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The Optimization of a Numerical Steel Foundry Simulation Through a Characterization of the Thermal Properties of the Materials

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Abstract

In many foundries, numerical simulation is used to determine the origins of different defects as this tool allows the acceleration of the design process. However, the databases provided by different software do not seem to tally with the actual properties of the material. In fact, every foundry uses a different grade of steel and varying mixtures of sand. An evaluation of the impact of different material properties showed the importance of measuring every physical property to improve the database of the software. Following this, an experiment was conducted to evaluate the gap between numerical simulations and the results obtained through experimentation. This experiment, called thermal analysis, consists in measuring the solidification and cooling of a cylinder filled with liquid steel. After the calculation of the steel properties and a simulation with real experimental parameters, a comparison between each cooling curve was realized. This comparison shows that the calculated properties provide a simulated cooling curve which is closer to the experimental curve than the properties in the original database. We did not explore all of the metal properties in this study, but the modification of the sand properties was explored, together with the thermal conductivity of the steel and sand. These other measurements will be obtained in a future study.

Keywords:

foundry simulation, low-alloyed steel, green sand, thermal analysis, CALPHAD

1. INTRODUCTION

In the foundry process, high temperature liquid metal is poured into a mold before it cools and solidifies. The solidification of molten metal induces contraction and this contraction takes place from outside to inside, which can lead to a lack of metal in the center of the part, in a process known as shrinkage. Numerical foundry simulation is used to predict manufacturing defects, especially shrinkages. It is possible to anticipate and eliminate shrinkage defects by adding a sacrificial element called risers. Risers are cylindrical parts that concentrate the shrinkage and are removed from the final product to make the cast free of any defects. Some basic rules exist which govern the design of foundry parts [1, 2] with handmade calculation, but the more complex the part is, the more complex the calculations. To reduce the time needed for these calculations and increase their accuracy, foundries use numerical simulation. Moreover, these tools are able to calculate filling, solidification, and cooling.

Commercial software like Magma®, NovaFlow&Solid® (NFS), TherCast®, ProCast®, Flow3D® or QuickCast® make the designer's work easier, faster, and more precise. These tools have become essential, but require accurate entry data [2, 3]:

- process parameters: initial temperature of metal and mold, type of ladle, height of the ladle, dimension of the metal jet, etc.
- material parameters: chemical composition, density, specific heat, latent heat, conductivity, viscosity, etc.
- the measurement of physical properties is a very complex process for a steel foundry due to the high temperatures of processing (up to 1700°C). There is also a lack of information existing in databases [4]. Without accurate data, it is unthinkable that good simulation results can be obtained.

Software is available which includes a database containing physical properties of some metals and mold material. The user choses the closest material to its own, but this material does not usually match the requirements as the composition could be slightly different and the specific process of the user might affect the real physical properties. Sometimes differences between reality and simulation are observed and as references [5] and [6] show, substituting material properties included in the original database with measured properties can really improve the results.

2. PRELIMINARY NUMERICAL STUDY

The first step of this work was to set the limitations of the NFS software. Firstly, a mesh study was conducted to reduce the influence of numerical parameters on thermal simulation results. Secondly, a sensitivity study was performed to evaluate the impact of material properties on simulation results. The second point will eventually help to highlight the prevalence of some properties in comparison to others.

For these two studies, the geometry used is a cube with sides of 50 mm with a virtual thermocouple placed in its center. The simulations were realized between 1600°C (standard temperature for low-alloyed steel casting) and 500°C; we will mainly analyze solidification in this paper. The steel grade used is "G20Mn5", a standard alloy in industrial foundry. The cube is surrounded by green sand in a layer of 40mm thick, where it serves as the molding material.

2.1. Meshing

NFS is based on a finite volume method meshing method. The software offers two methods to define the meshing that can be applied automatically: selecting the mesh count or choose the mesh size in mm. There is no way to select another parameter like local refinement.

