framatome

Modeling of thermal expansion and metallurgical phases of a material during its cooling

A. CLARISSOU, V. BRUYERE, P. NAMY,
I. CRASSOUS

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SIMTEC

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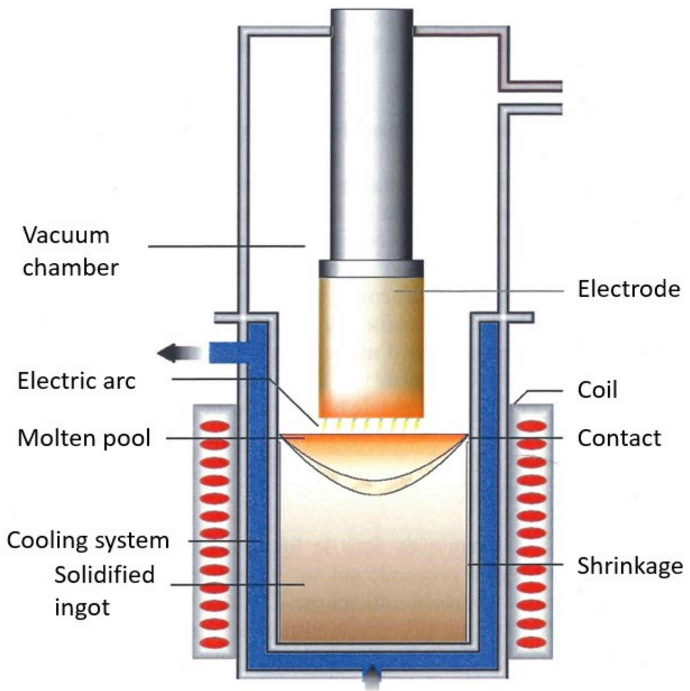
1 Context

Context

Foundry Processes

- Various melting processes



A schematic diagram of the VAR process

"Modélisation mathématique et simulation numérique du procedé de refusion à arc sous vide", Alain Jardy, 2005

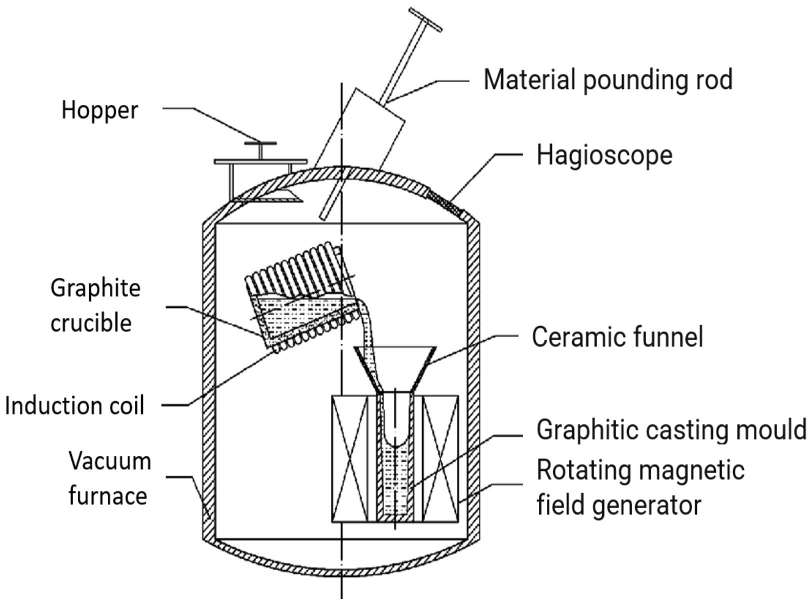
Vacuum Arc Remelting (VAR)

Vacuum Induction Melting (VIM)

To predict the resulting metallurgy

↓

Understand and model precisely thermal exchanges during the process



A schematic diagram of the VIM process.

« *The effect of rotating magnetic field on the microstructure of in situ TiB 2 /Cu composites.*» Zou, Cunlei & Kang, Huijun & Li, Rengeng & Li, M & Wang, Wei & Chen, Zongning & Wang, Tongmin. (2016). IOP Conference Series: Materials Science and Engineering. 117. 012043. 10.1088/1757-899X/117/1/012043.

