Investigating the suitability of using a single heat transfer coefficient in metal casting simulation: An inverse approach

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Abstract. In metal casting simulation the Heat Transfer Coefficient (HTC) is unknown as it depends on melt and mold materials, on the casting modulus at different regions of the casting and on local conditions at the mold-casting gap. In this paper, thermocouple measurements at three regions of a brass investment casting provided reference cooling curves. A genetic algorithm (GA) determined the optimum 3-step time-dependent HTC for the whole of the casting in a simulation program for which cooling curves are as close as possible to the reference curves. The resulting prediction of solidification times is satisfactory but prediction of qualitative characteristics such as start / end of solidification in different regions was not accurate enough.

Introduction

Casting simulation can assist in selection of optimal process parameters, namely melt temperature, mold preheat temperature, melt inlet pressure and velocity, as well as design of the feeding system. The computational power which is available nowadays allows ‘virtual casting’ involving thermal, mechanical and flow domains, thus replacing costly real-life experiments [1]. Although the definition of the model is dictated by experimental conditions [2], heat transfer through the casting-mold interface is to be guessed; this is described by the “Interfacial Heat Transfer Coefficient (IHTC)” or simply “Heat Transfer Coefficient (HTC)”. Heat transfer across the interface is determined by solid-to-solid conduction, conduction through the gas phase and radiation [3]. HTC is affected by the thermo-physical properties of the materials at the interface (cast metal, mold, coating) such as fluidity or solidification range [4]. At least three different representations of the HTC evolution have been proposed, namely: a step function of temperature, a step function of time (which is implicitly associated with solidification phases) [4] and an exponential function of time as a continuous approximation of the latter [5,6].

The well-known Chvorinov’s rule [7] depicts a strong relation between solidification time and casting modulus (volume over surface area of the casting) implying that the different regions of the casting exhibit different solidification times [8]. Although it is commonly acknowledged that different HTCs should be assigned to regions of the casting with “significantly different” geometrical characteristics [9], only few publications investigate this issue [1,4,10,11].

In determining HTC, most commonly, temperature transients are measured close to the metal/mold interface using thermocouples despite their embedding close to the interface. This data can then be used combined with either an inverse calculation [12] or with repetitive simulations

[13], until an HTC is identified that results in good agreement with the experiment. These methods can become substantially complex by employing, e.g., 3D instead of 2D models, various "local" HTCs tied to corresponding casting moduli or intricate optimization algorithms. Partitioning the casting shape into different complementary regions differing to a significant enough extent in casting modulus might be challenging, therefore an approach adopting a single HTC is a welcome simplification.

In order to avoid such complexity the present paper aims to answer the following questions: (a) Is it feasible to determine one 'equivalent' HTC and apply this to the whole casting domain during simulation instead of applying several different HTCs for different sub-domains? (b) How efficient is the use of genetic algorithms in the determination of HTCs?

The next section describes the experiment that provided the reference cooling curves. This is followed by two sections presenting the numerical simulation setup that was used in the evaluation function of the genetic algorithm that determines the optimum HTC and the setting up of this algorithm as well. Results and their discussion in the context of alternative genetic algorithm hyperparameters follow. Last, conclusions and further work are briefly summarized.

Experimental

A particular experiment was conducted to provide reference cooling curves to be used in the simulation through which optimum HTC is to be determined.

Lost wax investment casting was performed for a part with a stepwise increase in cross section made of CuZn33 alloy (brass), Fig. 1(a,b). The casting consists of three coaxial consecutive cylinders, namely a large (L), a medium (M) and a small (S) one. Length of the cylinders is 8 mm and their diameter measures 16 mm, 10 mm and 4 mm, respectively. Thus, casting modulus results as 2.30, 1.98 and 0.89, for L, M and S regions respectively.

