Simulation of the Casting and Quenching Process of a Laboratory AlSi7MgCu05 Casting

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1 Abstract

The goal of this work is the numerical simulation and experimental validation of the temperature field in an A356 laboratory scale casting during quenching. A standard Eulerian two-fluid model, being implemented into the commercial CFD software ANSYS (Fluent 6.3) and extended by user defined subroutines is used. The CFD calculation includes the two phase water/vapor-flow and the temperature field in the quenching medium and in the casting component. The formation of the vapor due to boiling is also taken into account. The heat transfer at the interface between the casting component and the quenching medium is governed by the so-called film boiling regime at the initial stage and the nucleate boiling regime in the later stage. The established Bromley-correlation is modified by a correction factor and used to calculate the heat transfer coefficient in the film boiling regime. To estimate and optimize the heat transfer for all regimes a reverse optimization task was solved based on experimental temperature curves. The water/vapor mass transfer rate due to boiling is correlated with the particular heat transfer coefficient. The condensation of vapor is ignored. The predicted cooling curve in the laboratory casting shows acceptable agreement with the experimental results. This indicates that the model can be further developed e.g. for the calculation of the temperature field during quenching of 3D industrial castings.

2 Introduction

A typical heat treatment applied to sand and gravity die-cast Al-Si alloys is the so called T6 heat treatment [1]. The casting is first heated to a high temperature close to the solidus temperature (~535°C) and then quenched by immersing into a liquid bath [2]. Due to the superheated walls of the casting a stable vapor film forms along the hot surface which exhibits an insulating effect, so that the cooling rate during this film boiling period is relatively low. This leads to a nearly linear relation between wall temperature and time. When the temperature of the surface falls below the so called Leidenfrost-temperature the vapor film collapses and nucleate boiling begins [3]. During this stage, the highest cooling rate is observed. The curve of wall temperature versus time turns into hyperbolic shape [4]. At this period large thermal gradients appear and might cause significant thermal stresses. In many cases, this thermal stresses can result in serious distortion of the casting [5]. The problem cannot be solved by choosing a lower cooling rate. Because of thermodynamic reasons a lower cooling rate would have negative impacts on the effectiveness of the heat treatment process [6]. Because of these contradictory goals, there is a big demand from casting industry to optimize the cooling conditions during quenching.

In the context of computational fluid dynamics Wang and co-workers [2] proposed a numerical model for the quenching process. A preliminary simulation on a laboratory casting has demonstrated that the flow dynamics as observed in experiments could be reproduced by the numerical model. The further development of this model was applied to calculate the water quenching of an engine cylinder head [4]. The authors were able to obtain good qualitative agreement between the calculated and the measured cooling curves in the casting. Srinivasan and co-workers presented a code coupling approach for the numerical simulation of the direct immersion quenching process. In this new approach numerical simulations within the fluid and solid domain were linked via a code coupling interface and data was constantly exchanged across this interface [7]. The predictive capability of this model has been verified under a wide range of different quenchant temperatures.

The goal of the present work is to predict the temperature field in an A356 step plate casting during quenching by means of numerical simulation. A standard Eulerian two fluid model being implemented into the commercial CFD software ANSYS (Fluent 6.3) and extended by user defined subroutines is used. Additionally the open source optimization tool DAKOTA [9] is used to inversely determine the model parameters namely the correction factor to the Bromley correlation and heat transfer coefficients in the nucleate boiling and convective

cooling regimes. The simulation results are evaluated against measured temperature time curves of a laboratory A356 step plate casting. Experimental curves for the A356 step plate used in the presented studies showed much steeper cooling rates in the film boiling regime than those based on the Bromley correlation [8]. This can be explained by the complex geometry of the sample, where different regimes in thinner and thicker parts occur simultaneously.

3 Mathematical Model

In the present paper a simulation approach is presented for modeling the quenching process based on the Eulerian two-fluid method with the commercial CFD software ANSYS (Fluent 6.3). The Eulerian multiphase model solves continuity, momentum and energy equations for each phase and is used to model multiple interpenetrating phases. The coupling among phases is achieved through inter-phase exchange terms [10]. The dynamic process of the immersion of the solid in the quenchant was not taken into account. The initial condition of the simulation is the submerged state.