2 Modeling

Modeling

Thermal Exchanges & Deformed Geometry

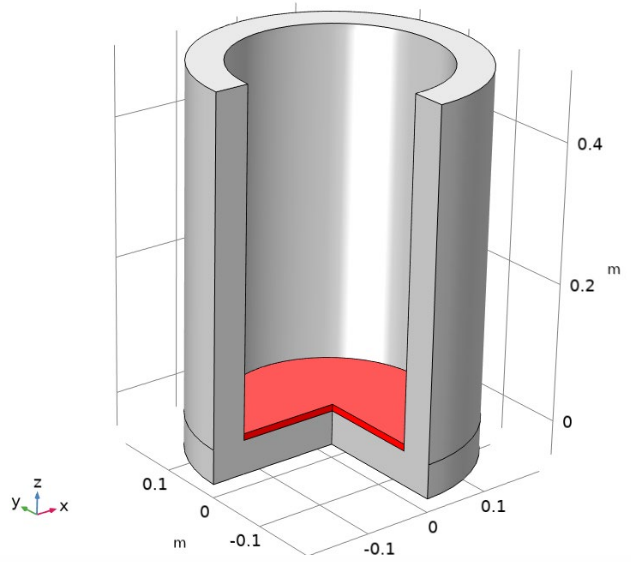
- 2D axisymmetric assumption
- **Heat equation** solved in a **deformed geometry** to model the growth of the ingot during mold filling

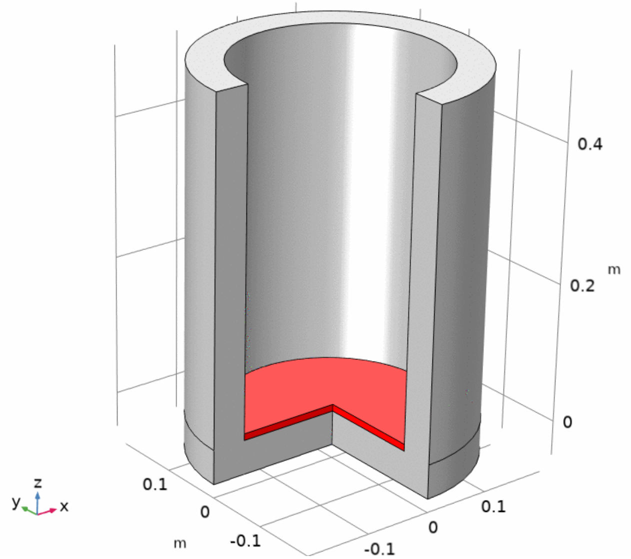
$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = 0$$

- Filling Velocity is known analytically, and **Mesh Deformation is prescribed**

$$\Delta Z_{top} = \frac{\left(v_{ingot} \cdot t \cdot f(t) + h_{ingot}\left(1 - f(t)\right)\right) \cdot Z}{h_{ingot}}$$

- Temperature of the top boundary of the ingot is maintained at $T = T_{melt} + 100$ during the filling with a heat flux condition





Modeling

Thermal Exchanges – Boundary Conditions

- Thermal Contact

$$-\boldsymbol{n}_1 \cdot \boldsymbol{q}_1 = -h_{ingot}(T_2 - T_1)$$
$$-\boldsymbol{n}_2 \cdot \boldsymbol{q}_2 = -h_{ingot}(T_1 - T_2)$$