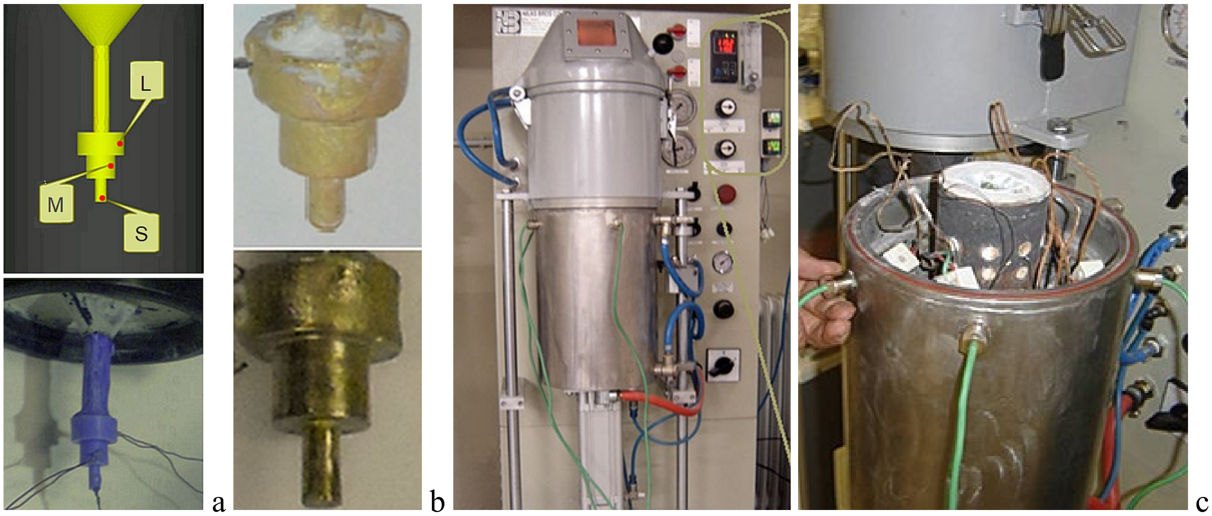

Fig. 1. Experiment setup (a) part/feeder: design (up), wax model with thermocouples (down) (b) casting: rough (up), cleaned (down). (c) casting machine: open with flask (left), closed (right)

The vacuum-pressure casting machine employed (NILAS BROS^{TM}) comprises a melting and a casting chamber, see Fig. 1(c). The former contains a graphite crucible with embedded thermocouple openings for temperature monitoring. Melting takes place under inert atmosphere of Ar. The mold is placed in the casting chamber which is sealed so that vacuum can be created and maintained. The machine is equipped with temperature and pressure displays allowing monitoring of the casting conditions in real time and performing corrections, as needed.

The casting parameters were as follows: casting chamber pressure: 0.03 bar (99.7% vacuum), pouring temperature: 990ºC and mold preheating temperature: 600ºC. One K-type thermocouple for each region was embedded in the mold cavity, as close to the metal-mold interface as possible, Fig. 1(a).

An A/D converter (Personal Daq/55 ^{TM}) fed raw temperature measurements to a laptop computer where they were processed by the Savitzky-Golay smoothing filter followed by cubic spline interpolation yielding the experimental temperature evolution curves. As shown in Fig. 2. each curve consists, as expected, of a short period of abrupt cooling (1st stage), a long period of mild cooling (2nd stage – solidification) and a third period of more pronounced cooling (3rd stage – post solidification).

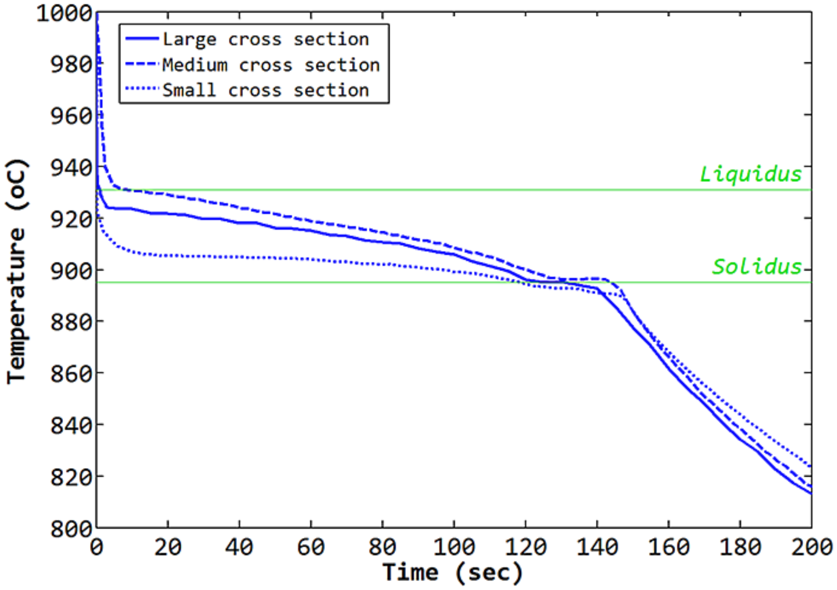

Fig. 2. Experimental temperature evolution curves.

