza egzaktno opisana i zadržava svojstvo dvofluidnoga modela na način da se proračun može provesti korištenjem grublje rezolucije mreže i većih vremenskih inkremenata tijekom simulacije.

Pregledom dosadašnjih istraživanja utvrđeno je kako su oba tipa numeričkoga modeliranja višefaznoga strujanja primjenjivana u kontekstu modeliranja procesa gašenja uranjanjem (**El Kosseifi, 2012; Srinivasan et al., 2010; Kopun et al., 2018**), dok se kod postupka gašenja prskanjem (engl. *spray quenching*) primjenjuje Eulerov dvofluidni model (**Subhash, 2017; Stark and Fritsching, 2015; Edelbauer et al., 2016**). Ključna uloga svih proračuna višefaznoga strujanja pripada načinu modeliranja prijenosa mase na granicama faza. Za modeliranje prijenosa mase ističu se tri glavna pristupa, koja sumiraju Kharangate i Mudawar (**Kharangate and Mudawar, 2017**): model energijskoga skoka (MES); Schrageov model (SM) i Leejev model (LM). Grafički prikaz tih modela, zajedno s jednadžbama za izračun prijenosa mase na granici faza, shematski je prikazan na **slici 3**.

Model energijskoga skoka (MES) prikazan na **slici 3** proizlazi iz jednostavnoga rezoniranja na temelju mehanike kontinuuma, a taj je da je gustoća toplinskoga toka koja se prenese u procesu promjene faze jednaka razlici gustoća toplinskoga toka provođenjem (Fourierov stavak s obiju strana granice faza, što opisuje termodinamički poznati Fourierov stavak). Takav pristup iziskuje definiranje inicijalnoga sloja pare (kod isparivanja) neposredno uz sâm uzorak jer se u jednadžbi prijenosa mase nalazi gradijent volumnoga udjela parne faze, ali pri tome nije nužno u jednadžbe uvoditi empirijske koeficijente ili faktore. S druge strane, Schrageov model (SM) prikazan na **slici 3** izveden je iz kinetičke teorije plinova te je za njegovo korištenje nužno definirati tzv. akomodacijski faktor kako bi se dobili ispravni rezultati proračuna. Međutim, i ovaj model iziskuje definiranje inicijalnoga sloja disperzne faze. Posljednji Leejev model (LM) naveden na **slici 2** po definiciji ne zahtijeva definiranje inicijalnoga sloja disperzne faze, što ga čini prikladnim za proračun s promjenom faze u stopostotnome monofaznom mediju (engl. *bulk fluid*). No, i ovaj model zahtijeva kalibriranje empirijskoga koeficijenta kako bi se postigla zadovoljavajuća točnost.

U ovome je radu stoga primijenjen pristup najsličniji metodi energijske bilance jer fenomenološki najbolje opisuje procese isparivanja kapljevitih medija kod gašenja uranjanjem. Prisutnost inicijalnoga sloja pare opravdana je činjenicom da je cilj rada modelirati filmsko isparivanje pri procesu gašenja uranjanjem, što za posljedicu ima da su rezultati numeričke simulacije pomaknuti za određeni vremenski interval koji je potreban za stvaranje parnoga omotača. Pregledom dosad provedenih istraživanja utvrđeno je samo nekoliko slučajeva u kojima se dvofluidnom formulacijom uspješno riješilo napredovanje granice faza na fundamentalnoj razini. Stoga će se u radu opisati razvoj nove metode numeričkoga proračuna prijelaza topline prikladne za matematičko modeliranje faze parnoga omotača u procesima gašenja uranjanjem ugrijanoga čelika u kapljevita sredstva za gašenje podložna Leidenfrostovu fenomenu.

U usporedbi s pristupom utemeljenim na metodi konačnih elemenata (MKE) koji se koristi za simuliranje

gašenja, predstavljenim primjerice u Demirel (**Demirel, 2009**) i Steuer (**Steuer, 2015**), unutar pristupa baziranoga na računalnoj dinamici fluida (engl. *computational fluid dynamics*, CFD) nema potrebe za ulaznim temperaturama iz eksperimenta, već su samo model turbulencije te inicijalne temperature uzorka i kupke dovoljne za dobivanje rješenja. Nadalje, koristeći se CFD pristupom, može se steći uvid u polja temperature i strujanja, dok je koeficijent prijelaza topline dio rješenja, a ne ulazni podatak dobiven, primjerice, metodom inverznoga prijenosa topline.

Općenito govoreći, prednost je primjene predložene metode u obuhvaćanju polja strujanja, posebice procesa isparivanja koristeći se predloženim modelom prijenosa mase, u proračunu temperaturnoga polja unutar uzorka i korespondirajuće integralne veličine.

2. Metoda za proračun prijenosa mase energijskim skokovima na graničnoj površini faza

Uspješno numeričko modeliranje procesa mjehurastoga isparivanja, jednako kao i procesa filmskoga isparivanja nužno zahtijeva učinkovito modeliranje prijenosa mase na graničnim površinama faza (u nastavku granica faza). U radu se predlaže nova metoda za proračun prijenosa mase, postavljena na temelju modela energijskoga skoka (engl. *energy jump model*) razvijenoga za slučaj čistoga provođenja topline unutar sloja pare uz prisutnost jedne zasićene i jedne nezasićene (pregrijane ili pothlađene) faze (npr. vrela kapljevina i pregrijana para) te toplinskoga modela promjene faza (engl. *thermal phase change model*, TPCM), dokumentiranoga u Ansys® Fluent (**Ansys® Fluent, 2019**). Predloženom se numeričkom metodom aproksimacijom određuje temperaturni gradijent u okolišu granice faza, pri čemu se udaljenost od granice faza tretira kao polovica duljine stranice kuboidnoga kontrolnog volumena numeričke mreže. Ovakva aproksimacija provodi se primjenom koeficijenta prijelaza topline, h_{pq}, dostupnoga u TPC modelu kao fiktivne varijable, kojom se u TCP model unosi lokalna duljina ćelije. Međufazna se površina računa kao gradijent volumnoga udjela faze, čime se osigurava primjena konstitutivnih relacija isključivo na granicama faza. Nadalje, ovim se pristupom osigurava i ponašanje metode nalik onome kod jednofluidne VOF formulacije, tj. jasno razgraničenje između dviju faza, odnosno modeliranje podvojenoga strujanja (engl. *separated flows*). Isto ponašanje numeričkih rezultata uočeno je i u drugim metodama, metodi algebarske gustoće međufazne površine (engl. *algebraic interfacial area density*, AIAD), koju predlažu Höhne i Vallée (**Höhne and Vallée, 2010**) i u metodi velikoga mjehura (engl. *large bubble method*, LBM), predložene u Denèfle et al. (**Denèfle et al., 2015**). Predložena numerička metoda implementirana je u računalni program ANSYS Fluent korištenjem korisnički definiranih funkcija (engl. *user-defined functions*, UDFs).

