Discovering optimal parameters for excellent casting simulations through

Ngadja Taha Niane, PSA Peugeot-Citroën
Stefano Mascetti, XC Engineering srl
XC Engineering presentation

- XC Engineering srl is a small company that works as a Flow Science associate and SigmaTech representative for European countries
- All engineers in XC Engineering are highly qualified fluid dynamics engineers
- Located 30km from Milan
- It has a growing cluster, to provide better support service also in HPC simulations.
Thanks to PSA for this test case!

This work has been developed with PSA, in particular thanks to:

**Mr. Ngadia Taha Niane**
*Specialist in numerical modeling of casting processes*
The question

This work started by trying to answer the following recurrent questions:

✓ How accurate can be my casting simulations with **FLOW-3D**?
✓ What to set for numerical parameters like the HOBS or others?

Sometimes when tuning numerical parameters it is difficult to know what to set and represent like a barrier between the simulation and potentially accurate results.
The test case

Thanks to Peugeot-Citroen we have available a good experiment to compare with:

A gravity casting pouring, with well known data and a mold fully filled of thermocouples. Having several thermocouples in the mold is helpful to track temperature history along the process time, as well as to give an idea of the filling dynamic.

- n° 15 thermocouples
- time available from t=0 to t=1000 s
The goal of this study is to optimize numerical parameters to set in *FLOW-3D* to match both the filling dynamic and the solidification behavior.
The tools

- To perform the best at this job, we coupled the cfd simulation software **FLOW-3D** with **IOSO Optimization Technology**, to allow the automatic calling of **FLOW-3D** simulations and the best optimization strategy to converge to the optimal solution.

- The physics involved and the amount of tuning parameters that we want to change are in fact too complex to be managed simply through human experience. \(<- \) not possible!

- An additional benefit of using optimization tools is that – while executing simulations and analyzing results – the user is free to do any other job.

**FLOW-3D**

**IOSO Technology**
Pre-simulation improvements

- Optimization tools, especially if good, have the natural tendency of «cheating»!

  To push the solution at really high extremes, these tools often make use of the smallest software deficiencies or weak points, not always correspondent to the real deficiencies of the system.

- Then, before running the job, we carefully improved the cfd setup making it:
  1. more accurate  -> we want search for a good comparison with thermocouples data
  2. more robust   -> to prevent IOSO from cheating
  3. faster        -> to run the highest number of simulations in a shorter time

With all of these improvements simulation speed was reduced from ~30 hours to 5 hours, keeping a high accuracy on the numerical results.
Optimization parameters – filling stage

For the filling stage, 10 independent variables are chosen as design parameters:

<table>
<thead>
<tr>
<th>Prepin variable</th>
<th>Meaning</th>
<th>Range (min-max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HFLV1</td>
<td>heat transfer between metal and void</td>
<td>5-80</td>
</tr>
<tr>
<td>CLHT1</td>
<td>latent heat of solidification</td>
<td>(nominal) ±10%</td>
</tr>
<tr>
<td>TSDRG</td>
<td>solidification drag coefficient</td>
<td>0 – 250</td>
</tr>
<tr>
<td>FSCO</td>
<td>coherent solid fraction</td>
<td>0 – 0.6</td>
</tr>
<tr>
<td>ROUGH</td>
<td>roughness for solid component</td>
<td>0.01 – 1 *e-3</td>
</tr>
<tr>
<td>TEMPI</td>
<td>initial metal temperature</td>
<td>720 – 750</td>
</tr>
<tr>
<td>HOBS(750)</td>
<td>htc between metal and mold at T=750°C</td>
<td>100 – 16000</td>
</tr>
<tr>
<td>HOBS(650)</td>
<td>htc between metal and mold at T=650°C</td>
<td>100 – 16000</td>
</tr>
<tr>
<td>HOBS(613)</td>
<td>htc between metal and mold at T=613°C</td>
<td>100 – 16000</td>
</tr>
<tr>
<td>HOBS(580)</td>
<td>htc between metal and mold at T=580°C</td>
<td>100 – 16000</td>
</tr>
</tbody>
</table>
# Optimization parameters – solidification stage

About the solidification stage, 12 independent variables are chosen:

<table>
<thead>
<tr>
<th>PrepIn variable</th>
<th>Meaning</th>
<th>Range (min-max)</th>
</tr>
</thead>
<tbody>
<tr>
<td>HFLV1</td>
<td>heat transfer between metal and void</td>
<td>8-25</td>
</tr>
<tr>
<td>CLHT1</td>
<td>latent heat of solidification (nominal)</td>
<td>(nominal) ±10%</td>
</tr>
<tr>
<td>TSDRG</td>
<td>solidification drag coefficient</td>
<td>100 – 250</td>
</tr>
<tr>
<td>FSCO</td>
<td>coherent solid fraction</td>
<td>0 – 0.49</td>
</tr>
<tr>
<td>FSCR</td>
<td>critical solid fraction</td>
<td>0.5 – 0.9</td>
</tr>
<tr>
<td>HOBS(613)</td>
<td>htc between metal and mold at T=613°C</td>
<td>100 – 16000</td>
</tr>
<tr>
<td>HOBS(580)</td>
<td>htc between metal and mold at T=580°C</td>
<td>100 – 100000</td>
</tr>
<tr>
<td>HOBS(560)</td>
<td>htc between metal and mold at T=560°C</td>
<td>100 – 100000</td>
</tr>
<tr>
<td>HOBS(540)</td>
<td>htc between metal and mold at T=540°C</td>
<td>100 – 100000</td>
</tr>
<tr>
<td>HOBS(490)</td>
<td>htc between metal and mold at T=490°C</td>
<td>100 – 100000</td>
</tr>
<tr>
<td>HOBS(450)</td>
<td>htc between metal and mold at T=450°C</td>
<td>100 – 100000</td>
</tr>
<tr>
<td>HOBS(20)</td>
<td>htc between metal and mold at T=20°C</td>
<td>100 – 100000</td>
</tr>
</tbody>
</table>
Definition of optimization objectives [1]

- from experiment there are n°15 independent curves of temperature vs. time
- each curve is composed by > 2000 temperature points, to be compared with their respective temperature point coming from simulation.

Problem: How to translate in an efficient mathematical equation the qualitative objective «minimize the error between the curves»?
Definition of optimization objectives [2]

The actual solution is based on a two objective solution:

**Objective #1:** minimize the difference between the temperature (numerical – experiment) recorded at a certain time of interests, or better:

\[
\min \left[ \sum_{1}^{15} |T_{\text{exp}}(t) - T_{\text{num}}(t)| \right] \quad \text{for } t = \text{(ex.: 16 s)}
\]

**Objective #2:** minimize the difference between the integral of each temperature curve, or better:

\[
\min \left[ \sum_{1}^{15} \int_{t=0}^{t=200} |T_{\text{exp}}(t) - T_{\text{num}}(t)| \, dt \right]
\]
Uncertainties on the experimental data

- About experimental data, we know there can be uncertainties both in the temperature value, and in the time.
- Hence, for the purposes of this work it is still considered good a value that is inside a range of ±10 °C, and an uncertainty on the time up to 1 second.
- Furthermore, observing the experimental curves, it seems that 3 thermocouples over 15 can be discarded.
Running the optimization task

- The two phases (filling and solidification) have been optimized separately.
- Each of them, brought to a Pareto curve, show all combinations of optimal points.
- Concerning solidification, the most interesting phase for this work, for example, **IOSO** took about 50 calls of the cfd model to get actual best solution:
Analyzing the optimal solutions

- The optimizer provided a specific set of values that give the optimal solution, but identifying what ranges are good is not an easy task.
- Some parameters exhibit a certain dependency on the output, while some others did not:

  examples:

![FSCO](image1.png) ![HOBVT1](image2.png)

This plot clearly shows a certain dependency on the optimal solution (y-axis) by the coherent solid fraction value. On contrary, the htc between mold and air seems to be quite arbitrary.
Results – Comparing temperature plots [1/12]

- By comparing the temperatures at the thermocouples point, between numerical (optimal filling and solidification) and experiment we get 10/12 excellent matching! (before using optimal parameter, the matching was quite poor)
Results – Comparing temperature plots [2/12]

Thermocouple #14

[1/2] not best match
Results – Comparing temperature plots [3/12]

Thermocouple #15

[2/2] not best match
Results – Comparing temperature plots [4/12]
Results – Comparing temperature plots [5/12]
Results – Comparing temperature plots [6/12]
Results – Comparing temperature plots [7/12]
Results – Comparing temperature plots [8/12]
Results – Comparing temperature plots [9/12]
Results – Comparing temperature plots [10/12]
Results – Comparing temperature plots [11/12]
Results – Comparing temperature plots [12/12]

Thermocouple #12

![Graph showing temperature over time for Thermocouple #12 with different conditions: Experiment, Initial, and Optimized #50.](image-url)
Results – The filling video
Results – Comparative video
Results – Optimal parameters [1]

...okay, but what are the optimal parameters to use then??