3.1 Boiling Model

The name film boiling, has been given to that type of boiling when a complete vapor film exists between the heated surface and the boiling liquid [8]. Bromley derived a correlation for the heat transfer coefficient (*HTC*) in the stable film boiling for natural convection from the outside of a horizontal tube. The same theory as for the horizontal tube may also be applied for a vertical tube [8]. In this work a dimensionless correction factor $C_{Bromley}$ was added.

$$HTC_{film} = C_{Bromley} \cdot 0.62 \cdot \left[\frac{k_v{}^3 \cdot \rho_v \cdot (\rho_w - \rho_v) \cdot g \cdot (H_{wg} + 0.4 \cdot C_{pv} \cdot \Delta T)}{D_0 \cdot \mu_v \cdot \Delta T}\right]^{1/4} \left[\frac{\mathrm{W}}{\mathrm{m^2 K}}\right] \quad (1)$$

In this equation k_v is the thermal conductivity of vapor in $W \cdot m^{-1} \cdot K^{-1}$, ρ_v ρ_w is the density for vapor and liquid water in $kg \cdot m^{-3}$ respectively. The latent heat of evaporation in $J \cdot kg^{-1}$ is H_{wg}, μ_v is the dynamic viscosity of vapor in $kg \cdot m^{-1} \cdot s^{-1}$. The diameter of the vapor bubbles D_0 is modeled with the constant value of 3mm. The specific heat of vapor is C_{pv} in $J \cdot kg^{-1} \cdot K^{-1}$.
The wall superheat ΔT [K] is the difference between the wall temperature and the saturation temperature of the quenching liquid. The saturation temperature of the liquid is 372 K and modeled as constant equal to the temperature of the vapor phase. No thermal energy exchange between liquid and vapor phase taken into account in the present model.

$$\Delta T = T_{wall} - T_{sat} \ [K] \tag{2}$$

Instead of the so called Leidenfrost-temperature a point in time was used as criteria for transition from the film boiling to the nucleate boiling regime. This time was based on experimental determined cooling curves. Also the transition from nucleate boiling to solely convective heat transfer was defined in the same way and is expressed by Eq. 3. So far this method is sufficient for the simplified calculation of the temperature field in the casting during the quenching process.

$$HTC = \begin{cases} \mathrm{C_{Bromley}} \cdot HTC_{film} \left[\frac{\mathrm{W}}{\mathrm{m^2K}}\right], & t < 1.53\ s \\ \text{Nucleate Boiling } HTC_1 \left[\frac{\mathrm{W}}{\mathrm{m^2K}}\right], & 1.53\ s \leq t \leq 4.5\ s \\ \text{Convective Boiling } HTC_2 \left[\frac{\mathrm{W}}{\mathrm{m^2K}}\right], & t > 4.5\ s \end{cases} \tag{3}$$

The CFD software Ansys FLUENT allows to define different phases and their interactions. Furthermore the CFD software provides the implementation of so called user defined functions (UDFs) for customizing the software for various types of problems. For modeling the mass transfer in this multiphase problem a UDF written in C is used. Since the mass transfer rate is coupled with the heat transfer, it is reasonable to model the mass transfer rate proportional to the heat transfer as shown in Eq. (4) [2]. The calculated value of the mass transfer is returned by the UDF to the FLUENT solver.

$$\dot{m}_{lg} = \frac{c_m \cdot HTC \cdot A_{int} \cdot \Delta T}{H_{wg}} \left[\frac{\mathrm{kg}}{m^3 \mathrm{s}}\right] \tag{4}$$

The coefficient c_m is a correction coefficient in the order of 0.02. The interfacial area concentration A_{int} in Eq. (5) is calculated from the volume fraction of the vapor phase α_v [%] and the diameter of the vapor bubbles:

$$A_{int} = \frac{6\alpha_v}{D_0} \left[\frac{1}{\mathrm{m}}\right] \tag{5}$$

As an initial volume fraction of the vapor phase 0.1 % are used to avoid getting a zero value for the interfacial area at the beginning of the calculation. The heat flux from the wall to the liquid was calculated as:

$$\dot{q} = HTC \cdot (T_{Wall} - T_{solid}) \left[\frac{J}{m^2 \cdot s}\right] \tag{6}$$

3.2 Optimization model parameters

To find the optimum parameters for the film and nucleate boiling regimes as well as the heat transfer coefficient for the convective cooling of the step plate casting, an optimization task was solved. The object function to be minimized for the right cooling parameters of the model was formulated using the least square method as:

$$S = \sqrt{\sum_{i=1}^{N}\left(T_i^{sim} - T_i^{exp}\right)^2} \rightarrow min, \tag{7}$$

where T_i^{sim} are the simulated temperature values at the point which correspond to the measured temperature T_i^{exp}. N is the number of thermocouple measurements done during the experiment. It should be noted, that the temperature history was recorded during trials with the time step 0.01 seconds. Corresponding data writing frequency was used in the simulation to be able to compare the results at exactly the same moments in time.