2.1. Matematički model, rubni uvjeti i računalni program korišten u proračunu

2.1.1. Matematički model

Dvofluidni model, prema de Bertodano et al. (**de Bertodano et al., 2017**), proizlazi iz Landauove teorije superfluidnosti helija II, i u sklopu ovoga modela jednadžbe očuvanja definirane su za pojedinu fazu, dok se interakcija među fazama modelira putem izvorskih članova. Ovi izvorski članovi, koji se pojavljuju u jednadžbama očuvanja, posljedica su procesa osrednjavanja, koji je primijenjen nad tim parcijalnim diferencijalnim jednadžbama i uslijed kojega je izgubljena informacija o granici faza. Jednadžbe očuvanja relevantne za problem razmatran ovim radom mogu se pronaći u Drew and Passman (**Drew and Passman, 1999**), a zapisane za *k*-tu fazu uključenu u višekomponentni sustav glase:

- zakon očuvanja mase:

$$\frac{d}{dt}\int \alpha_k \rho_k dv + \oint \alpha_k \rho_k \mathbf{v}_k \cdot \mathbf{n} ds = \int \Gamma_k dv \tag{1}$$

- zakon očuvanja količine gibanja:

$$\frac{d}{dt}\int \alpha_k \rho_k \mathbf{v}_k dv + \oint \alpha_k \rho_k \mathbf{v}_k \mathbf{v}_k \cdot \mathbf{n} ds =$$

$$= \oint \alpha_k \mathbf{t}_k ds + \int \left(\alpha_k \rho_k \mathbf{b}_k + \mathbf{M}_k + \Gamma_k \mathbf{v}_{ki} \right) dv \tag{2}$$

- zakon očuvanja energije:

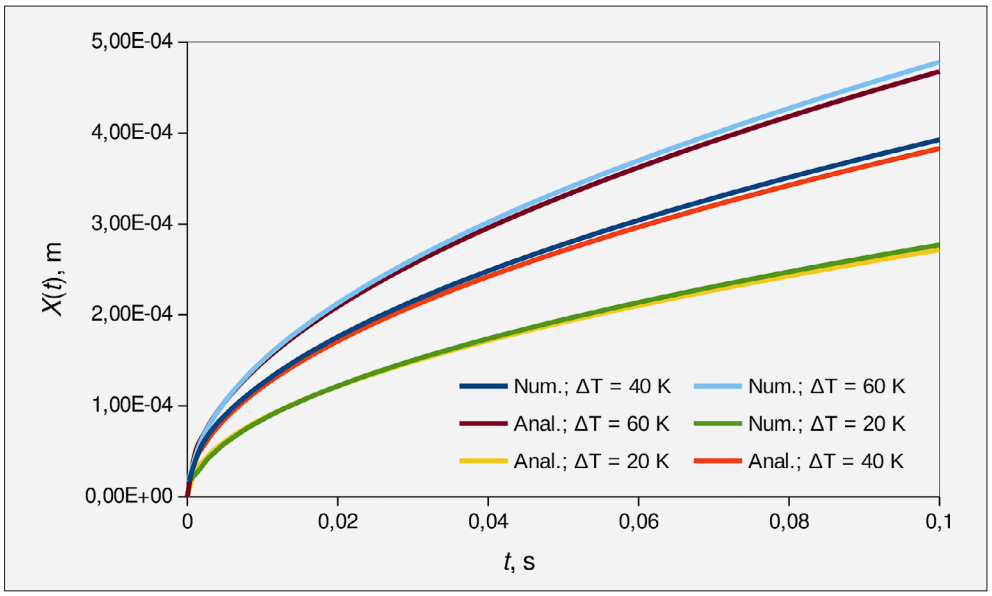
$$\alpha_k \rho_k \left(\frac{\partial u_k}{\partial t} + \mathbf{v}_k \cdot \nabla u_k \right) = \alpha_k \mathbf{T}_k : \nabla \mathbf{v}_k - \nabla \cdot \alpha_k \mathbf{q}_k +$$

$$+ \alpha_k \rho_k r_k + E_k + \Gamma_k \left(u_{ki} - u_k - \frac{1}{2} v_k^2 + \mathbf{v}_{ki} \cdot \mathbf{v}_k \right) \tag{3}$$

gdje je posebna pozornost u ovome radu, između ostalih veličina, posvećena članovima Γ_k, koji se odnosi na prijenos mase uslijed promjene faze, i $\mathbf{M}_k$, koji uključuje sile koje djeluju na fazu *k* u interakciji s drugim fazama prisutnima tijekom strujanja. Prvospomenuti je modeliran koristeći se modelom prijenosa mase predloženim u Cukrov et al. (**Cukrov et al., 2021**), dok je u potonjemu članu, koji proizlazi iz procesa osrednjavanja korištenoga pri izvođenju jednadžbi modela, uzet u obzir jedino međufazni otpor. U ovome je radu korišten pristup modeliranja višefaznoga strujanja koji slijedi izloženo u Štrubelj et al. (**Štrubelj et al., 2009**), gdje se primjenom iznimno velike vrijednosti međufaznoga otpora postiže jednakost brzina dviju faza na granici između faza. U sklopu ovoga rada to je provedeno primjenom modela anizotropnoga otpora koji je dostupan unutar računalnoga programa ANSYS Fluent.

2.1.2. Rubni uvjeti

Standardni Dirichletovi i von Neumannovi rubni uvjeti pridruženi su granicama proračunske domene te



Slika 4: Položaj granice faza pri različitim pregrijanjima stijenke. Usporedba numeričkoga i analitičkoga rješenja.

su istaknuti u prethodnim publikacijama (**Cukrov et al., 2021; Cukrov et al., 2023b; Cukrov et al., 2023a**). Važno je naglasiti kako je, s obzirom na dva skupa jednadžbi očuvanja koje su potrebne za opis višefaznoga strujanja načinjenoga od dviju faza, bilo obavezno pridružiti rubne uvjete svakoj fazi odvojeno, ali također i za mješavinu faza gdje je to bilo potrebno. Komunikacija između domene krutine i tekućine realizirana je korištenjem spregnutoga (eng. *coupled*) rubnog uvjeta, dostupnoga unutar programa ANSYS Fluent.

