

The Manufacturing Engineering Society International Conference, MESIC 2013

Adjustment of Numerical Simulation Model to the Investment Casting Process

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Abstract

This paper presents the adjustment process of a simulation model to improve the correlation between simulation results and parts industrially manufactured. It includes the data registration at foundry plant, the preliminary set-up of the model and the later adjustment process to reach a correlation level according to the industrial necessities.

The adjustment has been performed by means of inverse modelling. This technique uses thermal histories experimentally registered as base, and modifies the material properties and boundary conditions used in simulation until reaching a good correlation between numerical simulated cooling curves and they registered experimentally. The adjustment has been also focused on the shrinkage defects.

The simulation model is a FEM model developed in commercial software specifically focused on metal casting simulation. The case of study is an investment casting process, vacuum poured, of a nickel base superalloy designated Hastelloy X. Usual in the manufacture of components for aeronautical turbines.

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Selection and peer-review under responsibility of Universidad de Zaragoza, Dpto Ing Diseño y Fabricacion

Keywords: Numerical simulation; inverse problem; finite elements; investment casting; superalloy

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1. Introduction

Simulation methods have contributed since their origins to reach a better knowledge about the materials and the manufacturing processes, and as consequence to improve the manufacturing methods. Today, a big number of commercial codes are available to simulate a wide range of manufacturing processes including the metal casting.

Obviously, as Bonollo and Odorizzi (2001) state, the reliability of the simulation is significantly related to the accuracy adopted for defining the initial and boundary conditions and to the knowledge of the properties of the materials involved. Inaccurate input data can easily lead to poor or even misleading predictions.

In this sense, the ASM International Handbook Committee (2010) emphasizes the importance of the boundary conditions to produce accurate simulations. They state that each manufacturing process has unique boundary conditions that must be identified, understood and characterized for the specific application being simulated. Moreover, boundary conditions can be equipment specific, meaning that one furnace may not give rise to the same boundary conditions as another furnace of a similar type used under same nominal processing conditions.

Relating to material properties is a fact that they can vary significantly with temperature. So, this variation must be considered in the simulation but to obtain the necessary data is not a trivial task. The measurement of material properties, especially at high temperatures, is not only time consuming and costly but also very complex to achieve. Moreover, metal casting industry must also tackle with the usual variations in alloy compositions and with the evolution of the melt alloy, depending for example of the time in furnace. In case of investment casting another source of important variations is the mould. Due to the manufacturing method, it is not possible to assure a complete homogeneity along the whole ceramic shell. The typical solution consists in the use of material properties extracted from literature and handbooks. But they use to be standard values and not always correspond with the properties of the specific materials used at foundry.

The use of inverse modelling techniques is a helpful option to try to avoid these difficulties. These techniques permit to estimate some model parameters based on direct experimental measurements of related variables. In the case of metal casting simulation, instead of performing direct measurements of material properties or boundary conditions, experimental thermal histories are registered in a number of defined points. These thermal histories are used as base and some simulation parameters are modified until reaching a good correlation between numerical simulated cooling curves and they registered experimentally. This is the approach followed in this work to perform the adjustment between simulation models and experimental results obtained industrially at foundry.

The number of papers based in the application of inverse methods to metal casting simulation is high, existing references since the mid-90s, Rappaz et al. (1995), but the number of papers focused on investment casting is more reduced. Moreover the majority of them use to reflect works performed at laboratory scale and mainly focused on the determination of the heat transfer coefficients between the alloy and mould, as occurs in references Dong et al. (2011); J. M. Drezet et al. (2000); Jin et al. (2009) and O'Mahoney and Browne (2000).

The work presented here instead, is based on measurements registered at industrial level where the process is not as controlled as at laboratory scale. Additionally not only the heat transfer coefficients have been determined but also the rest of boundary conditions and material properties.

The numerical simulations have been performed by means of commercial software, more exactly with the software called ProCAST specifically focused on the simulation of metal casting processes. The prototypes have been manufactured at industrial plant following the industrial standards and procedures usual for this type of parts. The case of study is an investment casting process, vacuum poured, of a nickel base superalloy designated Hastelloy X. This material and process is usually employed in the manufacture of some components for aeronautical turbines.

