Understanding and improvement of ingot manufacturing process using a numerical sensitivity analysis

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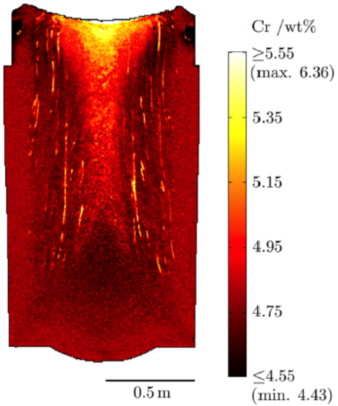
Introduction

- Ingot casting is used in many industrial sectors (aeronautics, nuclear, naval...)
- During solidification, **chemical heterogeneities**, or **segregations**, can appear at the ingot scale
- These defects may weaken the **mechanical properties** of the manufactured piece
- EDF has been confronted to this problem: some components of the reactor vessel have locally high carbon concentrations

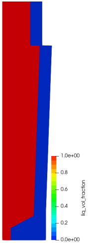


Need to understand and control the formation of segregations using experiments and simulations

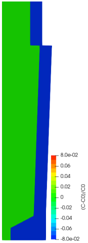
Introduction

- A solidification model with prediction of segregations is currently developped in **Code_Saturne**[1], the general purpose open-source Computational Fluid Dynamics (CFD) software developed and released by EDF R&D.

Solidification of a 3.3 tons ingot with Code_Saturne



Liquid Fraction



Carbon segregation

Goals of the present study:

- Identify (numerically) influential process parameters on segregations
- Specify (real) experiments on 500kg ingots to validate these sensitivities
- (Benchmark the sensitivities with two other codes)

[1] C. Demay et al., *Modelling and simulation of ingot solidification with the open- source software Code_Saturne*, MCWASP XV Proceedings, 2020.

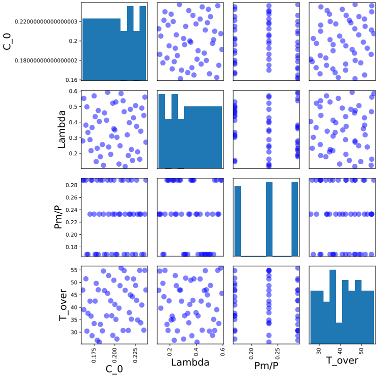
Outline

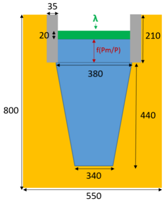
Design Of Experiments

Input: 4 process parameters

* Initial carbon concentration
  C_0 $(w.t.\%) \in [0.16, 0.24]$
  (uniform)
* Conductivity of isolation layer
  λ $(W.m^{-1}.K^{-1}) \in [0.1, 0.6]$
  (uniform)
* Hot top ratio
  $Pm/P \in [16.8\%, 23.3\%, 28.8\%]$
  (discrete uniform)
* Overheating temperature
  T_over $(^\circ C) \in [30, 60]$
  (uniform)

→ **Sobol Sequence, 50 simulations**
(should be 2^n...)





Rk 1: This list has been provided by experts and corresponds to parameters that can be varied experimentally

Rk 2: Model uncertainties are not taken into account in this study

Design Of Experiments

Outputs of interest

- **dC/C0** = max((C-C0)/C0) [scalar]
  - Maximum of carbon segregation rate over the domain
  - **dC/C0 all**: all over the ingot
  - **dC/C0 low**: only under the hot top (ingot body)

- **GM** $= \left(\frac{1}{V} \int \left(\frac{C - C_0}{C_0} \right)^2 dV \right)^{\frac{1}{2}}$ [scalar]
  - Global Macrosegregation Rate
  - **GM all**: all over the ingot
  - **GM low**: only under the hot top (ingot body)

- **Axis segregation rate** [vector]

Design Of Experiments

Workflow

Salome CFD 9.3

PERSALYS

DOE

Outputs

CODE SATURNE V6.0

Define:

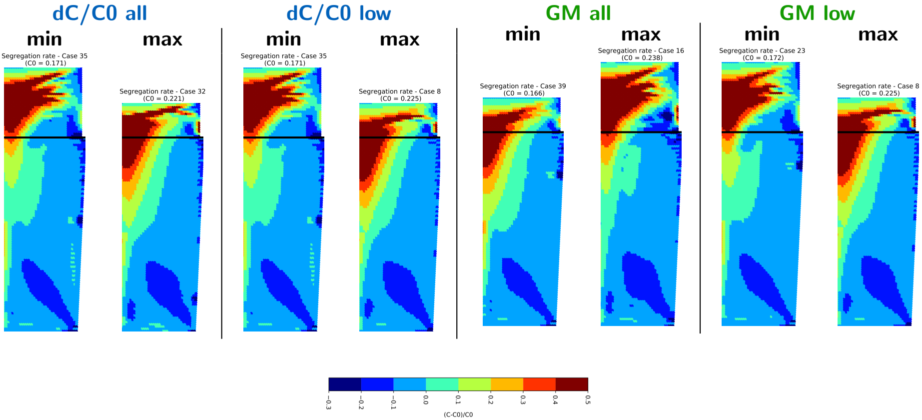
- Input distribution/Output
- Design Of Experiments
- Calculation resources

- 1 calculation/CPU
- 1 calculation: 3 days

- *Automatic* workflow between OT/PERSALYS and the cluster
- The CFD code is seen as a physical model by OT/PERSALYS

Design Of Experiments

Some pictures of carbon segregation



- Only the ingot body is used to build the final piece (under the black line)
- Preference for large hot top but loss of matter...