Numerical Simulation Setup

ProCAST 2004.1® was used as the dedicated simulation platform implementing Finite Element Analysis to model coupled heat transfer, fluid flow and stress.

Determination of the initial conditions and the boundary conditions of the problem, i.e. temperature and pressure values during casting (mold preheating temperature, temperature of the outer surface of the mould, vacuum chamber pressure) followed the pertinent experimental settings, see previous Section.

HTC in the part of the sprue section filled by the melt was assumed to be the same as that of the small cylinder part of the casting (S), Fig. 1(a). This is a valid assumption as only a very small height of the sprue is actually filled by melt. The free surface of the melt is assigned radiation losses with an emissivity coefficient equal to 0.3 [14] and convective losses corresponding to air at 600°C with a film coefficient of 20 W/m^2K [15]. The pouring cup as such is treated exactly as the outer wall of the flask, i.e. it is assigned a Dirichlet boundary condition.

Melt flow rate was calculated as 1.13 kg/s using Bernoulli equation and considering the dimensions of the vacuum casting machine and of the casting tree.

Cast material properties were defined by interpolating the corresponding data available in literature. For brass CuZn33, liquidus was 931ºC and solidus was 886ºC; latent heat was 205 KJ/kg. Variation curves of thermal conductivity, density, specific heat, viscosity and fraction solid as a function of temperature are taken from [11].

HTC is modelled as a step function of time corresponding to three stages as first documented in [16] and is depicted in Fig. 3(a) and represented by the five element vector [h_1 t_1 h_2 t_2 h_3].

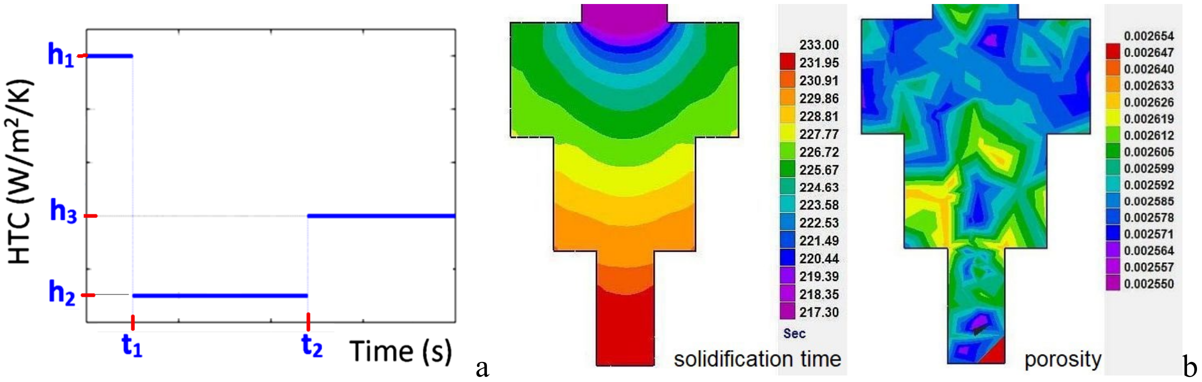

Fig. 3. (a) HTC representation (b) solidification time and porosity indicative simulation results.

Indicative simulation results regarding solidification time and porosity are shown in Fig. 3(b). Note that the right HTC needs to be employed if these results are to be credible, hence the need for inverse optimization approach.

The most valuable simulation result is temperature evolution at the three finite element mesh nodes corresponding to thermocouple locations by analogy to the experimentally obtained counterpart shown in Fig. 2.

Genetic Optimisation Setup

A classic GA was employed in order to determine the optimum HTC values that would cause the predicted temperature evolution curves to be as close as possible to the experimentally obtained ones. It was implemented on Matlab and made use of integer encoding of the chromosome.

The chromosome consists of the five variables that are necessary to define the HTC as a function of time, namely [h1 t1 h2 t2 h3], see Fig. 3(a). For each one of these variables its definition domain was discretised into 150 intervals. Each value is thus mapped to the corresponding interval, i.e. to a number from 1 to 150. The range of values for each variable was determined approximately from literature [11], thus for h_1, which is applicable during filling and generally above solidus, it is 200-30000 W/m^2K, whilst for h_2, which is applicable during solidification, it is 10 – 1500 W/m^2K; for h_3, which is applicable after the end of solidification, it is 20-3000 W/m^2K. The stepwise transitions occur at times t_1 and t_2 roughly corresponding to transition under liquidus and under solidus temperature respectively. Their value ranges are estimated by observing the experimental temperature evolution curves, Fig. 2, as 0.2-30 sec, and 105 – 165 sec respectively.