The main difficulties of the work performed are precisely related with the type of process modelled. The metal parts manufactured by this method typically are characterized by the complex geometry and by the thin wall thickness, which reach values of only 1 mm. These thin walls are the cause for which the mould needs to be preheated before pouring, as in other case the liquid alloy would freeze during filling and the mould would not result completely filled. The thickness of the mould walls is also small, with values between 5 and 12 mm. Moreover the pouring is performed under vacuum conditions. All these characteristics make very difficult the data

recording at foundry. Additionally, the high number of variables implied in the process and the existence of manual operations increase the variability of the process and the difficulty of the adjustment.

2. Methodology

2.1. Experimental phase

The experimental phase involves the design and manufacturing of dedicated prototypes, and the recording of the process parameters together with the temperature evolution in specific points. Later the cast prototypes have been cut in different fragments in order to check the location and magnitude of shrinkage defects. Every operation related with the experimental phase has been done into the industrial plant of the foundry where the project was developed, employing the same facilities used in the manufacture of industrial metal casting parts.

One of the main requirements to take into account in the prototype design is a simple geometry. The reason is not only to make easier the temperature measurements but also to reduce the calculation time of simulations. The only difference between the prototypes and real parts consists in their geometry. The materials and process conditions used in the manufacture are exactly the same that for industrial parts.

Temperature measurements have been registered by means of dedicated thermocouples inserted both into the mould and into the metallic part. To avoid difficulties with thermocouples during the mould preheating and the transfer to vacuum furnace, they have been fixed to the mould just after this transfer. Temperature recording has been performed by means of autonomous equipment able to work in vacuum conditions.

Fig. 1 shows a sketch of the prototype and one photograph took during experimental phase, where the location of one of the thermocouples can be observed.

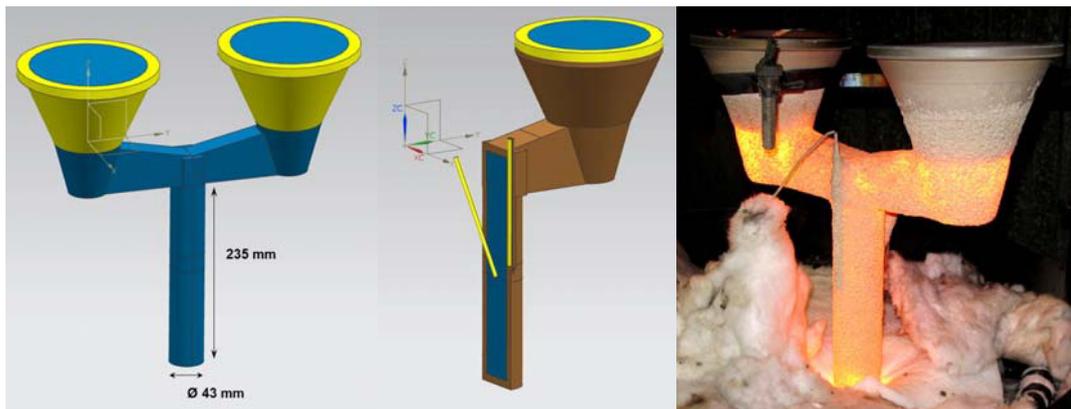


Fig. 1. Prototype sketch and prototype photograph during experimental phase.

The appropriate register of process conditions is essential for the correct definition of the boundary conditions to be applied on the simulation. Although every experiment has been performed in the same way trying to do all of them as similar as possible, the special characteristics of the process together with the execution at industrial level by the plant operators cause important variations in the process.

Table 1 summarizes the range of variation of the process parameters registered during the experimental phase. Relating to the shell mould it was made mainly of aluminium silicate and its thickness varied in a range between 6 and 9 mm depending not only on each mould but also on the area of the mould. All these data are into the typical ranges used industrially in this type of manufacture.

Table 1. Experiments process conditions.

