INNOVATIVE PROCESS SIMULATION OF TOOL STEEL PRODUCTION PROCESSES

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Abstract
Over many years, the liquid metal flow in steel continuous casting tundishes and molds, the cooling and solidification of the melt and the formation of segregation, as well as stresses and cracks, have been the subject of numerous projects in which the phenomena were analyzed by various measurement techniques, calculations and/or analytical or numerical simulations. The motivation for these efforts was the desire to understand the details of the phenomena influencing the casting process performance and the strand quality, in order to be able to optimize the casting process conditions.

Today, the combination of newest developments in coupled 3D numerical heat and mass transport simulation coupled with computational optimization methods based on genetic algorithms allows new approaches to answering various questions that arise in process optimization.

In this contribution, the authors show different examples of the use of genetic algorithms for autonomous multi-objective numerical optimization of the continuous casting process and in the second part of this paper for the prediction of filling, solidification, convection and segregation for a steel ingot of a typical tool steel.

Introduction

The simulation of tool steel manufacturing processes such as continuous or ingot casting have been developed in many ways over the last 20 years. Today, the high end numerical simulation technologies have gained a level, where many of the every day’s questions being asked by the production can be answered.

In continuous casting these questions are for example:
• What is the optimal casting velocity dependent on process temperatures, mould and secondary spray cooling?
• What kind of segregation can occur in the strand?
• How does the residual stress influence crack formation and strand distortion?

In ingot casting these questions are accordingly:
• What kind of flow occurs, driven by the filling process as well as by convection?
• What kind of segregation can occur in the ingot, taken convection and diffusion into consideration?
• What kind of porosities must be expected?
• How can a sufficient directional solidification be realized?
In its first part, this contribution presents a computational optimization methodology, based on 3D numerical simulations of the continuous casting process for the whole strand. This can be seen as a first step into the future of autonomous process optimization - recently being named as “the second generation of numerical simulation technologies” [1].

The best possible boundary conditions for the computational continuous casting process optimization have been evaluated by the use of inverse optimization methods [2]. The objectives for the optimization were to get the best possible coupling between casting speed, spraying nozzle layout and liquid pool depth. The use of a multi-objective optimization algorithm made it possible to follow all these objectives simultaneously. The Pareto-set from the optimization allows the evaluation of how the different versions that were simulated perform with respect to the given objectives – which means selecting a situation that makes the best possible compromise.

The second part of this paper deals with the prediction of the casting quality of an ingot casting process. Here the focus was to understand in detail, how process parameters influence the formation of porosities and segregations. The applied model considers details like the thermo-solutal convection occurring during the solidification and the temperature dependent diffusion of alloying elements. With this level of details the simulation can provide the necessary process understanding for any subsequent optimization measures.

1. Continuous casting optimization

1.1 Measured mould and strand temperatures

Even though it is common practice to measure temperatures and their gradients in the mould there is a lack in well documented plant data for continuous casting. For the purpose of developing and validating simulation models for the continuous casting process it is necessary to compare simulation results with recorded temperature curves from the moulds. In this paper the “measured” temperature/time plots are taken from a simulation study where such plots were generated [2]. This approach was necessary due to the above mentioned lack in well documented plant data.

1.2 Heat withdrawal of the mould

The transported heat from the strand surface to the cooling water is conducted through the solidified steel shell, the flux layer, the gas gap, the copper wall before convective dissipated to the cooling water. For a steady state heat transfer the heat flow is given by:

\[ Q = \alpha_{\text{eff}} \cdot (\dot{v}_u - \dot{v}_0) \cdot A \]

where \(1/\alpha_{\text{eff}}\) is the heat transmission resistance of the different layers between strand surface and copper wall. The heat flux through a layer of casting flux is complicated due to the complex structures of the flux layer, the glassy and
crystalline state, respectively, the mushy and liquid part as well as microscopically gas gaps. In order to simplify the details of the radiation and convection heat transfer through a slag layer with several sub layers an engineering approach is considered, where the conduction and radiation properties of the slag layer, and the contact resistance are concentrated in an average “system conductivity” $\lambda_{\text{sys}}$ [3]. To measure the system conductivity in laboratory scale, experimental setups where developed and the dependence of slag composition was investigated [4]. Among the composition, the system conductivity depends on temperature.