2.1.3. Računalni program korišten u proračunu

Računalni program korišten u proračunu provedenom u ovome radu jest ANSYS Fluent (**Ansys® Fluent, 2019**), komercijalni CFD računalni program. Ovaj računalni program ima relativno dugu povijest u proračunima isparivanja. Počevši od rada Sun et al. (**Sun et al., 2012**) provedeni su različiti pokušaji modeliranja procesa isparivanja koristeći se modelom prijenosa mase iz skupine MES modela, koji su fizički najtočniji jer proizlaze iz temeljnih principa prijenosa topline primijenjenih na granici faza. Nadalje, cilindrični uzorak stvarnih dimenzija proučavan je u Arevalo et al. (**Arévalo et al., 2014**), koristeći se izvedenicom MES modela za numeričku simulaciju filmskoga isparivanja oko sfere. U radu Perez-Raya i Kandlikar (**Perez-Raya and Kandlikar, 2018**) istaknuta je potreba za učinkovitom evaluacijom temperaturnoga gradijenta na granici faza unutar spomenutoga računalnog programa te su autori predložili novi pristup računanja udaljenosti između tzv. G-ćelije (gradijentna ćelija) i granice faza. U ovome istraživanju udaljenost između granice faza i središta susjedne ćelije uključena je u model te involvirana unutar računalnoga programa korištenjem korisnički definiranih funkcija (engl. *user-defined functions*, UDF).

2.2. Verifikacija metode

Model za predviđanje temperaturne raspodjele unutar metalnoga materijala na čijoj površini dolazi do pojave Leidenfrostova fenomena verificiran je rješavanjem Štefanova problema, nestacionarnoga napredovanja fazne granice, pri čemu je rezultat numeričke simulacije uspoređen s analitičkim rješenjem položaja granice faza, $X(t)$ te distribucije temperature uzduž prostorne koordinate x. Proračun je proveden na trima različitim mrežama: jednolikoj pravokutnoj, nejednolikoj (gradiranoj) pravokutnoj i hibridnoj mreži. Hibridna mreža bila je sastavljena od nejednolikih pravokutnih i trokutnih kontrolnih volumena. Detaljan opis korištenoga pristupa iznesen je u radu Cukrov et al. (**Cukrov et al., 2021**). Za svaki od navedenih tipova mreže provedena je studija utjecaja rezolucije mreže na dobivena rješenja te je potvrđena ranije poznata pretpostavka kako prilikom korištenja Eulerova dvofluidnoga modela rezolucija mreže nema bitan utjecaj na konačni rezultat simulacije. Isto je potvrđeno u studiji koju provode Gauss et al. (**Gauss et al., 2016**), dok irelevantnost rezolucije mreže na točnost rješenja prilikom korištenja Eulerova dvofluidnoga modela navode Pointer i Liu (**Pointer and Liu, 2017**). Položaj granice faza pri trima različitim pregrijanjima stijenke vidljiv je na **slici 4**.

Dobiveni rezultati pokazuju dobro slaganje predložene numeričke metode s analitičkim rješenjem te otkrivaju kako povećanjem pregrijanja stijenke sloj pare brže napreduje. Uzrok je navedenom veći temperaturni gradijent na graničnoj liniji kapljevina-para pri višim pregrijanjima stijenke.

2.3. Validacija metode

Eulerov dvofluidni model nestacionarnoga napredovanja fazne granice kapljevina-para validiran je korištenjem eksperimentalnih rezultata dostupnih u Mo-

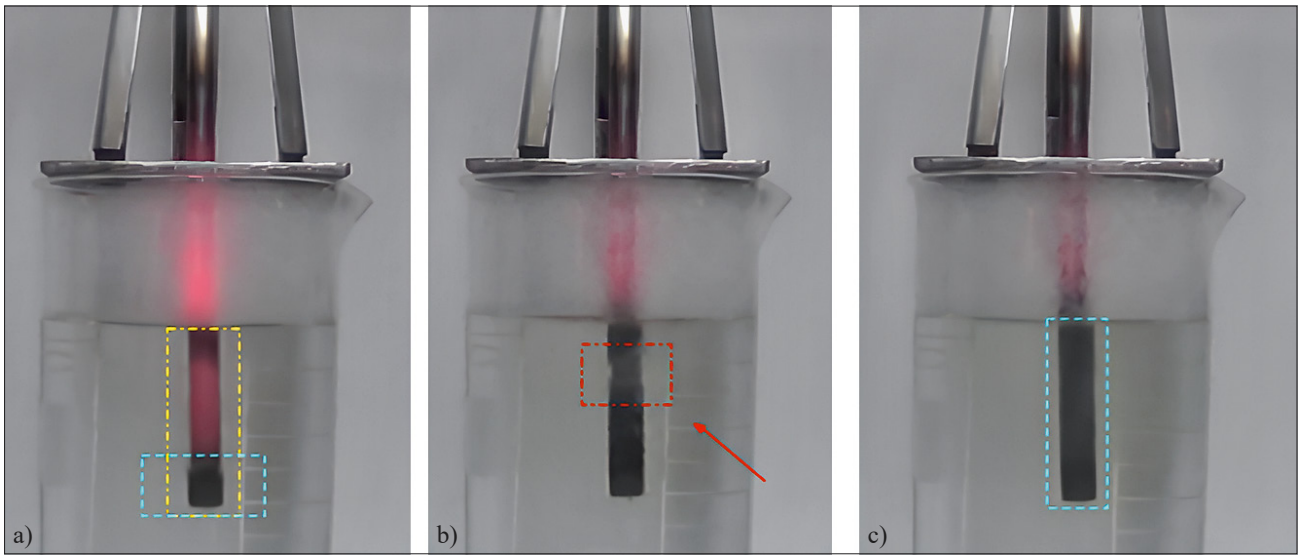
moki et al. (**Momoki et al., 2007**), koji su dobiveni za cjelokupan proces hlađenja srebra u kapljevitoj vodi pri temperaturi zasićenja. Cjelokupan proces validacije modela detaljno je iznesen u Cukrov et al. (**Cukrov et al., 2023b**) te je ukratko opisan u nastavku. U provedenoj numeričkoj simulaciji srebrni uzorak izložen je vreloj kapljevini s tankim filmom pare, koji inicijalno okružuje uzorak. Uzorak je inicijalno ugrijan na 600 °C, dok je vrela kapljevina temperature 100 °C. Nadalje, kako bi se inducirao adekvatan toplinski tok iz uzorka, turbulentno strujanje uzeto je u obzir unutar domene. Proračun je proveden za približno 10 % ukupnoga vremena trajanja filmskoga isparivanja prijavljenoga u Momoki et al. (**Momoki et al., 2007**) za slučaj hlađenja srebra u vreloj kapljevini pri atmosferskome tlaku, tj. ukupno vrijeme simulacije iznosi 15 s. Pri modeliranju filmskoga isparivanja uočena je važnost modeliranja turbulentnoga strujanja kapljevine oko filma vodene pare. Utvrđeno je kako disperzirani model turbulencije, tj. model turbulencije u kojemu se jednadžbe očuvanja veličina strujanja rješavaju jedino u kontinuiranoj fazi, dok se unutar dispergirane faze turbulencija modelira korelacijom, adekvatno opisuje fiziku procesa filmskoga isparivanja sa spregnutim prijenosom topline (engl. *conjugate heat transfer*, CHT). S obzirom na kompleksnost modeliranja turbulentnoga strujanja za ovakav slučaj pretpostavljena je vrijednost kinetičke energije turbulencije unutar domene te je ova vrijednost zadana konstantnom tijekom proračuna, tzv. „zamrznuta turbulencija". Određena se vrijednost kinetičke energije turbulencije zadaje unutar glavnine domene, izuzev sloja ćelija neposredno uz ohlađivani materijal, čime se modelira laminarno strujanje u filmu pare uz sam predmet. Na temelju provedenih proračuna utvrđeno je kako vrijednost kinetičke energije turbulencije u iznosu 0,25 m^2/s^2 adekvatno modelira spregnuti prijenos topline jer se s tom vrijednošću postiže zadovoljavajuće slaganje temperaturnoga polja unutar krutine dobivenoga numeričkom simulacijom s rezultatima eksperimenta, za prvih 15 s trajanja procesa. Potvrđeno je kako se primjenom Kelvin-Helmholtzove teorije nestabilnosti može dobiti adekvatna vrijednost kinetičke energije turbulencije, koristeći se izrazom izvedenim u Hillier et al. (**Hillier et al., 2020**), ako se za relativnu brzinu, prisutnu u brojniku toga izraza, uzme vrijednost brzine strujanja unutar filma pare. Brzina strujanja izračunava se iz teorije graničnoga sloja predstavljene u Yamada et al. (**Yamada et al., 2001**), uz pretpostavku glatke granice kapljevina-para te da je brzina na rubu parnoga omotača jednaka nuli (engl. *no slip condition*). Primijećeno je kako koeficijent turbulentne viskoznosti, koji je svojstvo strujanja, idealno prati tijek formiranja pare. Navedeno se može objasniti primjenom tenzora brzine deformacije, koji se nalazi unutar definicije turbulentne viskoznosti odabranoga modela turbulencije.