Parameters	Minimum	Maximum
Mould pre-heating temperature (°C)	1050	1150
Pouring temperature (°C)	1480	1564
Room temperature (°C)	18	25
Transfer time (s)	95	140
Time until pouring (s)	155	165
Pouring time (s)	1	3

Finally, after numerous trials, a set of measurements corresponding to nine experimental cases has been obtained. The corresponding curves are shown in Fig. 2, where red curves correspond to the alloy and blue curves to the ceramic shell mould. The alloy curves shown a preliminary cooling that correspond to the cooling of the cover inserted into the mould, where thermocouple is located. The next fast heating until reaching values near the pouring temperature corresponds to the pouring process. After that, the cooling of the alloy takes place, first in form of slow cooling during metal solidification and later in form of faster cooling once the alloy is completely solidified. Relating to the mould curves, the mould suffers also a cooling at the beginning until pouring takes place, then its temperature is increased in contact with the melt alloy and later the cooling restarts again. One of the shell curves presents a pronounced local minimum around 200 seconds. This temperature drop seems to be caused by a measurement anomaly, as several seconds later the temperature returns to logical values, but the reason is unknown. The curve has been included as an example of the anomalies that use to happen in this kind of measurements.

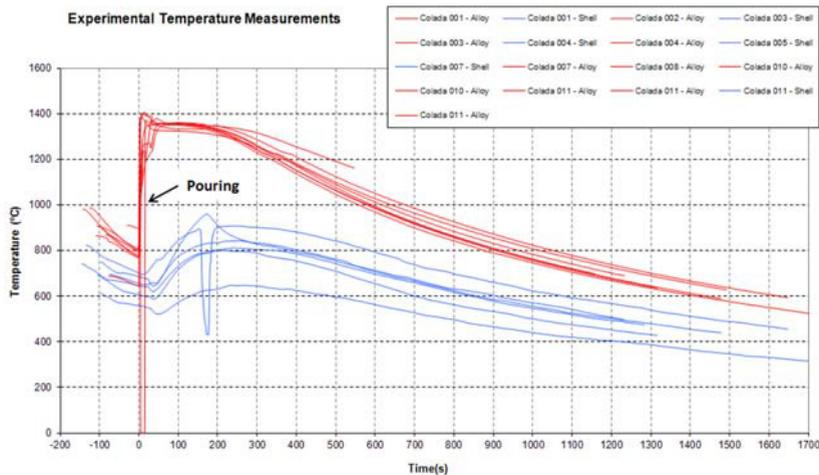


Fig. 2. Experimental temperature measurements.

2.2. Simulation adjustment

The first step once experimental data are available is the treatment of the raw values. The procedure followed in this case is quite standard in the treatment of functional data: Remove functional data which present high levels of measurement anomalies; smoothness of the curves to reduce noise; and synchronization of the curves to align the pouring instant in all cases.

Almost all the variables included in the simulation model present some level of uncertainty, so they have been subjected to variations in order to reach the adjustment of the model. It includes the alloy and mould material properties, the heat transfer coefficient between alloy and mould, and boundary conditions related to heat exchange and to pouring conditions.

Due to the iterative nature of the adjustment methodology, the number of simulations to be performed during the process is very high, so the calculation speed is an important aspect. In this case thanks to the symmetry present in the prototype only one half of the geometry has been modelled by means of 36,327 nodes and 167,061 elements. This model has been used during preliminary phases of the adjustment where only heat transfer calculations have been performed. Once a reasonable adjustment has been reached, simulations combining filling and heat transfer have been executed and the adjustment has been refined using a model representative of the complete geometry, formed by 50,644 nodes and 237,059 elements. The model reproduces the complete process, since the extraction of the mould from preheating furnace until the final cooling of the part.

2.2.1. Preliminary model

The preliminary model should be based on our best approximations to the problem, taking into account the process data recorded at industrial plant combined with the values obtained from bibliography or from the team experience.