1.3 Use of genetic algorithms

The application of genetic algorithms requires the definition of a start generation consisting of several individuals. In this context “individual” is just another word for design resp. a variant of the involved project. The individuals can be generated by using different DOE strategies like random, quasi-random (Sobol), full/reduced factorial, Taguchi or Monte Carlo methods [5].

The algorithm now starts for any of these individuals a casting process simulation and evaluates the results for their compliance with the given constraints and optimization targets. After that the algorithm creates a new generation following the genetic rules of heredity, mutation and selection. Out of the total number of designs (a given number of generations multiplied by a given number of individuals), being defined and evaluated by the algorithm the good designs can be selected.

The optimization described in this paper was performed using the software module MAGMAfrontier. The optimization problem has to be defined by the following boundary conditions:

- design variables with their corresponding ranges of variation (these are the parameters of the simulation that will be varied)
- output variables (they contain the results of the simulation in concentrated form)
- constraints
- objectives (maximize or minimize certain combinations of output variables)

Based upon this information an optimization loop can be started.

1.4 Continuous casting case study

As an example the production of a bloom with a square section of 160 x 160 mm was analysed. Six cooling zones with different heat transfer coefficients in each zone were modelled. As casting velocity 3 m/min was chosen. Results of the influence of casting velocities on the depth of the liquid pool were already shown in earlier publications [6/7]. For the first part of the project the focus was on the heat withdrawal in the mould. The complex heat transfer coefficient $\lambda_{\text{sys}}$ was determined with an inverse optimization method based on measured temperatures in the mould [1].

The heat transfer coefficients between mould and strand and its characteristics can be described by just a few parameters. These parameters are varied by the optimization algorithms until a minimum of the deviation between measured and calculated temperature/time plots is stated. The set of heat transfer coefficients that leads to the minimum is then the parameter set what leads - same meaning, just different words – to the best fit between simulation and measurements.
In the here described project the melt level in the mould is at ca. 150 mm. So the starting point at 6000 W/m²K is only an approximation, but in general such a curve should have a shape as shown in Fig. 1.

Fig. 1: Typical plot of heat transfers between a water cooled copper mould and a strand.

After the optimization the measured and the calculated temperature plots show a good matching (Fig. 2) and the heat transfer coefficient have been identified well.

Fig. 2: The two temperature curves (left) are in a good agreement. The corresponding heat transfer coefficient is show on the right.

The results of the inverse optimization were used in the second step for the optimization of spray cooling conditions with the objective of a stable liquid pool...
depth. The objective function was defined by minimizing the difference between a liquid pool depth resulting from particular secondary cooling parameters and the desired liquid pool depth of 16.5 meters. The variants were the characteristics of the secondary cooling zones (Fig. 3).

Fig. 3: The secondary cooling is partitioned into 6 different zones; the left picture shows the cooling zones in total.

An important medium to study the results of the optimization project is the so called scatter chart. Here the position of the liquid pool tip is plotted over a water spray nozzle in zone 3 (Fig. 4). A clear tendency can be found. Changing the heat transfer coefficient to higher amounts will decrease the depth of the liquid pool.

Fig. 4: Scatter chart for a water spray nozzle which belongs to the zone 3. On the x-coordinate the heat transfer coefficient [W/m²K] of a spray nozzle is plotted and the y-coordinate shows the liquid pool depth [mm]. A clear tendency can be found.

After this optimization loop the user has now the possibility to choose a design which is corresponding to the desired liquid pool depth.
2. Ingot casting quality assurance

The quality of cast tool steel ingots can often be discovered not before the ingot ran through several cost intensive forging steps. For this reason an accurate prediction of the ingot quality, particularly what concerns porosity and segregations, of course before the ingot will be cast would be very welcome. Modelling of the casting and solidification process is the way to get this forecast of the casting quality. Many analytical and numeric models representing certain parts of the complete process have been proposed over the years. But the only future oriented approach is a simulation of the complete casting and solidification process as it is known from the shape casting processes for many years now with the addition of features to model and predict the microstructure.