To reduce the influence of meshing on the simulation results, a preliminary study on the cooling curve of the cube was carried out. The simulations were realized by varying the mesh size from the high size of 5 mm to the low size of 0.5 mm. This allows to determine the minimum size of meshing to use for the simulations to follow.

Protocol

All parameters remained constant except the mesh size:

- metal: “G20Mn5”,
- mold material: “green sand”,
- start temperature: 1600°C,
- ending temperature: 500°C,
- mesh size: 5 mm, 2.5 mm, 1.5 mm, 1 mm, 0.75 mm, 0.5 mm.

After simulation, the shapes of the cooling curves will be compared to examine the time for total solidification and the simulation duration.

Results

The different cooling curves are presented in Figure 1. Concerning the influence of the mesh size, the impact is quite low and below 1mm, the results are equivalent.

When comparing the different simulation times in Table 1, it is observed that the time of simulation is dependent on the mesh size; for these reasons, it is necessary to do a simulation with the roughest meshing, but with the consideration of the least influence on solidification time.

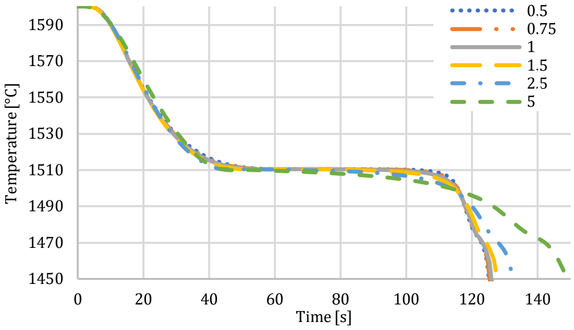

Fig. 1. Mesh study impact on the cooling curve

Table 1
Time of simulation by size of meshing

Mesh size [mm]	5	2.5	1.5	1	0.75	0.5
Simulation time [s]	1	11	90	1286	3555	29,500

This part shows that the mesh size has an impact on both solidification and simulation time. To obtain the lowest influence of the mesh on the result we need to refine it, but the simulation time grows as a consequence. That is why we need to choose a mesh size that offers limitation in simulation time, with little impact on the time of solidification. We will use a 1 mm mesh thereafter.

2.2. Sensitivity

Some results from the literature [7–9] have shown that physical properties do not have the same impact on the solidification time. In order to confirm this (or not) and to see the impact of some modifications, a number of simulations were completed using the cube described earlier.

Protocol

The reference simulation was done using “G20Mn5” steel grade and “Green sand” as the mold material from the NFS database. The simulations were done with 1 mm mesh size as determined in the previous section. For each property, five simulations have been realized, its value varying from 80% to 120% around the original value from NFS database with 10% steps, while the other properties were kept constant. For each calculation, the complete solidification of the cube was determined.

Results

The corresponding results are presented in Figure 2. At first, it seems that none of the properties were predominant: a variation of 10% of any of these properties involves a variation of approximately 5% on the solidification time. These results are valuable and close to the initial properties (more or less 20%) and if no coupled interaction between them exist. This means that for each of these properties, experimental measurements or calculation by means of software like ThermoCalc® or JMatPro® will be necessary to check if the accuracy of the NFS database properties.

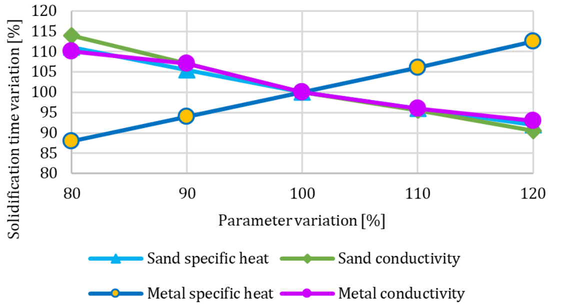

Fig. 2. Curve of time variation of the solidification of cube depending on the sensitivity of material

3. EXPERIMENTATION

The numerical study shows that exact properties are required to obtain good results. The exact chemical composition of the cast steel was measured by glow discharge optical emission spectroscopy (GDOES). A difference of composition between "G20Mn5" from NFS and cast steel (Tab. 2) is noticed.