3. Numerička simulacija gašenja metalnog materijala uranjanjem u kapljevinu

U ovome radu proveden je proračun gašenja uranjanjem valjka od superlegure Inconela 600, pri čemu su poznati: temperatura medija za gašenje i inicijalna temperatura valjka. Detaljan opis numeričkoga postupka nalazi se u Cukrov et al. (**Cukrov et al., 2023a**) te će ukratko biti opisan u nastavku. Dvofluidna VOF metoda primijenjena na hibridnoj proračunskoj mreži sastavljenoj od kvadratičnih i trokutastih ćelija zahtijevala je promjenu interpolacije iz interpolacije između središta kontrolnih volumena (engl. *cell based interpolation*) u interpolaciju između čvorova kontrolnoga volumena (engl. *node based interpolation*), nakon što je provedena inicijalizacija zavisnih varijabli unutar domene. U promatranome se slučaju radi o pothlađenoj kapljevini temperature 60 °C te je radi jednostavnosti proračuna pretpostavljena ista temperatura i za okolni medij unutar kojega se uzorak nalazi neposredno prije uranjanja. Bitno je napomenuti da su, radi jednostavnosti, materijalu odabranom kao okolni medij iznad slobodne površine kapljevine pridružena svojstva vodene pare i da je njegova temperatura 60 °C. Na taj se način pojednostavnjuje matematički model jer nije potrebno uzimati dodatni skup jednadžbi za modeliranje prijenosa topline na okolni zrak. U protivnome bi bila potrebna još jedna skupina jednadžbi očuvanja za zrak, čime bi se proračun bitno usporio. Ova je aproksimacija opravdana zbog izrazito niskih vrijednosti koeficijenta prijelaza topline s užarene krutine (temperature preko 800 °C) na okolni medij. Nadalje, na ovaj je način u numeričkome modelu primijenjenom u ovome radu osigurana jednolikost temperature unutar računalne domene te je, stoga, izbjegnuta mogućnost induciranja prijenosa mase preko granice faza velikih razmjera (eng. *large-scale interface*) na granici kapljevina-okolni medij, do koje bi moglo doći uslijed temperaturnoga gradijenta.

Valjak od Inconela 600 inicijalno se nalazi na temperaturi 855 °C, što je u suglasju s normom ISO 9950 koja propisuje uvjete pod kojima bi se trebao provoditi takav eksperiment. Uz navedene vrijednosti, inicijalne temperature medija i uzorka, zadana je i vrijednost kinetičke energije turbulencije u iznosu od 0,1 m^2/s^2 na temelju prijašnjih istraživanja. Definirane su dvije zone s obzirom na režim strujanja (turbulentni ili laminarni) unutar domene. Prva je međufazna zona 1, koja oplakuje površinu uzorka i proteže se samo jedan sloj ćelija u domenu. Unutar te se zone pretpostavlja laminarno strujanje, tj. kinetička energija turbulencije teži k nuli.

Druga zona obuhvaća zonu neposredno uz sâm objekt, ali ne i samu zonu 1, te se unutar nje definira ranije navedena vrijednost kinetičke energije turbulencije. U ostatku domene pretpostavlja se laminarno strujanje, na način naveden za međufaznu zonu 1. Također, primijenjena je metoda pomične mreže s topološkom pro-



Slika 5: Napredovanje fronte kvašenja tijekom gašenja legure Inconel 600 u kapljevitoj vodi približne temperature 52 °C

mjenom, tj. tijekom gibanja mreže (objekta) dolazi do generiranja novih ćelija i brisanja nekih postojećih, pri čemu se provodi interpolacija rezultata sa stare mreže na novu. Uzorak se uranja konstantnom brzinom uranjanja, 0,13 m/s, pri čemu je za gibanje uzorka u numeričkoj simulaciji korišten tzv. ALE (engl. *arbitrary Lagrangian-Eulerian*) pristup, kod kojega se unutar svake od domena rješava Eulerov skup jednadžbi (praćenje promjena unutar kontrolnoga volumena), dok se sama granica između dviju domena opisuje Lagrangeovom formulacijom (praćenjem gibanja materijalnoga volumena). Posebnost niklove superlegure Inconel 600 dobro je predvidljiva promjena fizičkih svojstava, toplinske provodnosti, λ_s, i specifičnoga toplinskog kapaciteta, c_s, s promjenom temperature uzorka, što je potrebno uzeti u obzir pri proračunu. Materijal je izrazito visoke toplinske prodornosti (engl. *thermal effusivity*), što znači da su prilikom gašenja uranjanjem prisutni svi režimi Leidenfrostova isparivanja (npr. filmsko i mjehurasto isparivanje i prijenos topline konvekcijom).