2.1 Modelling approach

Today the modelling people still live in two worlds: One is the “macroscopic” model world, where the mould filling and solidification simulation leads to quite reliable predictions of temperatures, gradients, cooling and solidification rates. Here it is possible to predict different kinds of porosities and some microstructures based on criteria functions.

The other is the “microscopic” model world, where the microstructure is modelled under consideration of phase building kinetics. The limitation here is the microscopic scale, so that there are no predictions possible for the complete ingot.

In the following an approach is shown in which both worlds were bound together targeting for accurate microstructure predictions in a macroscopic scale. The model takes the following phenomena into consideration:

- diffusion of alloying elements in the melt and in the solid phase
- temperature depending distribution coefficients of the characteristic alloying elements
- melt density as a function of temperature and content of alloying elements

2.2 Tool steel ingot case study

The objective of the simulation project presented here was the determination of possible shrinkage defects and segregations of the characteristic alloying elements of a tool steel. The first step of the simulation project always is the set up of the complete process relevant geometry model (Figure 5).
The mould filling process is controlled by a pressure boundary condition at the
down sprue. The filling process shows the characteristic fountain that is typical for
an unoptimized bottom pouring system and that leads to some turbulence during
the filling process (Fig. 6).

Fig. 6: Due to the quite simple shape of the bottom pouring system a fountain –
like filling can be observed (a-c). The temperature loss during the filling
process is quite low. The occurring turbulences are visualized by tracer
particles (d).
The simulation result shows some room for improvements of the bottom pouring system in order to get a smooth and turbulence free mould filling.

For the prediction of porosities a Niyama criterion has been used. Even if the solidification is ideally directional from the ingate to the riser of the casting, kinetic phenomena might lead to centreline shrinkage such as detected by applying the Niyama criterion (Fig. 7). This criterion reacts on critical high solidification rates in casting sections where the volume increment during solidification can not be compensated fast enough.

![Fig. 7: Although the solidification is directional as indicated by the plot of the local solidification times (left), centre line shrinkage will appear due to insufficient risering. This can be detected with the Niyama criterion (right).](image)

The model applied for the segregation prediction demonstrated here takes thermo-solutal convection, temperature dependent distribution coefficients for alloying elements and the diffusion of alloying elements in liquid as well as in solid phases into consideration.

In this contribution the segregation of carbon, tungsten and vanadium are shown (Fig. 8). With the existing models it is possible to predict also the segregation of the other alloying elements. The chemical composition of the tool steel is:

<table>
<thead>
<tr>
<th>Element (wt%)</th>
<th>C</th>
<th>Si</th>
<th>Mn</th>
<th>V</th>
<th>W</th>
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<tbody>
<tr>
<td>Content</td>
<td>0.9</td>
<td>0.3</td>
<td>0.3</td>
<td>1.85</td>
<td>6.25</td>
</tr>
</tbody>
</table>
3. Conclusions and outlook

It was shown that simulation of continuous and ingot casting processes can distinctly improve and optimize the process conditions and the product quality. This potential is gained from two new features implemented in the software applications having been used here:

- The autonomous computational optimization of casting processes based on genetic algorithms and
- The integration of porosity and segregation building kinetics to the macroscopic casting process simulation.

It should be stated here that the doors have just been opened. The autonomous optimization technologies will in the near future be applied to improve more process phenomena than porosity and segregations like for example residual stress. For the ingot casting process the typical applications of the autonomous optimization technology are:

- The optimization of mould wall thicknesses to support a directional solidification
- The optimization of the bottom pour system to support a smooth turbulence free filling process
- The optimization of the mould shape to improve its life time
Finally it should be clear that with increasing computational power several models describing the microscopic phase building kinetics can be implemented by the macroscopic process simulation models.

References