Table 2
Steel grade composition [% weight]

Element	Fe	C	Mn	Si	Cr
Grade measured	98.47	0.31	0.81	0.41	0
Grade NFS	98	0.15	1.2	0.45	0.2

This difference is very important, firstly, the weight percentage of carbon of "G20Mn5" from the NFS database implies no peritectic transformation during solidification, contrary to the casted sample grade. Secondly, the liquidus and solidus are quite different and finally, each difference in composition could bring a modification of physical properties. It is for this reason that it was decided to determine most of them.

While analyzing the sand, it was found that the heat capacity curve of the silica sand (87.4% of green sand) [10] is different from the property given in the NFS database. As shown in Figure 3, the endothermic phase change of quartz-α into quartz-β (573°C) and the transformation of quartz into tridymite (≈870°C) and into crystobalite (≈1100°C) are not taken in account [11]. Water contained in the green sand, which induced high endothermic vaporization, was observed not to simulate and led to errors [12, 13].

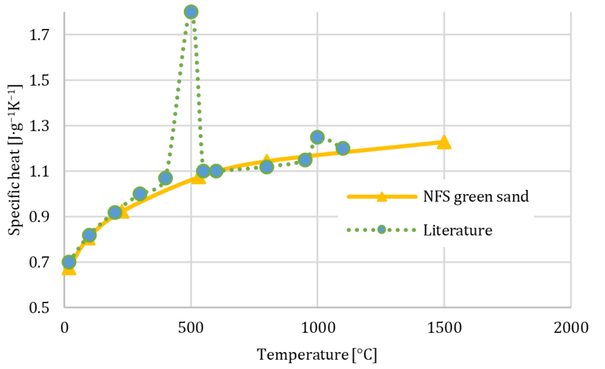

Fig. 3. Silica sand specific heat from literature [10] compared to NFS green sand

3.1. Property measurement and calculation

To obtain the physical properties, it is possible to measure each property based on temperature. However this requires expensive material and a lot of time. However, the properties of metal can be calculated with the use of its chemical composition calculated with the CALPHAD method [14]. This method is used for the calculation of properties thanks to the phase diagram [15]. The properties obtained seem to be suitable for improving the simulation results.

After the calculation of different properties using software such as JMatPro® and ThermoCalc®, for the composition given in Table 2, a difference between properties from the NFS database and the calculated properties were observed. The results given in Figure 4, for example, show a difference between the calculated density obtained by mens of the CALPHAD method and NFS database density. This difference seems to be low, but also exists in other properties: specific heat and latent heat.

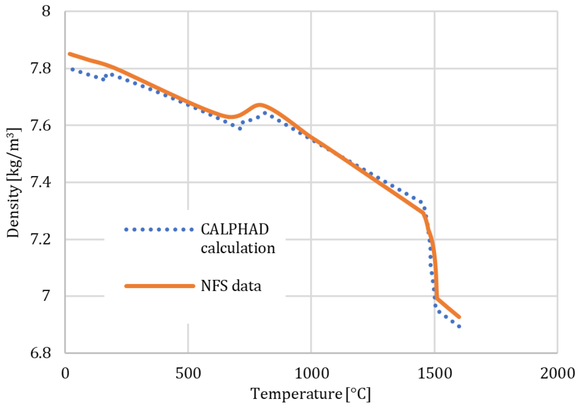

Fig. 4. Curve of density obtain by calculation compared to NFS database properties

The amount of water contained in the sand was measured to simulate its vaporization with the method of addition of specific heat around the water vaporization temperature (100°C) [12]. To obtain the amount of water, a precision scale is used to measure the loss of weight of the green sand after being dried between room temperature and 120°C. This measure gives us the weight percentage of water in the green sand, which resulted in approximately 4% for this study. With the use of this value and the water vaporization latent heat (2257 J · g⁻¹), the energy absorbed by this phase transformation for 1 g of green sand can be calculated:

$$2257\cdot\frac{4}{100}=90.28\ \mathrm{J}\cdot\mathrm{g}^{-1} \qquad (1)$$

For comparison, the specific heat of the sand at 100°C is approximately 0.8 J · K⁻¹ · g⁻¹, which means that it needs around one hundred times more energy to increase the green sand temperature with 4% of humidity by 1°C at 100°C than it needs for the rest of the temperature range. To consider this phenomenon, this energy was added to the specific heat with a temperature range of 10°C from the vaporization temperature as had been observed in the literature [12].