Hastelloy X material properties has been defined after the study of diverse bibliography. The main sources taken into account are the ASM International Handbook Committee (1990), the Military Handbook for Metallic Materials for Aerospace of the Department of Defense of USA (1998) and the thermodynamic database included in ProCAST called CompuTherm LLC (2012). Finally, the material properties provided by the mentioned thermodynamic database have been used. These properties have been calculated based on the Scheil micro-segregation model, which assumes that no diffusion takes place in solid phase, and assuming that the chemical composition is equal to the average values of the typical range defined for this type of alloy. The material properties defined for the mould have been estimated based on the information found in several journal articles: Browne and Sayers (1995), Connolly et al. (2000), Kovac et al. (2008), O'Mahoney and Browne (2000), Rafique and Iqbal (2009); within some confidential information extracted from prior research projects.

The value of the heat transfer coefficient between alloy and mould has been estimated following the typical values recommended in bibliography by Calcom (2002), that for metallic alloy with sand moulds is between 300 W/m²K and 600 W/m²K.

The heat exchange between the mould and the alloy with the environment takes place by means of convection and radiation. Convection coefficient has been defined as time dependant, taking into account if the mould is in movement or in vacuum conditions and based on the typical values considered for air convection in Chapman (1984): between 5 and 25 W/m²K for free convection, and between 10 and 500 W/m²K for forced convection. Relating to radiation heat transfer, emissivity values according to the estimated material properties have been used. Apart from that, the software requires the definition of an enclosure to be able to include the view factor calculation into the analysis. This enclosure has been defined with an emissivity value of 0.7. Ambient temperature has been fixed to 20°C.

The initial mould temperature has been fixed at 1100°C and the pouring temperature at 1520°C. The pouring starts at time 160 seconds and corresponds to a flow rate equal to 10.5 kg/s.

Results obtained in this first approximation are shown in Fig. 3. As can be observed, the simulation results before pouring, match quite well with experimental values. After pouring, temperatures predicted by the simulation for ceramic shell mould are not very far from the expected, but their values are higher than the average observed experimentally. The main difference with experimental values is found on the alloy curve, where the simulation not only gives a slower cooling but also predicts higher solidification temperatures.

Of course these results correspond to our best first approximation based on our expertise. Probably a different research team would get a first different model depending on the decisions adopted, which could provide better or worse results.

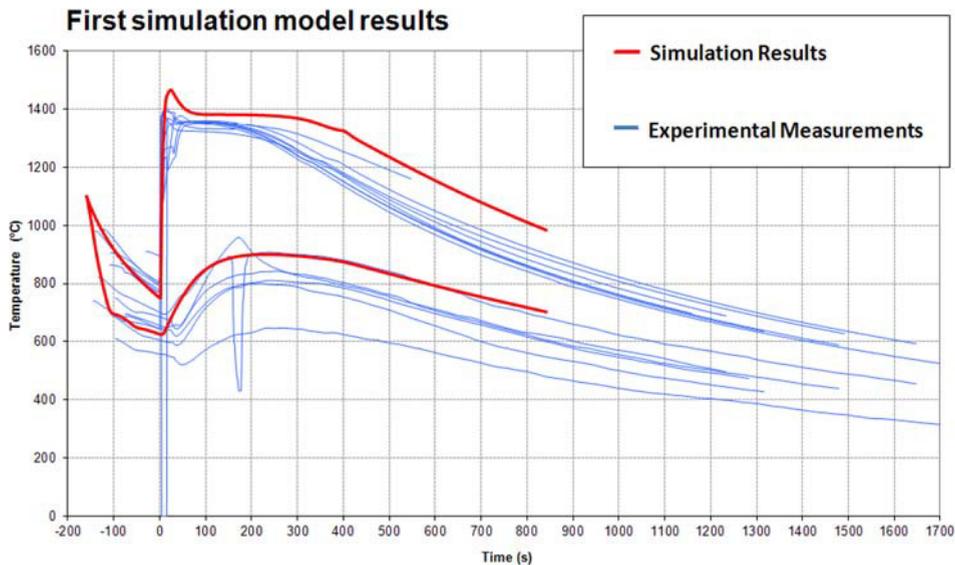


Fig. 3. First simulation results vs experimental temperature measurements.

2.2.2. Adjustment process

The adjustment methodology consists in an iterative process where some parameters are modified, the simulation is run, results are checked and some parameters are modified again until results are good enough.