To perform the optimization simulation the open-source software DAKOTA was used along with the FLUENT multiphase solver. Preprocessing module of DAKOTA package permitted to modify FLUENT starting files by varying input parameters. The required number of CFD batch-mode simulations was automatically performed for the optimization task. The Fletcher-Reeves conjugate gradient method from the CONMIN library [11] was used to estimate optimal model parameters.

4 Simulation Setup

The A356 step plate casting used in the experiments had step heights of 4, 6, 10 and 16 mm respectively. For the Euler-Euler multiphase flow simulation of the quenching process a computational domain of 300×120 mm in size was chosen. The boundary conditions used in the current simulations are shown in Fig. 1 (a). The grid (Fig. 1 (b)) consisted of 4000 cells of which 3813 were located in the fluid domain. An initial temperature of 761 K was patched to the solid domain as initial condition whereas the liquid domain was initialized with 332 K. Laminar flow assumptions were applied in the simulation and the resulting contributions of the turbulent heat fluxes were neglected.

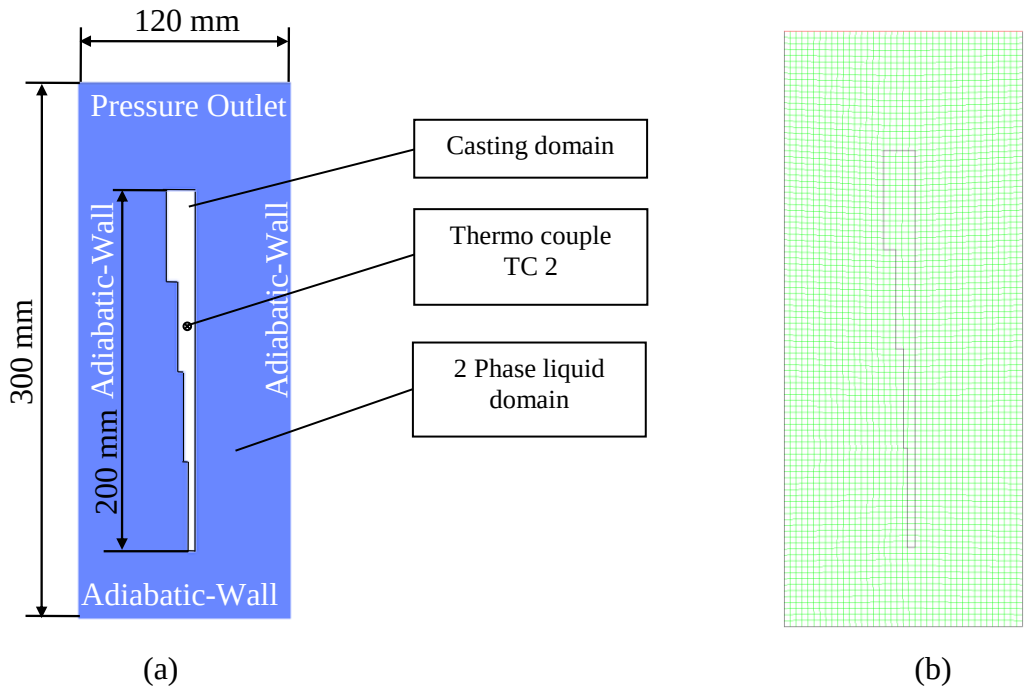


Figure 1: (a) Computational domain and boundaries with the position of the thermocouple 2 within the 10 mm step and (b) corresponding structured grid.

Vapor and water were assumed to be incompressible fluids with constant properties as shown in Table 1.

	ρ [kg·m^{-3}]	C_P [J·kg^{-1}·K^{-1}]	k [W·m^{-1}·K^{-1}]	μ [kg·m^{-1}·s^{-1}]
Water	998.2	4182	0.6	$1.003 \cdot 10^{-3}$
Vapor	0.5542	2014	0.0261	$1.34 \cdot 10^{-5}$

Table 1: Physical properties from the Ansys (Fluent 6.3) database

A constant time step of 0.01 seconds was used where maximum 100 iterations per time step were allowed in order to reduce the residuals to $1 \cdot 10^{-4}$. The simulation was stopped at a flow time of 7 seconds.