3.2. Protocol

Physical experimentation

In order to control the improvements of the simulation due to the database modifications described previously, a specific trial based on a standard thermal analysis cup was developed. Thermal analysis is currently employed for the determination of the physical properties of steel or cast iron like liquidus and solidus [16, 17]. For simulation, the designed cylinder with a similar geometry to a standard thermal analysis bucket with a virtual thermocouple was placed in the same position to the real one in the experimental trials (Fig. 5).

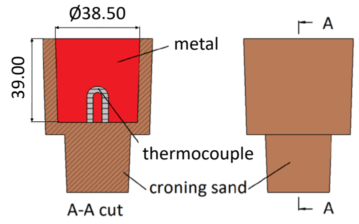

Fig. 5. Design of a thermal analysis used for the study of steel properties

Usually, for thermal analysis, experiments are conducted in air. The cup is placed on a support to facilitate filling: the cavity is filled with a ladle by the upper part. However, this generates lot of heat exchange by radiation, which is poorly simulated by NFS because this condition is rarely seen in foundry. Indeed, NFS only takes into account a fixed emissivity, when in reality, this property depends on the temperature and the state of the metal: liquid, solidified, clean or oxidized and depend on the surface state. That is why it was decided to cover the metal with a lid of green sand: just after the filling (directly in the cup), a lid is placed on top to close the mold. Furthermore, to study the impact of the green sand parameters, the sides of the thermal analysis bucket were cut, as in Figure 6, to remove the lateral part made of Croning sand, which is different from green sand. The lower part of the thermal analysis bucket was kept for practical reasons.

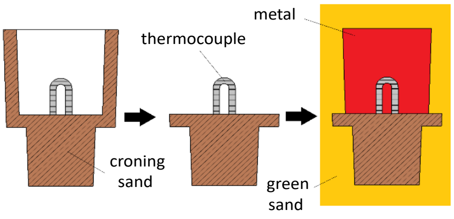

Fig. 6. Plan of cutting of sides of thermal analysis bucket

After cooling, the casts parts were weighed in order to carry out simulations with a precise amount of steel. This step is crucial because the time of solidification depends on the mass of the metal. Moreover, the starting temperature of the simulation is a key parameter; it is for this reason that the temperature of the alloy was directly measured in the crucible outside of the oven. It is necessary to subtract 40°C from the measured temperature to take into account the loss of heat due to the transportation of the crucible. The loss of heat has been the subject of a previous test campaign to measure it precisely.

Numerical experimentation

To compare the experimentations and simulations, the same cylinder was simulated, with the same mass of metal in it. A mesh size of 1 mm was chosen in accordance with the first experimentation and only the solidification and cooling of the metal was simulated, not the filling. For the simulation, Croning sand was not taken into account and it was replaced with green sand. Four different simulations were realized:

- standard grade: steel grade "G20Mn5" from the NFS database,
- standard grade exact composition: steel grade "G20Mn5" from NFS database with composition modified (measured by GDOES),
- calculate grade: exact composition and properties from the CALPHAD method,
- calculate grade + modified sand: exact composition and properties from CALPHAD method + sand with specific heat modified to take into account water vaporization.

4. RESULTS

As Figures 7 and 8 shown, the modification of metal properties changes the shape of the solidification curve whereas the modification of sand properties only modifies the speed of the cooling process. When observing the experimental curve, a difference in the shape at the beginning due to the process is observed: the mold is filled at room temperature whereas metal simulations are carried out at 1515°C.