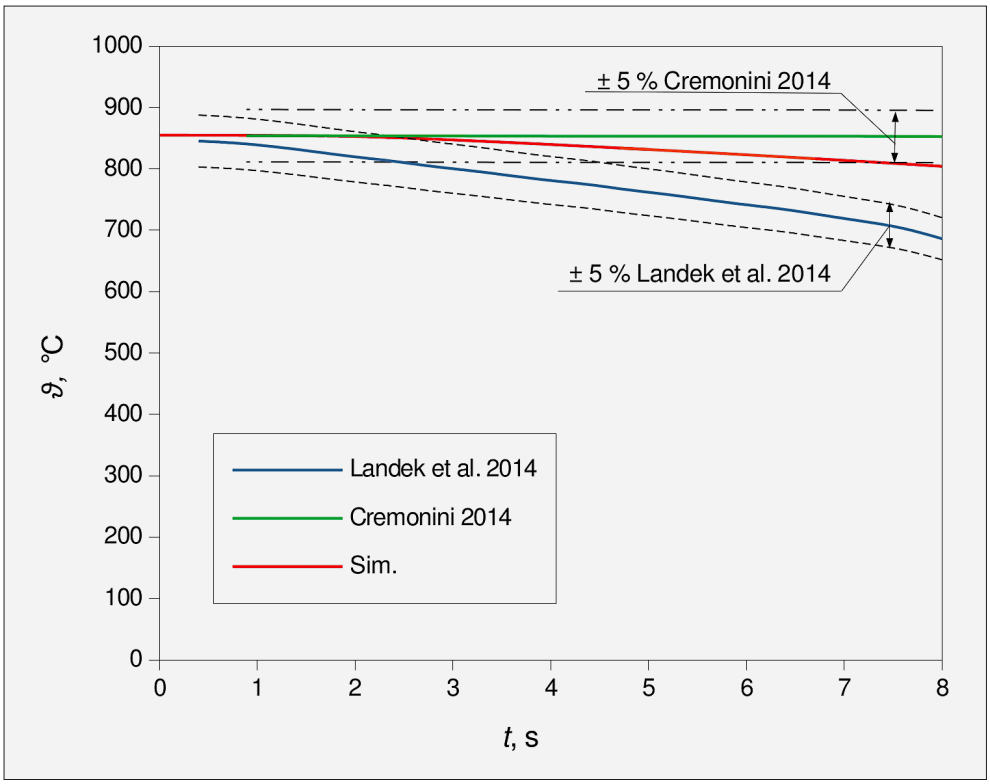
Za potrebe kvalitativne analize polja temperature unutar materijala i ponašanja parnoga omotača proveden je eksperiment s približnom temperaturom vode od 52 °C. Tako je ponašanje parnoga omotača vidljivo na **slici 5**.

Slika 5a otkriva kako se radi o prisutnosti prostornih temperaturnih gradijenata unutar materijala uslijed nejednolike temperaturne raspodjele, tj. prisutne su zone s povišenom temperaturom (istaknuta crvena boja materijala) i tamne zone s nižom temperaturom (označeno linijom crta-točka-crta žute boje). Navedeno implicira slučaj $Bi \rightarrow +\infty$, kada su znatni prostorni temperaturni gradijenti unutar krutine. Nadalje, **slika 5a** (plavi crtkani pravokutnik) otkriva začetak fronte kvašenja na donjoj strani uzorka. Napredovanjem fronte kvašenja, kako je pokazano na **slici 5b**, uočava se njezina egzistencija na objema stranama uzorka. Naposljetku, filmsko isparivanje završeno je kada su se susrele fronte kvašenja, **slika 5c**. S obzirom na to da su ove fotografije izrađene pri temperaturi kupke 52 °C, ova su razmatranja kvalitativne naravi. Za rigoroznu usporedbu sposobnosti numeričke metode za procjenu nestacionarne temperaturne raspodjele u središtu uzorka, u okviru ovoga istraživanja korišteni su eksperimentalni rezultati dobiveni za gašenje u kapljevitoj vodi temperature 60 °C, koji su dostupni u Landek et al. (**Landek et al., 2014**).

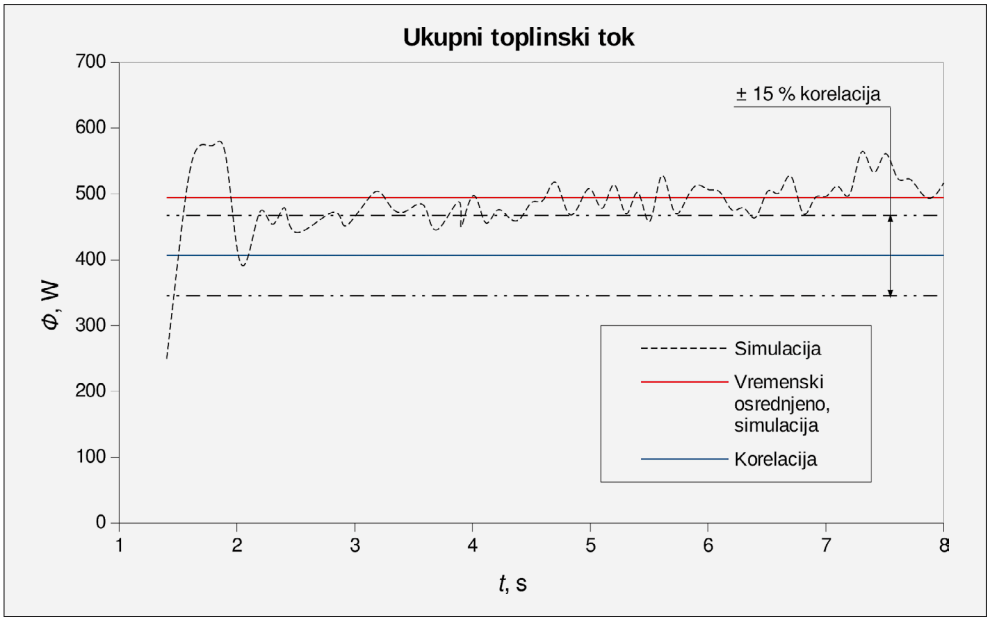
4. Rezultati

Za razliku od studije Cukrov et al. (**Cukrov et al., 2023a**), u kojoj su temperature iz središta uzorka dobivene numeričkom simulacijom uspoređene s rezultatima dostupnim u Landek et al. (**Landek et al., 2014**), u ovome je istraživanju provedena dodatna usporedba s mjernim rezultatima koje navodi Cremonini (**Cremonini, 2014**), a koji su dobiveni korištenjem vode temperature 60 °C, s razlikom da se u tome istraživanju koristi destilirana voda. Prikaz nestacionarne promjene temperature u središtu uzorka nalazi se na **slici 6**.