5 Results and Discussion

5.1 Optimization reuslts

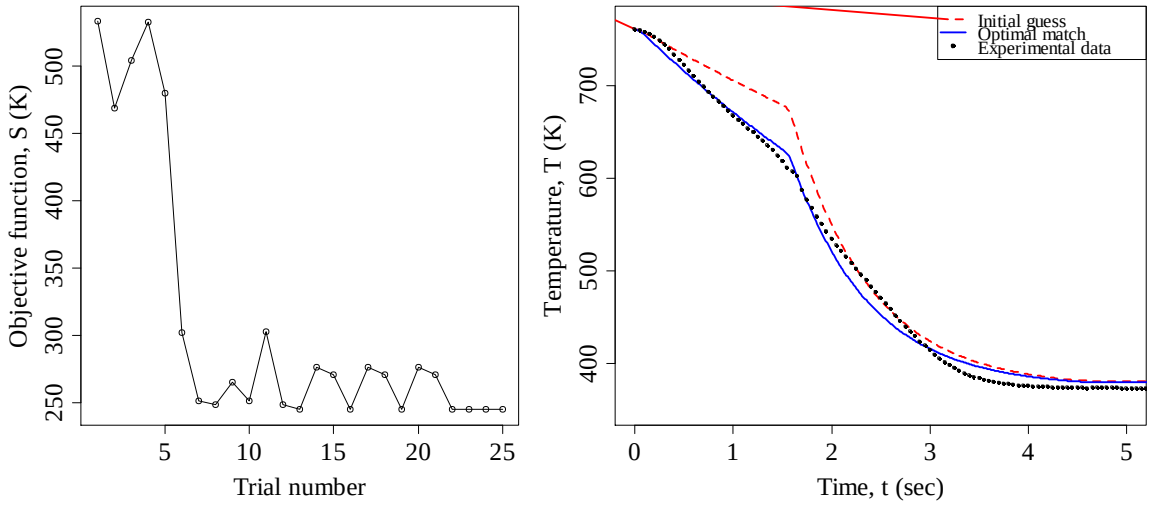
As the cooling at the position of TC2 depends on (i) the correction factor $C_{Bromley}$ of the Bromley correlation (Eq. (1)), (ii) the heat transfer coefficient for nucleate boiling (HTC_1) and (iii) that of the convective cooling regimes (HTC_2) also the object function (Eq. (3)) depends

on these quantities. The initial and final model parameters are presented in the Table 2. The results of the simulation are presented in Fig. 2, where the object function was evaluated for 25 points in times.

It is notable, how the simulated and experimental cooling curves, which do not fit each other at the beginning (red curve in Fig. 2(b)), meet quite well, with the best model parameters obtained (blue curve Fig. 2(b)).

	$C_{Bromley}$ [-]	HTC_1 [W·m^{-2}·K^{-1}]	HTC_2 [W·m^{-2}·K^{-1}]
Lookup range	8-30	10000-20000	1000-4000
Initial value	10	15000	2000
Optimal value	14,772	17500	2500

Table 2: Lookup range, initial and optimal parameters of the model



(a) (b)

Figure 2: Evolution of the objective function *S* (a) and the cooling curves for the initial guess and final solution compared to experimental data at thermo couple 2 (b)

It should be mentioned, that to obtain the presented results the coupling of the optimization tool with the CFD software was performed, which is of the great importance for the wide application range in engineering and simulation fields.

5.2 Simulation results with optimized HTC's

The movement from the heating furnace to the quenching basin took approximately 50 seconds and caused a temperature loss in the order of 40 K and an inhomogeneous temperature distribution. For the simulation the starting temperature casting was set to 761 K for the whole casting. In Fig. 3 the volume fraction of the vapor phase in the film boiling regime is shown at t = 0.1s and t = 1.5s. At the initial stage vapor starts to form in the corners of the steps. At t = 0.1s the casting is partially surrounded by a vapor film with only a low volume fraction of vapor. The correction coefficient $C_{Bromley}$ which is a result of the least squares optimization loop shows that the *HTC* in the film boiling regime is approximately 15 times higher than calculated by Bromleys equation for stable film boiling. This discrepancy can be explained by the fact that there is not a complete vapor film covering the whole casting surface and acting as an isolating. The relative small amount of vapor phase (Fig. 3a), which is only partially covering the casting surface leads to much higher HTC than predicted by equation (1) which is only valid if a complete vapor films exists between heated surface and boiling liquid.