The fitness of any chromosome is calculated as the RMS metric of the difference in ordinates between 200 points defined on the experimental cooling curve and its simulation counterpart. This is done at the same time for all three curves corresponding to the small medium and large sections, see Fig. 2 and Fig. 1(b). The points are denser in regions where more sudden changes of temperature are expected. The fitness value is stored in a database so that the former does not have to be calculated anew each time the same input vector values are required. Obviously, fitness evaluation presumes that simulation curves of temperature evolution are obtained, which requires running the casting simulation programme with the particular HTC.

Several values were tried for the GA's hyperparameters, namely: for mutation rate: [0.1, 0.4, 0.7] for crossover rate: [0.2, 0.4, 0.5 , 0.8], for maximum iterations: [10, 20, 40, 100] and for population size: [4, 10, 20, 100]. The best result (best coincidence of experimental and simulation cooling curves) was obtained for mutation rate=0.1, population size = 20, crossover rate = 0.8, max iterations=100 and the evolution of the objective function is shown in Fig. 4. Note that if a much higher number of generations were allowed, e.g. 1000, a further decrease in the value of the objective function might have resulted, since GAs cannot guarantee convergence to the minimum. However, such extravagance is not practical, in view of the high computational cost of each evaluation, as this requires execution of a casting simulation scenario typically lasting several minutes depending on the hardware employed.

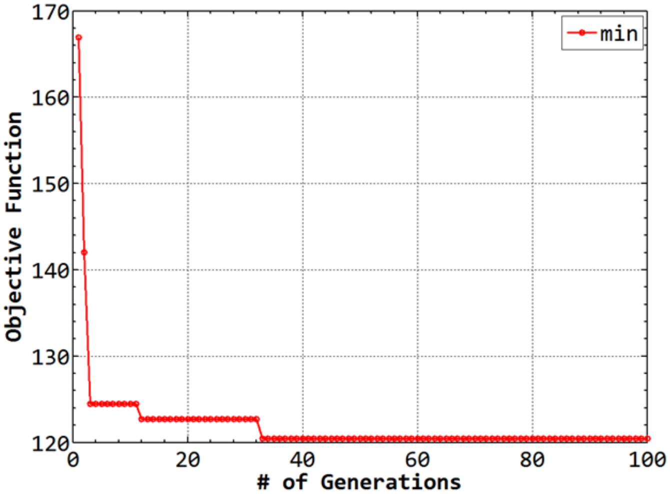

Fig. 4. Genetic algorithm cost evolution for the best chromosome in each generation.

HTC Optimisation Results and Discussion

The optimum HTC value determined by the GA is: [h1 t1 h2 t2 h3] = [102 38 70 3 35] in integer form, whilst in real number terms it is: h1=20400 W/m^{2}K, h2= 6 W/m^{2}K, h3=700 W/m^{2}K, t1=7 sec, t2=117 sec. This solution corresponds to a minimum in objective function equal to 120.4.

Fig. 5 depicts the cooling curves obtained by running the casting simulation for the optimum HTC in comparison to the experimental curves obtained by the corresponding thermocouples.

Referring to Fig. 5 comparison of experimental and simulation curves is generally satisfactory. The slope of the experimental and simulation cooling curves in the 2nd stage (during solidification) and in particular in the 3rd stage (post solidification) are similar.

Regarding the μ section, approximation of the experimental by the simulation curve is fairly good. Regarding the M section, approximation is good for the 2nd stage (solidification) but not so good for the 3rd stage (post solidification). Regarding the m section, approximation is unsatisfactory in the 1st and 2nd stages but fairly good in the 3rd stage. Furthermore, the lag in cooling of the m section with respect to the μ and M sections is not clearly captured by the simulation.

The end of solidification stage as determined by simulation at all three points is not far from the corresponding one that has been experimentally determined. However, the solidification start is not predicted so accurately by simulation.