Iz dobivenih se rezultata vidi kako se primjenom predložene metode mogu postići zadovoljavajuće točna rješenja temperaturne distribucije u središtu uzorka. Naravno, daljnjim radom na modeliranju turbulencije moglo bi se postići još bolje slaganje s eksperimentalnim rezultatima. Međutim, cilj je ovoga rada izbjeći bilo kakvo ugađanje rezultata te primjenom bazičnih principa doći do zadovoljavajuće točnoga rješenja za inženjersku primjenu. Metoda je ograničena na slučaj filmskoga isparivanja te je daljnji rad usmjeren na pronalaženje načina modeliranja raskidanja parnoga omotača. Učinkovitost predložene metode vidljiva je u pojasu pogreške ± 5 %, koji je pridružen dostupnim eksperimentalnim podatcima. Očito je da blaga razina turbulencije, uočena u Cremonini (**Cremonini, 2014**), gdje je eksperiment proveden s destiliranom vodom temperature 60 °C, bolje

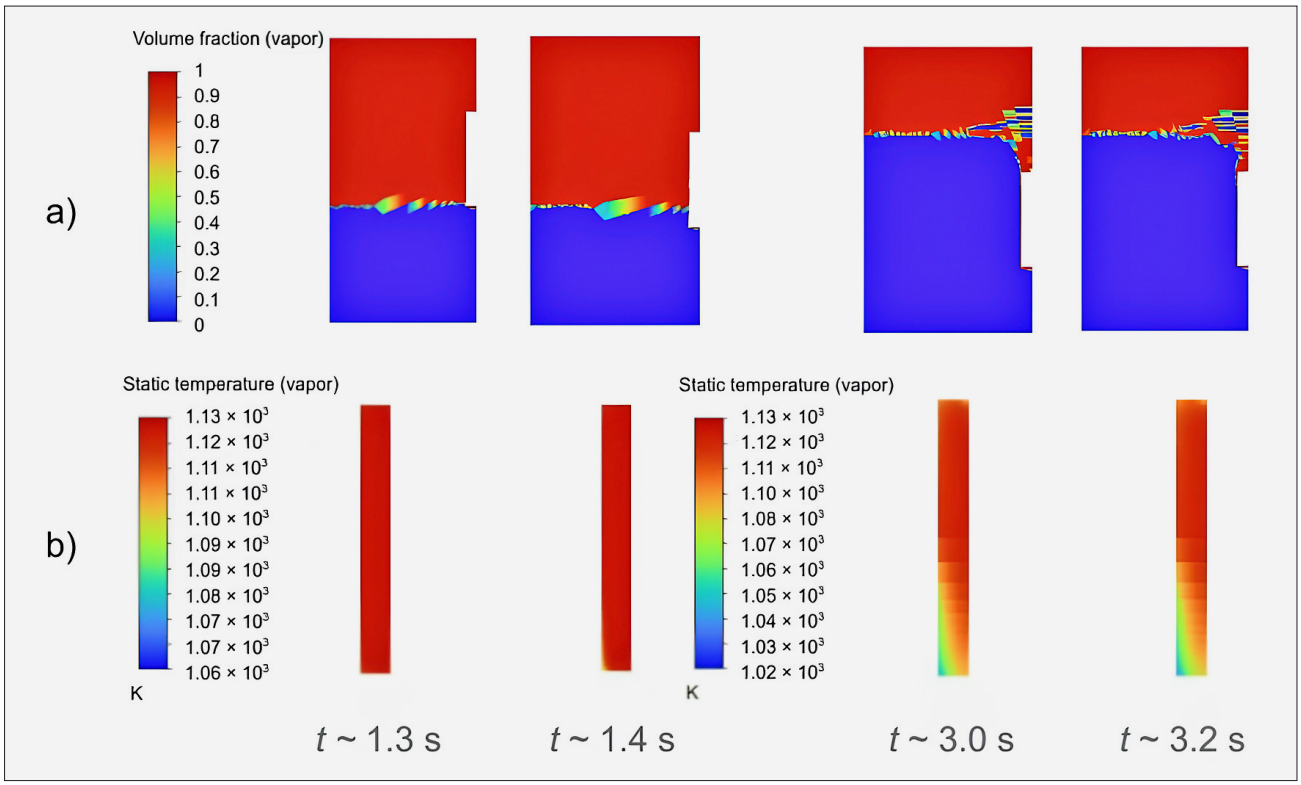


Slika 6: Usporedba rezultata proračuna s eksperimentalnim rezultatima dostupnim u Landek et al. (**Landek et al., 2014**) i Cremonini (**Cremonini, 2014**). Eksperimentalni rezultati očitani su korištenjem softvera (**Rohatgi, 2021**).



Slika 7: Ukupni toplinski tok prenesen s površine uzorka na okolni medij tijekom prvih 8 s procesa gašenja uranjanjem u kapljevinu. Usporedba s rezultatima dobivenim korištenjem korelacija u Momoki (**Momoki et al., 2007**).

odgovara numeričkom rješenju dobivenom korištenjem vrijednosti kinetičke energije turbulencije 0,1 m^2/s^2. S druge strane, u eksperimentu koji provode Landek et al. (**Landek et al., 2014**) turbulencija je snažnija, pa numeričko rješenje dobiveno predloženom metodom ulazi u zadani interval pogreške proračuna samo unutar prvih ~ 2,5 s ukupnoga trajanja ove simulacije. Nadalje, analizom toplinskoga toka, trenutačnoga i vremenski osrednjenoga po cjelokupnoj površini valjka, utvrđeno je njegovo dobro slaganje s proračunom korištenjem korelacija dostupnih u Momoki et al. (**Momoki et al., 2007**), kako je prikazano na **slici 7**. Može se uočiti, s obzirom na točnost proračuna i učinkovitost modela, da je nadmašena vrijednost dobivena korelacijom malo iznad 15 %, kao što je vidljivo iz propisanoga pojasa pogreške, odabranoga prema pojasu pogreške u Momoki et al. (**Momoki et al., 2007**), koji je, međutim, pripisan procijenjenoj vrijednosti koeficijenta prijelaza topline u njihovu istraživanju filmskoga isparivanja. Trenutačne vrijednosti toplinskoga toka upadaju periodički u pripisani pojas pogreške, kao što je također prikazano na **slici 7**. Ove nestacionarne oscilacije prisutne su uslijed oscilira-



Slika 8: Rezultat numeričke simulacije procesa gašenja uranjanjem: razvoj a) volumnoga udjela parne faze; b) temperaturnoga polja krutine, oboje tijekom gašenja (t ~ 1,3 i 1,4 s) i nakon što je materijal uronjen u kapljevitu kupku za gašenje (t ~ 3,0 i 3,2 s).

juće prisutnosti tzv. suhih točaka (eng. *dry spots*) tijekom procesa isparivanja (više o tome u nedavnoj studiji koju provode Tecchio et al. (**Tecchio et al., 2024**)).