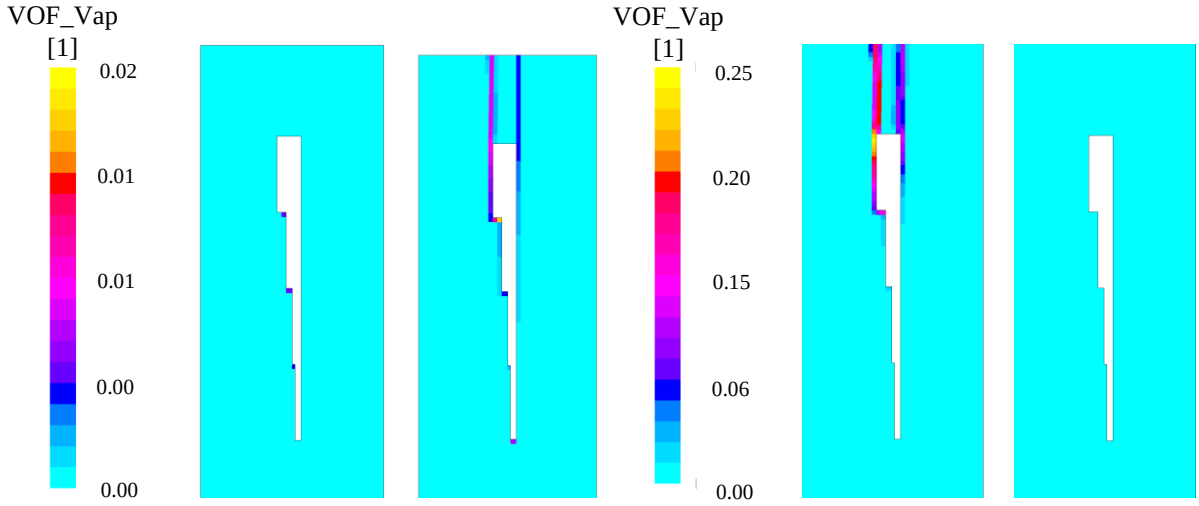


Figure 3: Phase fraction of the vapor phase in the (a) film boiling regime ($t \leq 1.53$ s) and (b) during the nucleate boiling regime ($t > 1.53$ s)

The velocity field at t = 1.5s (Fig. 4a) causes mixing of hot fluid originated near the surface of the casting with cooler fluid farer away from the hot solid surface. The experimental cooling curves and also the simulation results of the vapor volume fraction and the velocity field show that there is no pure film boiling regime during quenching of the step plate geometry.

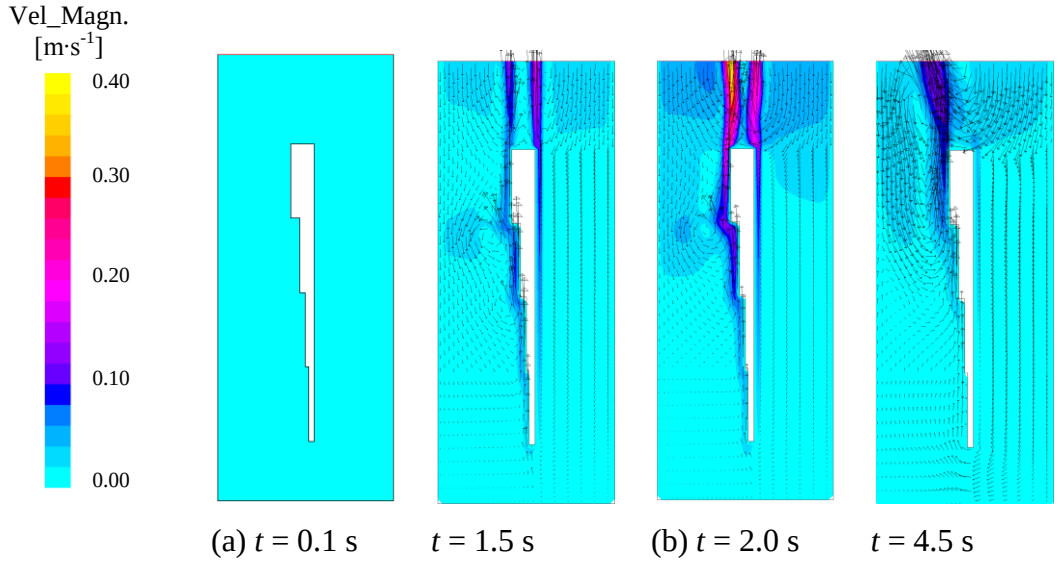


Figure 4: Contour of velocity magnitude and velocity vectors of the liquid phase in the (a) film boiling regime ($t \leq 1.53$ s) and (b) the nucleate boiling regime ($t > 1.53$ s)