- Three zones :

$$h_{ingot} = 10^4 \frac{W}{m^2 \cdot K} \; if \; T_1 > T_{liquidus}$$

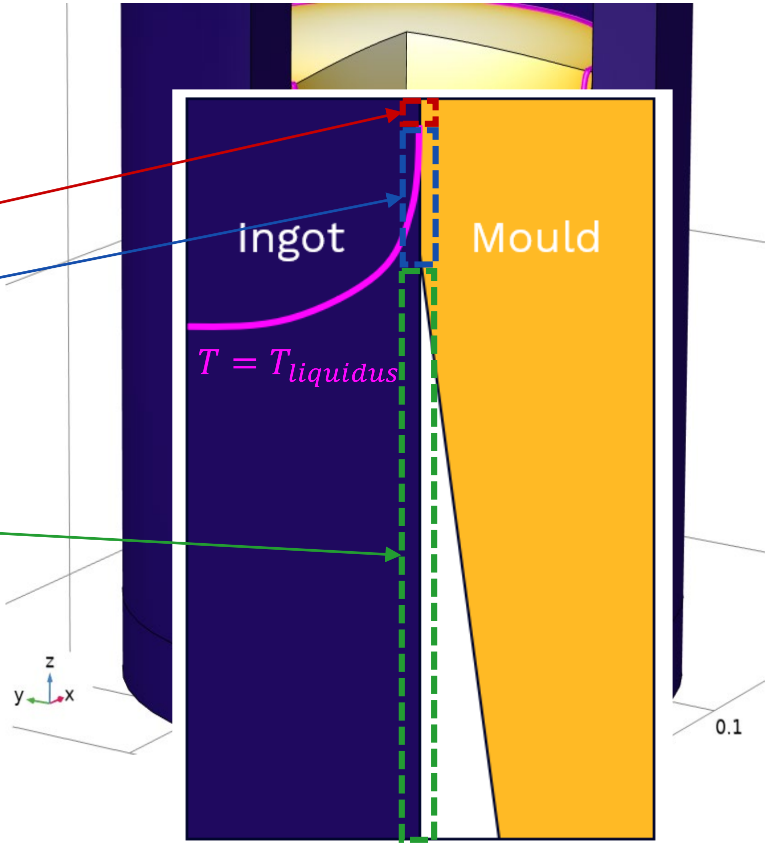
$$h_{ingot} = 800 \frac{W}{m^2 \cdot K} \; if \; contact$$

$$h_{ingot} = \varepsilon_1 \sigma \left(T_1^2 + {T_2}^2\right)(T_1 + T_2) \; if \; no \; contact$$

- Cooling conditions

$$-\boldsymbol{n} \cdot \boldsymbol{q} = h_{cooling}(T_{fluid} - T)$$

$h_{cooling}$ obtained with Comsol Multiphysics relations



Modeling

Metallurgy

- **Austenite** to **ferrite** and **pearlite** (diffusion behavior):

$$\frac{dz_i}{dt} = K_i(T)z_{austenite} - L_i(T)z_i$$

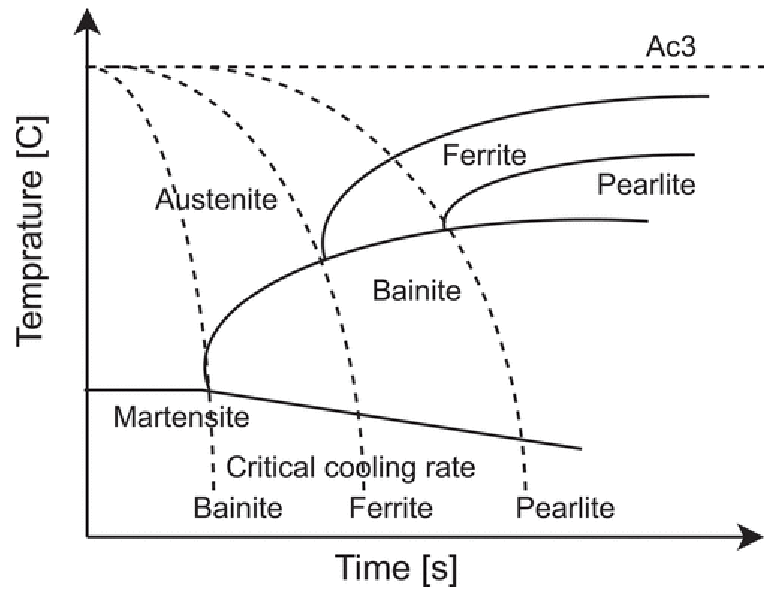
- Austenite to **bainite** (diffusion behavior but function of the thermal kinetics)

$$\frac{dz_{bainite}}{dt} == F(T)H\left(\frac{dT}{dt}\right)z_{austenite} - G(T)H\left(\frac{dT}{dt}\right)z_{bainite}$$