Iz dobivenih rezultata također je uočljivo kako su simulacijom obuhvaćeni i mnogi detalji vezani uz sâm proces uranjanja. Tako je razvidno naglo povećanje toplinskoga toka s površine uzorka kada se uzorak nalazi neposredno iznad slobodne površine medija za gašenje.

Praćenjem polja volumnoga udjela parne faze (**slika 8a**) može se uočiti eksplozija pare koja se događa nakon što materijal dotakne slobodnu površinu kapljevite kupke preko promjene polja volumnoga udjela parne faze. Ovo dovodi do spomenutoga naglog porasta toplinskoga toka, prikazanoga na **slici 7**. Problem razmazane distribucije volumnoga udjela parne faze za t ~ 1,3 i 1,4 s (**slika 8a**) vidljiv je u području podalje od krutoga tijela. Ovo je posljedica korištenja neortogonalne mreže u ovome istraživanju, tj. linija mreže ne poklapa se s razinom kapljevine. Međutim, s obzirom na to da se razmazanost ne pojavljuje u neposrednoj blizini krutoga tijela, smatramo da ima mali utjecaj na proces gašenja. Za t ~ 3,0 i 3,2 s (**slika 8a**) stratificirana kapljevita faza uočena je iznad krutoga tijela, koja je također razmatrana kao numerička pogreška. Vjerujemo da je ova pogreška rezultat oblika mreže i modela neprekinute površinske sile (eng. *continuum surface force*, CSF; **Brackbill et al. 1992**) korištenoga za površinsku napetost, koja može biti popravljena korištenjem modela neprekinutoga površinskog naprezanja (eng. *continuum surface stress*) umjesto toga, kako je objašnjeno u Kharangate i Mudawar (**Kharangate and Mudawar, 2017**), ali ostavljamo ovo pitanje za daljnja istraživanja.

Iz temperaturne distribucije unutar krutine (**slika 8b**) može se uočiti uspješnost metode u procjeni temperaturne distribucije unutar materijala tijekom gašenja uranjanjem u kapljeviti medij, posebno nakon što je materijal uronjen neko vrijeme u kapljevitu kupku za gašenje. Ovo napredovanje smanjenja temperature odozdo prema gore može se, barem kvalitativno i u određenoj mjeri, usporediti s distribucijom u Demirel (**Demirel, 2009**), koja je dobivena primjenom metode konačnih elemenata (MKE).

5. Zaključak

U provedenome istraživanju razvijen je novi model prijenosa mase na granicama faza temeljen na toplinskoj bilanci na granici faza, u kojemu se kao fiktivna varijabla koristi koeficijent prijelaza topline time što se putem te veličine aproksimira udaljenost središta kontrolnoga volumena koji sadržava granicu faza i same granice faza te uvodi toplinska provodnost u aproksimativni izraz za izračun gustoće toplinskoga toka na granici faza. Rezultati provedenih proračuna potvrđuju sljedeće:

- Provedenim rješavanjem Štefanova problema pri višim pregrijanjima stijenke uočeno je dobro slaganje s analitičkim rješenjem.

- Uočeno je brže gibanje granice kapljevina-para pri višim temperaturama pregrijanja stijenke kod većega temperaturnog gradijenta na strani parne faze (kapljevita je faza pri temperaturi zasićenja, pa u njoj nema temperaturnoga gradijenta).
- Relativno položit temperaturni tijek dobiven numeričkom simulacijom također je potvrđen eksperimentalnim podatcima dostupnim u literaturi te označava blagu turbulenciju u okolnome mediju tijekom režima filmskoga isparivanja.
- Praćenjem distribucije toplinskoga toka u vremenu uočen je njegov skokovit rast neposredno nakon što materijal uzorka dolazi u kontakt sa slobodnom površinom medija za gašenje. Pri tome je prosječna vrijednost toplinskoga toka, dobivena numeričkom simulacijom, 494,3 W.
- Analizom polja fizičkih veličina, volumnoga udjela parne faze i temperaturnoga polja unutar krutine potvrđena je relevantnost predložene numeričke metode za numeričko modeliranje filmskoga isparivanja prilikom gašenja uranjanjem u kapljeviti medij.

Navedeno implicira kako se razvijeni numerički postupak može sa sigurnošću primijeniti u industrijskim proračunima filmskoga isparivanja tijekom procesa gašenja uranjanjem, uz napomenu da je potrebno inicijalno zadati početnu temperaturu predmeta i medija za gašenje te vrijednost kinetičke energije turbulencije, koja ovisi o zadanim uvjetima strujanja. Pri tome treba voditi računa modelira li se matematički isparivanje u mirujućoj kapljevini (engl. *pool boiling*) ili je riječ o isparivanju uz prisutnost prisilne konvekcije (engl. *forced convection boilin*g).

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6. Literatura

Ansys® Fluent, 2019. ANSYS Fluent Theory Guide, Release 19.2, Help System. ANSYS, Inc.

Arévalo, R., Antúnez, D., Rebollo, L., Abánades, A., 2014. Estimation of radiation coupling factors in film boiling around spheres by mean of Computational Fluid Dynamics (CFD) tools. International Journal of Heat and Mass Transfer 78, 84–89. https://doi.org/10.1016/j.ijheatmasstransfer.2014.06.063

Brackbill, J.U., Kothe, D.B., Zemach, C., 1992. A continuum method for modeling surface tension. Journal of Computational Physics 100, 335–354. https://doi.org/10.1016/0021-9991(92)90240-Y

Cremonini, G.E.S. de O., 2014. Aplicação do método inverso de condução de calor na avaliação de fluidos de resfriamento para têmpera.