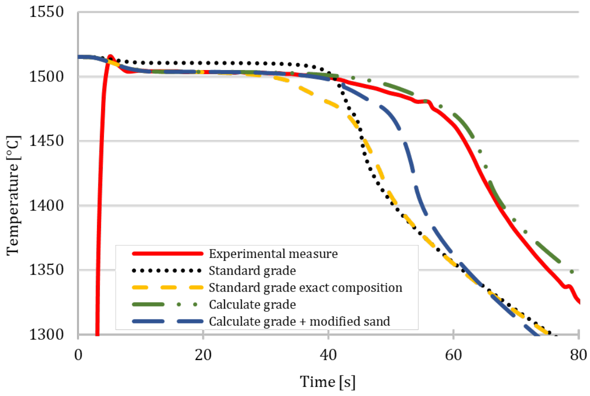

Fig. 7. Solidification curve of experimentation and simulations

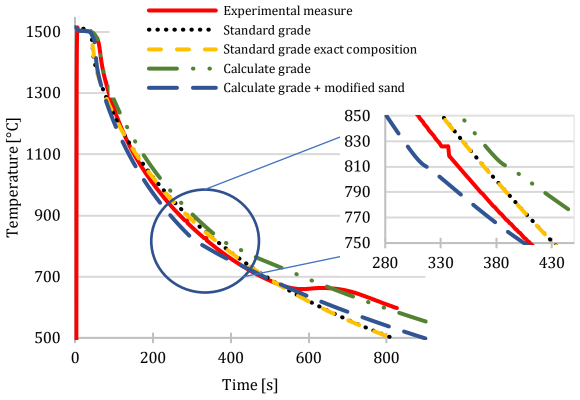

Fig. 8. Cooling curve of experimentation and simulation

Firstly, it is possible to see that the "Standard grade" has a change phase temperature different from the "Experimental measure". The liquidus temperature is also different. After modification of the chemical composition in the NFS database, the "Standard grade exact composition" change phase temperature seems similar to the "Experimental measure" but the solidification takes place too quickly. The "calculate grade" seem to be really close to the "Experimental measure", with the same solidus temperature and even the peritectic transformation at 1480°C observed. Unfortunately, changing the properties of sand (calculate grade + modified sand) leads to a worse match between the simulation and the experimental results. This was expected because of the heat absorption of water which is highly endothermic. The water vaporization absorbs a part of the heat and, as a result, the metal cools (and solidifies) faster. This means that for a better fitting between the simulation and the experiment, other parameters have to be taken into account, such as sand conductivity for example.

In Figure 8, the complete cooling curve is presented. The biggest difference between simulation and experimentation is the eutectoid transformation around 680°C. Indeed, NFS does not simulate this exothermic transformation. The use of properties calculated using data from the CALPHAD method ("calculated grade" and "calculated grade + sand modification") leads to a break in the slope around 800°C. This result is expected and is due to a solid/solid transformation ($\gamma \rightarrow \gamma + \alpha \rightarrow \alpha + Fe_3C$). This transformation is less visible on the experimental curve.

5. CONCLUSION

To improve the thermal simulation of a piece of casting simulation software (NovaFlow&Solid), metal properties in the database are modified. These properties are: composition, density, specific heat and latent heat. The impact on solidification and cooling of steel are studied; to estimate this impact, a thermal analysis experimentation has been used.

The first study (mesh size + sensitivity) showed the need to take all the physical properties (metal and sand) into account. The modification of steel's chemical composition in the NFS database leads to an improvement of the solidification temperature but did not change the solidification time. Improvement for future experiments can be obtained by modifying the physical properties with the use of the CALPHAD calculation. Nevertheless, the eutectoid transformation is still not observed on simulation curves. Future work will focus on the artificial implementation of exothermic heat during the eutectoid transformation (as was done for water vaporization) and experimental measurements of the thermal conductivity of steel and sand to obtain a more precise accuracy of the database regarding this property. Finally, a point to consider would be taking thermal resistance into account due to the presence of a layer of air between the metal and the mold [18].

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