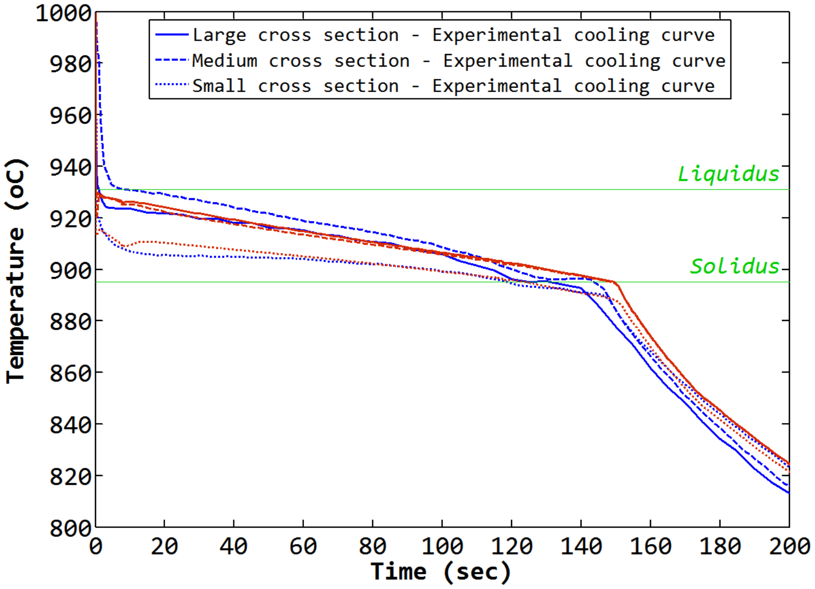

Fig. 5. Experimental and simulation cooling curves comparison.

Table 1 provides quantitative evidence for these observations. Note that the first few seconds after pouring are very important due to their influence on microstructure formation of the casting. Yet, the predicted duration of the 2^{nd} stage (solidification) is in relatively good agreement with the experiment.

For comparison purposes, Table 1 also provides the respective results from a similar exercise considering three separate HTCs that have been reported earlier [11]. Three HTCs are a better alternative to a single HTC but the difference is tolerable especially for the larger sections. The corresponding objective function attains a significantly lower value than that attained in the single HTC case, i.e. 38.50 compared to 120.4. Recalling that this metric denotes the RMS of the ordinate differences between experimental and simulation cooling curves, i.e. a representation of temperature difference in time at the particular points monitored, this improvement is important but not spectacular.

Table 1. Solidification start (S) and end (E) times and duration (D) for large, medium and small (M, m, μ index) according to experiment and simulation.

		Single HTC			3 separate HTCs		
	Experiment	Simulation	Error (sec)	Error (%)	Simulation	Error (sec)	Error (%)
S_M (sec)	0.97	0.13	0.84	86.6%	1.97	-1.10	-103.09%
E_M (sec)	131.8	149.7	-17.9	-13.6%	147.5	-147.64	-11.91%
D_M(sec)	130.83	149.57	-18.74	-14.3%	145.53	-145.67	-11.24%
S_m (sec)	8.5	0.12	8.38	98.6%	2.75	-1.76	67.65%
E_m (sec)	144.1	148.7	-4.6	-3.2%	149.35	-149.38	-3.64%
D_m(sec)	135.6	148.58	-12.98	-9.6%	146.6	-146.70	-8.11%
S_μ (sec)	0.28	0.09	0.19	67.9%	0.24	0.44	14.29%
E_μ (sec)	119.2	124.1	-4.9	-4.1%	119.2	-119.24	0.00%
Dμ(sec)	118.92	124.01	-5.09	-4.3%	118.96	-119.00	-0.03%

Summary

In this work the suitability of simulation modelling vacuum casting of brass with a single HTC that is applicable throughout a casting different casting moduli of different regions was investigated.

An acceptable single HTC can be determined using a single casting experiment for reference, but this of course is case-dependent, i.e. it should be repeated every time any of the process parameters change, e.g. melt temperature, mold temperature and even pouring rate and, of course, if casting or mold geometry or materials change. However, the methodology of determining the HTC is generic and universally applicable

In general, agreement between simulation predictions and experimental measurements concerning temperature evolution at characteristic points of the different regions is fair. In particular, prediction of solidification duration is acceptable. However, qualitative characteristics such as the differences in solidification starting time between different regions are not captured accurately. Yet, predictive performance of the simulation when using a single HTC is tolerably inferior to that achieved when using 3 HTCs as revealed by comparison to pertinent work reported before. However, this is certainly connected to the relatively moderate differences in casting moduli.

In cases of intense differences in casting moduli, most probably different HTCs should be assigned to different regions, but this has to be proved in future extension of this work.

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