Design Of Experiments

Goals

- Numerical Sensitivity analysis
  - How the input parameters influence the outputs ?
    - **Spearman Correlation** (for scalars)
  - What are the most influential input parameters on the outputs ?
    - **Sobol indices**

- Guiding for the experimental DOE: 4 ingots to specify
  - Validate (or not) the numerical sensitivities on experimental results

1 Design Of Experiments

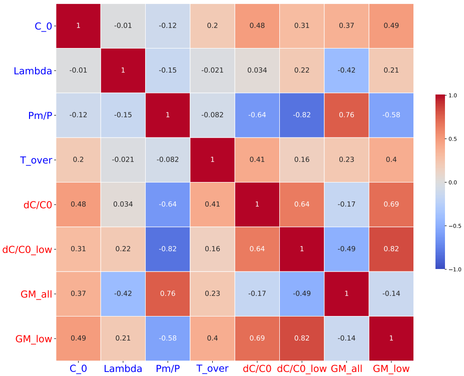
2 Sensitivity Analysis
- Segregation indicators
- Axis segregation rate
- Synthesis

3 Conclusion and perspectives

Sensitivity Analysis: segregation indicators

Spearman correlation

- Rank correlation to identify monotonic relationship between two random variables
  - ★ $r_s > 0$: increasing relationship
  - ★ $r_s < 0$: decreasing relationship



- Significant correlations are obtained with the **hot top ratio (Pm/P)**: less segregation in the ingot body when the hot top is larger (OK)
- The effect of C_0 should also be studied: the physical interpretation is less straightforward

Sensitivity Analysis: segregation indicators

Sobol indices

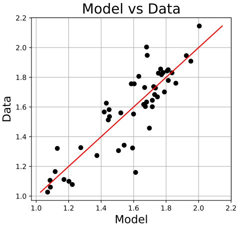
- Compute First Order and Total Order Sobol indices:
  Y: output, X_i: input
  - First order: $S_i = \frac{var(E(Y|X_i))}{var(Y)}$
  - Total order: $ST_i = 1 - \frac{var(E(Y|X_{-i}))}{var(Y)}$
  - Evaluation of uncertainty with bootstrap strategy (confidence interval)

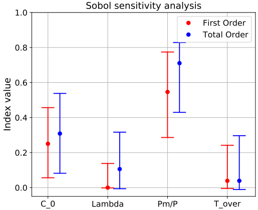
- ...using a Polynomial Chaos Expansion of the output (metamodel):
  - Suitable for discrete probabilistic law (Pm/P)
  - Link between projection coefficients and Sobol indices
  - 2nd Order with sparse strategy
  - Evaluation of Q^2 with Leave-One-Out

Sensitivity Analysis: segregation indicators

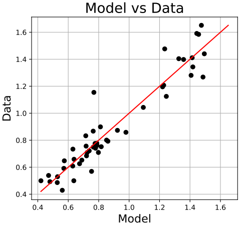
Sobol indices: dC/C0

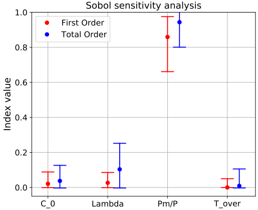
dC/C0 all
Q2-LOO = 0.68





dC/C0 low
Q2-LOO = 0.80





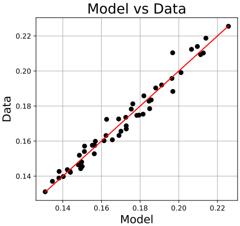
- The metamodels are quite satisfactory for this study (NB: difficulties to numerically get a reliable estimate of the maximum carbon concentration).
- The most influential parameter is the hot-top ratio, with some interactions (especially with lambda). The impact of C_0 is also worth mentioning.