The differences between simulation results and experimental data will show very different behaviours depending on the case studied. Also during the process of adjustment these differences will evolve in a different way. For this reason, is not possible to give standard rules for the adjustment procedure but only some general advises based on the work followed in this case.

The software used includes a specific tool that makes possible to perform the iterative process of adjustment automatically, but results obtained not always are good enough. Sometimes a correlation level good enough is not obtained and sometimes the values of the adjusted parameters have not physical sense. In the case of manual adjustment, each step of the process should be performed manually by the analyst, but this makes possible a better control of the parameter modifications. Depending on the difference observed between simulation results and experimental temperatures, it is more advisable to use the automatic tool included in the software or to use manual adjustments. In general, if the distance between results is high, the automatic tool has more problems to converge to reasonable solutions. So, in these cases it has resulted better the use of manual modifications of the parameters in order to get a better approximation before to use the automatic adjustment.

The decision about which parameter should be modified in each trial depends also of the behaviour observed. In this point the expertise of the analyst to evaluate which parameter should modify is essential. In general, the modification of only one parameter in each trial seems more interesting because it permits to see more clearly the influence of this parameter in the thermal behaviour.

Once the model has been adjusted relating to cooling curves, it is time to follow on the adjustment of the shrinkage defects. The parameters modified to adjust the magnitude of the shrinkage defects prediction are mainly the alloy density and the parameters that control the porosity model used by the software, which are specific of it.

3. Results and discussion

The comparison between simulation results once the model has been adjusted and experimental data is shown in Fig. 4. As can be observed the simulation results match well with experimental measurements along the whole process. The number of iterations performed to achieve these results has not been registered, but an estimation of about 500 iterations is a reasonable value taking into account the time dedicated to this task.

Relating to shrinkage defects, Fig. 5 shows the comparison between experiments and simulation. Simulation provides shrinkage predictions in form of porosity values, in this way areas with values near to zero implies almost none porosity and they have been removed from the picture. Results predicted by simulation match well with they observed experimentally, according to industrial necessities.

Relating to the adjusted parameters is not possible to include here the values obtained for each of them due to they are subjected to confidentiality. In spite of that, it is possible to include some indications about the differences between the values used in the preliminary model and they resulted after the adjustment. This information may serve as guide for other researches or users interested in this kind of simulation.

There are important differences between the alloy material properties used in the initial model and they used in the adjusted model. In the case of thermal conductivity and specific heat, only the values at low temperatures match with them assumed in the preliminary model. At higher temperatures the values varies until 20%, but while the values of thermal conductivity and emissivity result higher than they used as first approximation, in the case of specific heat the values result lower. The values of density present small variations with increases about 4% at some temperatures. The solidification range has resulted more similar to the values found in the handbooks from ASM International Handbook Committee (1990) and the Department of Defense of USA (1998).

In the case of the ceramic shell mould, the values obtained in general are lower than they used in the first model, with variations between 5 and 35 %. The higher variation corresponds to the thermal conductivity and the emissivity, and the lower to density.

The heat transfer coefficient values obtained from the adjusted model are included into the range assumed for the first model but nearer from the lower values of the interval.

Relating to the heat exchange by convection, the values estimated for the first model have resulted slightly higher during times where forced convection has been assumed whereas the values assumed for natural convection have resulted slightly lower. The emissivity applied in the enclosure has been slightly increased. Also it has been needed to include an additional condition of radiation to the environment in the interface of the alloy which is in contact with the mould, in order to incorporate to the model the transparency effect observed in the shell mould during the experimental phase (see Fig. 1).