- Remember that optimal parameters may be linked to the case of a gravity casting of aluminum in sand molds!
### Results – Optimal parameters [2]

<table>
<thead>
<tr>
<th>Prepin variable</th>
<th>Meaning</th>
<th>Decisive</th>
<th>Suggested values</th>
</tr>
</thead>
<tbody>
<tr>
<td>HFLV1</td>
<td>heat transfer between metal and void</td>
<td>!</td>
<td>(15-25)</td>
</tr>
<tr>
<td>CLHT1</td>
<td>latent heat of solidification</td>
<td>!</td>
<td>(nominal) +2-4%</td>
</tr>
<tr>
<td>TSDRG</td>
<td>solidification drag coefficient</td>
<td>~</td>
<td>150 – 200</td>
</tr>
<tr>
<td>FSCO</td>
<td>coherent solid fraction</td>
<td>!!</td>
<td>&gt; 0.4</td>
</tr>
<tr>
<td>FSCR</td>
<td>critical solid fraction</td>
<td>!</td>
<td>0.65 &lt; x &lt; 0.9</td>
</tr>
<tr>
<td>ROUGH</td>
<td>roughness for solid component</td>
<td>!! (filling)</td>
<td>0.55 – 0.8 *e-3</td>
</tr>
<tr>
<td>TEMPI</td>
<td>initial metal temperature</td>
<td></td>
<td>(735 – 745)</td>
</tr>
<tr>
<td>HOBVT1</td>
<td>htc between void and mold</td>
<td>~</td>
<td>(15-25)</td>
</tr>
</tbody>
</table>

~= objective is a little sensitive from this value
!= objective is quite sensitive from this value
## Results – Optimal parameters [3]

<table>
<thead>
<tr>
<th>Prep in variable</th>
<th>Meaning</th>
<th>Decisive</th>
<th>Suggested values</th>
</tr>
</thead>
<tbody>
<tr>
<td>HOBS(750)</td>
<td>htc between metal and mold (T=750 °C)</td>
<td>~</td>
<td>(3000 - 6000)</td>
</tr>
<tr>
<td>HOBS(650)</td>
<td>htc between metal and mold (T=650 °C)</td>
<td>~</td>
<td>3000 – 9000</td>
</tr>
<tr>
<td>HOBS(613)</td>
<td>htc between metal and mold (T=613 °C)</td>
<td>~</td>
<td>3000 – 8000</td>
</tr>
<tr>
<td>HOBS(580)</td>
<td>htc between metal and mold (T=580 °C)</td>
<td>~</td>
<td>(5000 &lt; x &lt; 20000)</td>
</tr>
<tr>
<td>HOBS(560)</td>
<td>htc between metal and mold (T=560 °C)</td>
<td>~</td>
<td>&lt; 10000</td>
</tr>
<tr>
<td>HOBS(540)</td>
<td>htc between metal and mold (T=540 °C)</td>
<td>~</td>
<td>&lt; 25000</td>
</tr>
<tr>
<td>HOBS(490)</td>
<td>htc between metal and mold (T=490 °C)</td>
<td>~</td>
<td>50000 &lt; x &lt; 90000</td>
</tr>
<tr>
<td>HOBS(450)</td>
<td>htc between metal and mold (T=450 °C)</td>
<td>~</td>
<td>(50000 &lt; x &lt; 80000)</td>
</tr>
<tr>
<td>HOBS(20)</td>
<td>htc between metal and mold (T=20 °C)</td>
<td>~</td>
<td>70000 &lt; x &lt; 90000</td>
</tr>
</tbody>
</table>

~ = objective is a little sensitive from this value
! = objective is quite sensitive from this value
Results – Final remarks

- With a good tuning of numerical/physical parameters it is possible to reach state-of-the-art filling and solidification behaviors, with an excellent matching with experimental thermocouples.

- During filling stage, for sand molds, it seems crucial to set up a proper roughness factor (quite different from the default).

- Also it seems important to take into account for heat transfer with void, giving an average range for ht coefficient.

- Default values for coherent and critical solid fractions seems also reasonable, and their sensitivity to final objective is present but minimal (using values around the default ones).

- During solidification, heat transfer coefficients seem important, but only as a range, not through a high accuracy.

- Latent heat given by JMatPro database seems also an excellent number, with an optimal value in a range of < +4% of the nominal value.
Results – Open questions...

As often happens, this work opened new questions other than closing the initial one:

- In the present work, HTC coefficients are given through a long tabular input (temperature-dependent): it would be of great interest to try to condense the tabular input into a single input. More user-friendly!

- Also: the initial question of setting optimal HTC is partially answered, because it seems that the fitting curve is not so sensitive from HOBS coefficients. What about then leaving the default HOBS=-1 value?

- To perform accurate HPDC simulation: would these coefficients work well as well? (need for a test-case to compare with)

- What about using the rapid shrinkage model after the filling? How large is the error?
End of presentation
- thanks for your attention -