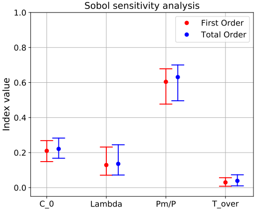
Sensitivity Analysis: segregation indicators

Sobol indices: GM

GM all

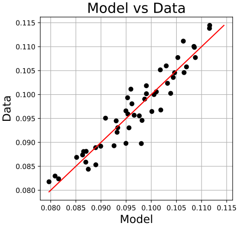
Q2-LOO = 0.93

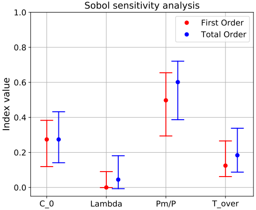




GM low

Q2-LOO = 0.80





- Better models are obtained on integrated data
- The most influential parameter is the hot-top ratio, followed by C_0

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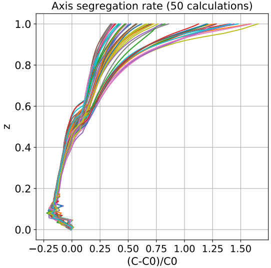
Sensitivity Analysis: axis segregation rate

Approach for multivariate output

- Dimension reduction using a Karhunen-Loève expansion (functional PCA):



$$\mathrm{Y}(z,\mathbf{P}) = \sum_{\alpha\geq 1}\sqrt{\lambda_\alpha}\xi_\alpha(\mathbf{P})\phi_\alpha(z),$$

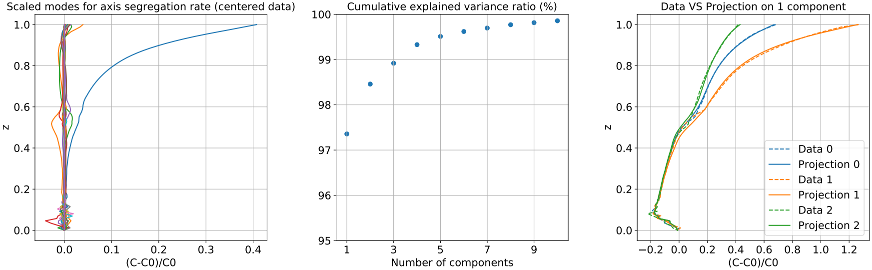
$$\begin{cases} \mathrm{Y}(z,\mathbf{P}) : \text{second-order, zero-mean stochastic process,} \\ \text{(centered segregation rate at altitude z for input paratemers } \mathbf{P}) \\ \lambda_\alpha : \text{principal values,} \\ \phi_\alpha : \text{principal factors,} \\ \xi_\alpha : \text{principal components.} \end{cases}$$

$\rightarrow$ Expansion usually truncated for $\alpha > N$ ensuring a sufficient explained variance ratio

- Compute Sobol indices on principal components $(\xi(\mathbf{P}))_{\alpha\leq N}$
  - First order and Total order for each component + aggregated indices if $\alpha > 1$
- ...using a Polynomial Chaos Expansion of the principal components $(\xi(\mathbf{P}))_{\alpha\leq N}$:
  - 2nd Order with sparse strategy
  - Evaluation of Q^2 with Leave-One-Out

Sensitivity Analysis: axis segregation rate

Dimension reduction

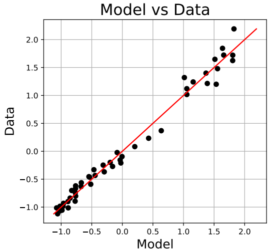


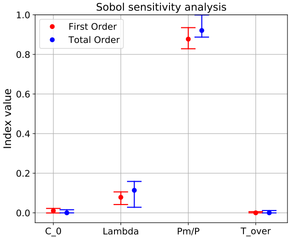
- The first component of the KL expansion explains 97.3% of the output variance
  - The sensitivity analysis on the axis segregation rate can be reduced to one scalar

Sensitivity Analysis: axis segregation rate

Sobol indices: axis segregation rate

Axis segregation rate
(first principal component)
Q2-LOO = 0.97





- The metamodel is very efficient
- The most influential parameter is the hot-top ratio (expected)

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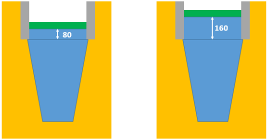
Sensitivity Analysis

Synthesis

- For all the considered segregation outputs, the most influential parameter is the hot top ratio, generally followed by the initial carbon concentration C_0
- These sensitivities has to be verified experimentally: physical and numerical validation. A two-step program is proposed:
  - First experimental campaign (2 ingots): high and low hot-top ratio
    - ⋆ $C_0 = 0.18$ (nominal concentration for alloys of interest)
    - ⋆ Max value of T_{over} and Min value of λ
      $\rightarrow$ Maximize the solidification time (transposability to larger tonnage)



  - Second experimental campaign (2 ingots) on the best quality ingot of the first campaign:
    - ⋆ High initial Carbon concentration C_0
    - ⋆ High initial Silicon concentration Si_0 (parameter studied with other codes)

Conclusion and perspectives

Conclusion

- A numerical sensitivity analysis has been performed using a coupling between OpenTURNS/PERSALYS and *Code_Saturne* (CFD code)
- A Sobol analysis relying on the metamodelling the code is proposed:
  - The 2 most influential process parameters are identified (hot-top ratio, initial carbon concentration)
  - Guiding for experimental program

Further work

- Comparison between experimental and numerical results
- Include model uncertainties in the sensitivity analysis (thermo-physical properties)
- Development of a robust approach for a joint experimental/numerical sensitivity analysis
- Transposability of the results to larger ingots