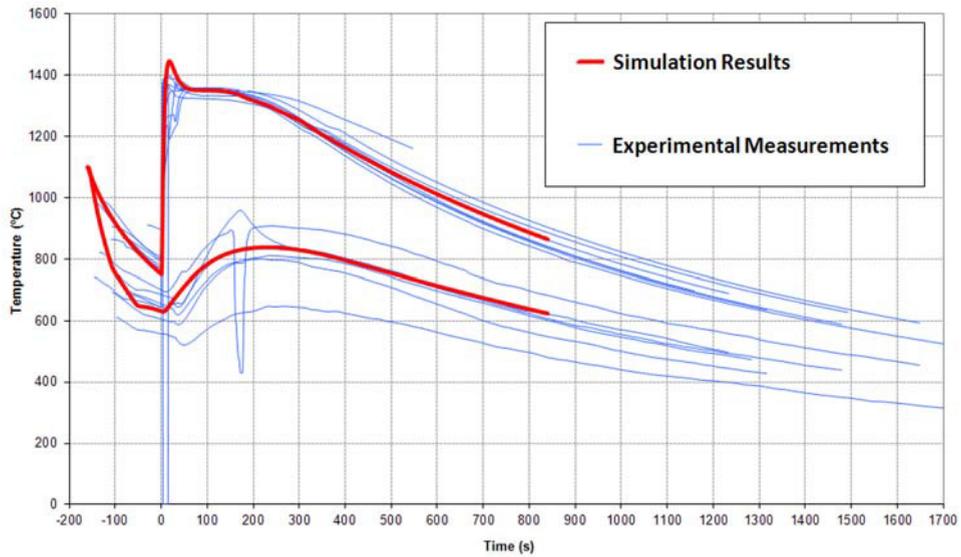


Fig. 4. Experimental cooling curves vs final simulation results

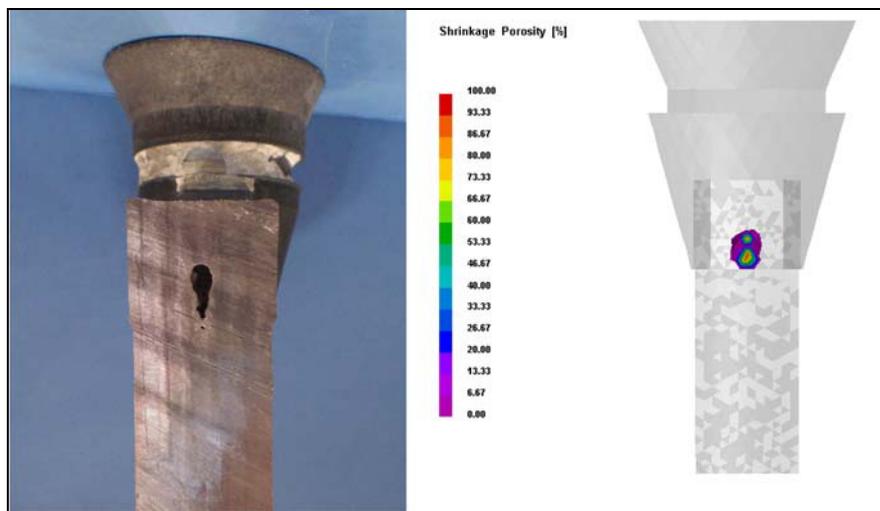


Fig. 5. Experimental shrinkage defect vs final simulation results

4. Conclusions

An adjusted simulation model of the investment casting process has been obtained so that simulation results match with experimental data measured at foundry, according to the necessities of the industry. The adjustment has been performed by means of inverse methodology, obtaining values for the adjusted parameters that can be considered reasonable compared with bibliographic values.

The model covers the whole casting process, since the mould extraction from preheating furnace to the final part cooling after the pouring. The simulation is a transient analysis combining fluid dynamics and heat transfer analysis, including heat latent release during solidification and radiation with view factor calculation.

Although numerous papers based on the application of inverse methods to metal casting processes exist, the number of them focused on investment casting is quite reduced. Moreover the majority of them use to reflect works performed at laboratory scale where the process is very controlled and not at industrial level as the work presented here. The contribution of this work consists in checking the viability of the application of this type of techniques over industrial processes. Apart from that, this paper contains information that may serve as guide for other researches or users interested in the investment casting simulation and in techniques to correlate the simulation models with experimental data.

Acknowledgements

This work has been developed as part of the GALDATEK project, funded by the INNOTEK program of the Basque Government (Department of Industry and Innovation).

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