- **Martensite** formation if $\frac{dT}{dt} < 0$ and $T < M_s$

$$\frac{dz_{martensite}}{dt} == -z_{austenite}\beta\frac{dT}{dt}$$

4 Distributed ODEs are added



A CCT diagram for steel

"Prediction of continuous cooling transformation diagram for weld heat affected zone by machine learning",, Satoshi Minamoto, 2022

Modeling

Mechanics

- **Equation** $\nabla \cdot \underline{\underline{\boldsymbol{\sigma}}} = \mathbf{0}$

- **Lemaitre & Chaboche [*]** model

$$\underline{\underline{\sigma}} = \underline{\underline{\underline{\underline{\mathbb{E}}}}}(T) : \left(\underline{\underline{\varepsilon}} - \underline{\underline{\varepsilon}}^p - \alpha(T, z_i) \cdot (T - T_0) \underline{\underline{\boldsymbol{I}}} \right)$$

$$\underline{\underline{\varepsilon}} = \frac{1}{2} (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T)$$

$$\underline{\underline{\dot{\varepsilon}^p}} = \dot{p} \frac{3}{2} \frac{\underline{\underline{\sigma}}' - \underline{\underline{X}}'}{J_2 \left(\underline{\underline{\sigma}}' - \underline{\underline{X}}' \right)}$$

$$\underline{\underline{\dot{X}}} = \frac{2}{3} C(T) \underline{\underline{\dot{\varepsilon}^p}} - \gamma \underline{\underline{X}} \, \dot{p}$$

$$\dot{p} = \left\langle \frac{J_2 \left(\underline{\underline{\sigma}} - \underline{\underline{X}} \right) - \sigma_y(T)}{K(T)} \right\rangle^{\mathrm{n(T)}}$$

[*] J. Lemaitre et J.-L. Chaboche, Mécanique des matériaux solides, Dunod, 2001.