Cukrov, A., Landek, D., Sato, Y., Boras, I., Ničeno, B., 2023a. Water Entry of a Heated Axisymmetric Vertical Cylinder. Energies 16. https://doi.org/10.3390/en16247926

Cukrov, A., Sato, Y., Boras, I., Ničeno, B., 2023b. Film Boiling around a Finite Size Cylindrical Specimen – A Transient Conjugate Heat Transfer Approach. Applied Sciences 13. https://doi.org/10.3390/app13169144

Cukrov, A., Sato, Y., Boras, I., Ničeno, B., 2021. A solution to Stefan problem using Eulerian two-fluid VOF model. Brodogradnja : Teorija i praksa brodogradnje i pomorske tehnike 72, 141–164. https://doi.org/10.21278/brod72408

de Bertodano, M.L., Fullmer, W., Clausse, A., Ransom, V.H., 2017. Introduction, in: Bertodano, M.L. de, Fullmer, W., Clausse, A., Ransom, V.H. (Eds.), Two-Fluid Model Stability, Simulation and Chaos. Springer International Publishing, Cham, pp. 1–8. https://doi.org/10.1007/978-3-319-44968-5_1

Demirel, C., 2009. Experimentelle Untersuchung und Simulation des Abschreckprozesses von bauteilähnlichen Geometrien aus G-AlSi7Mg.

Denèfle, R., Mimouni, S., Caltagirone, J.-P., Vincent, S., 2015. Multifield hybrid approach for two-phase flow modeling – Part 1: Adiabatic flows. Computers & Fluids 113, 106–111. https://doi.org/10.1016/j.compfluid.2014.07.018

Drew, D.A., Passman, S.L., 1999. Continuum Balance Equations for Multicomponent Fluids, in: Theory of Multicomponent Fluids. Springer New York, New York, NY, pp. 65–80. https://doi.org/10.1007/0-387-22637-0_7

Edelbauer, W., Zhang, D., Kopun, R., Stauder, B., 2016. Numerical and experimental investigation of the spray quenching process with an Euler-Eulerian multi-fluid model. Applied Thermal Engineering 100, 1259–1273. https://doi.org/10.1016/j.applthermaleng.2016.02.131

El Kosseifi, N., 2012. Numerical simulation of boiling for industrial quenching processes, Simulation numérique de l'ébullition pour les procédés de trempe industrielle. Ecole Nationale Supérieure des Mines de Paris.

Gauss, F., Lucas, D., Krepper, E., 2016. Grid studies for the simulation of resolved structures in an Eulerian two-fluid framework. Nuclear Engineering and Design 305, 371–377. https://doi.org/10.1016/j.nucengdes.2016.06.009

Hillier, A., Doorsselaere, T.V., Karampelas, K., 2020. Estimating the Energy Dissipation from Kelvin–Helmholtz Instability Induced Turbulence in Oscillating Coronal Loops. ApJL 897, L13. https://doi.org/10.3847/2041-8213/ab9ca3

Höhne, T., Vallée, C., 2010. Experiments and Numerical Simulations of Horizontal Two-Phase Flow Regimes Using an Interfacial Area Density Model. The Journal of Computational Multiphase Flows 2, 131–143. https://doi.org/10.1260/1757-482X.2.3.131

Kharangate, C.R., Mudawar, I., 2017. Review of computational studies on boiling and condensation. International Jour-

nal of Heat and Mass Transfer 108, 1164–1196. https://doi.org/10.1016/j.ijheatmasstransfer.2016.12.065

Kopun, R., Škerget, L., Hriberšek, M., Zhang, D., Edelbauer, W., 2014. Numerical Investigations of Quenching Cooling Processes for Different Cast Aluminum Parts. Strojniški vestnik - Journal of Mechanical Engineering.

Landek, D., Župan, J., Filetin, T., 2014. A Prediction of Quenching Parameters Using Inverse Analysis. Matls. Perf. Charact. 3, 229–241. https://doi.org/10.1520/MPC20130109

Momoki, S., Yamada, T., Shigechi, T., Kanemaru, K., Yamaguchi, T., 2007. Film Boiling Around a Vertical Cylinder With Top and Bottom Horizontal Surfaces, in: HT2007. ASME/JSME 2007 Thermal Engineering Heat Transfer Summer Conference, Volume 2, pp. 611–619. https://doi.org/10.1115/HT2007-32733

Perez-Raya, I., Kandlikar, S.G., 2018. Discretization and implementation of a sharp interface model for interfacial heat and mass transfer during bubble growth. International Journal of Heat and Mass Transfer 116, 30–49. https://doi.org/10.1016/j.ijheatmasstransfer.2017.08.106

Pointer, W.D., Liu, Y., 2017. Eulerian two-fluid RANS-based CFD simulation of a helical coil steam generator boiling tube, in: Proc. 17th International Topical Meeting on Nuclear Reactor Thermal Hydraulics. Xi'an, China, p. 19.

Rohatgi, A., 2021. Webplotdigitizer: Version 4.5.

Srinivasan, V., Moon, K.-M., Greif, D., Wang, D.M., Kim, M., 2010. Numerical simulation of immersion quench cooling process using an Eulerian multi-fluid approach. Applied Thermal Engineering 30, 499–509. https://doi.org/10.1016/j.applthermaleng.2009.10.012

Stark, P., Fritsching, U., 2015. Simulation of the impinging liquid jet cooling process of a flat plate. International Journal of Numerical Methods for Heat & Fluid Flow 25, 153–170. https://doi.org/10.1108/HFF-04-2013-0151

Steuer, R., 2015. Ultraschallunterstütztes Flüssigkeitsabschrecken bei der Wärmebehandlung metallischer Werkstoffe, Forschungsberichte des Lehrstuhls für Werkstofftechnik der Universität Rostock. Shaker Verlag, Aachen.

Štrubelj, L., Tiselj, I., Mavko, B., 2009. Simulations of free surface flows with implementation of surface tension and interface sharpening in the two-fluid model. International Journal of Heat and Fluid Flow 30, 741–750. https://doi.org/10.1016/j.ijheatfluidflow.2009.02.009

Subhash, M., 2017. Computational modelling of liquid jet impingement onto heated surface (Ph.D. Thesis). Technische Universität, Darmstadt.

Sun, D.-L., Xu, J.-L., Wang, L., 2012. Development of a vapor–liquid phase change model for volume-of-fluid method in FLUENT. International Communications in Heat and Mass Transfer 39, 1101–1106. https://doi.org/10.1016/j.icheatmasstransfer.2012.07.020

Tecchio, C., Cariteau, B., Houedec, C.L., Bois, G., Saikali, E., Zalczer, G., Vassant, S., Roca i Cabarrocas, P., Bulkin, P., Charliac, J., Nikolayev, V.S., 2024. Microlayer evaporation during bubble growth in nucleate boiling. International Journal of Heat and Mass Transfer 231, 125860. https://doi.org/10.1016/j.ijheatmasstransfer.2024.125860

Yamada, T., Shigechi, T., Momoki, S., Kanemaru, K., 2001. An Analysis of Film Boiling around a Vertical Finite-Length Cylinder. Reports of the Faculty of Engineering, Nagasaki University 31, 1–11.

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