As mentioned above the model was set such that the nucleate boiling regime starts at t = 1.53 s. Due to the strong cooling of the 4, 6 and 10 mm steps during the first 1.5 seconds, only in the surrounding of the 16 mm step a region of intense vapor formation is predicted. At t = 2.0 s the vapor film disintegrates due to the drag forces of the bubbles resulting in a noticeable upstream flow. The increasing fluid velocity causes a good mixing of the liquid resulting in strong cooling. After t = 4.5 s (Fig. 4b) there is no noticeable vapor formation any longer which is typically for the convection regime. The measured and simulated cooling curves show a qualitatively agreement at the point TC2.

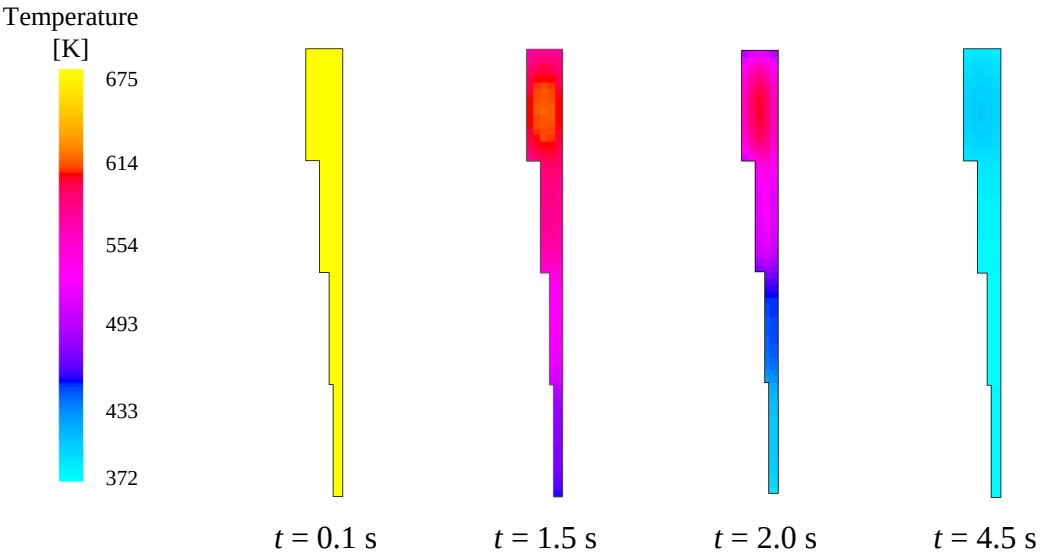


Figure 5: Contour of the casting temperature at different moments, the initial temperature of the casting is 761.19 K.

In Fig. 5 the temperature fields within the casting at different points in time are shown. Due to the non-uniformity of the temperature distribution in the casting thermal stresses are induced

during cooling. The temperature history could be further used for calculating stress and distortion with a FEM model. To create a supersaturated state with respect to Mg/Cu concentration it is necessary to cool the material rapidly to avoid kinetic processes where precipitations occur [12]. So the cooling rate which can be calculated from the temperature history is an important parameter to control the quality of the quenching process.

6 Conclusion

An Eulerian two-fluid model extended by user defined functions has been used for the calculation of the temperature history in an A356 casting during quenching. The CFD calculation is embedded in an open source optimization code where the CFD software was running in batch mode. After 25 attempts the optimum parameters for the *HTC* were found. To take into account the transitions between film boiling, nucleate boiling and finally to the convective regime the implemented model switches at defined time steps between different HTCs. With the exception of the HTC for the film boiling which is calculated by Bromleys equation the HTCs in the other regimes are modeled constant. In reality all three regimes may appear at the same time at different areas of the casting. The quality of the numerical model was validated by comparison of calculated cooling curves with measured cooling curves obtained by quenching of a step plate casting into water. It has been shown that the cooling curves calculated by the presented methods show an acceptable agreement with the measured data in the casting.

7 References

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