3

Numerical Aspects & Validation

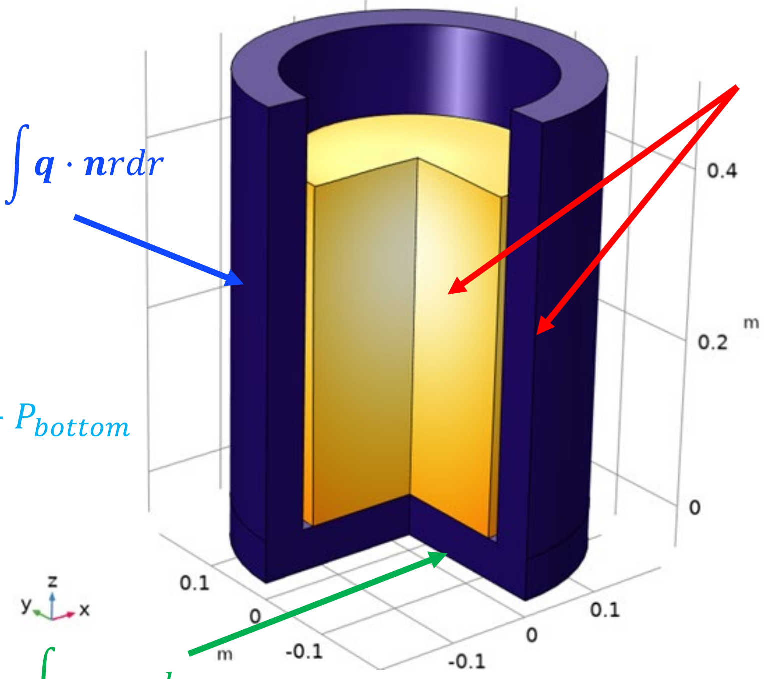
Numerical Validation

Energy Balance

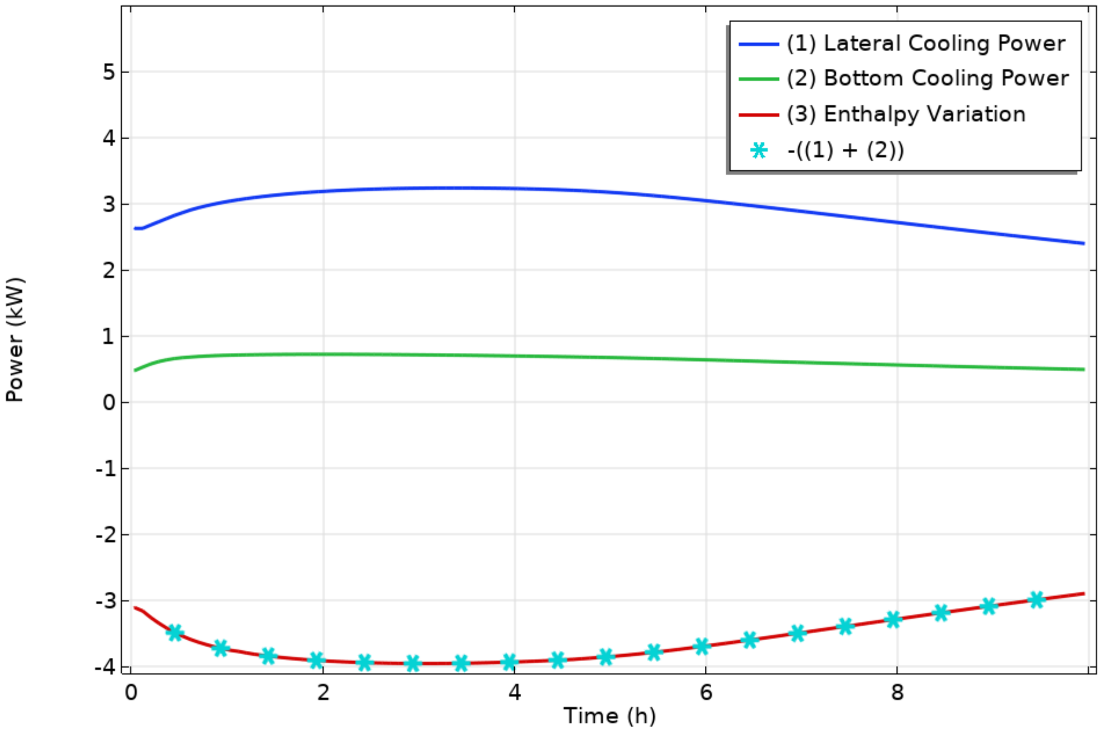
$$P_{enthalpy} = 2\pi \iint \rho C_p \frac{dT}{dt} r dr dz$$

$$P_{lateral} = 2\pi \int \boldsymbol{q} \cdot \boldsymbol{n} r dr$$

$$\sum = P_{lateral} + P_{bottom}$$



$$P_{bottom} = 2\pi \int \boldsymbol{q} \cdot \boldsymbol{n} r dr$$



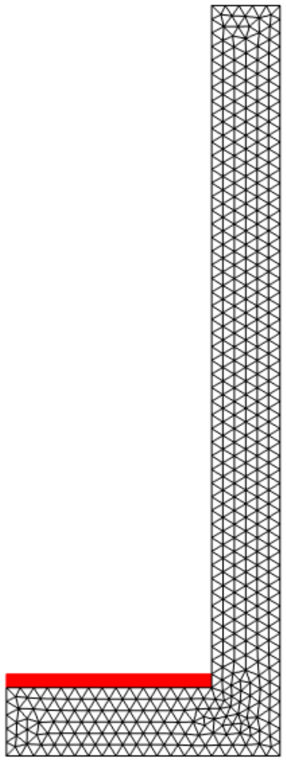
- Numerical Validation with energy balance verifications

Numerical Aspects

Mesh and Solvers

- Mapped Mesh
- Refinement near the lateral contact conditions
- Deformation analytically controlled

- Segregated Resolution Technique
- Time-Step control



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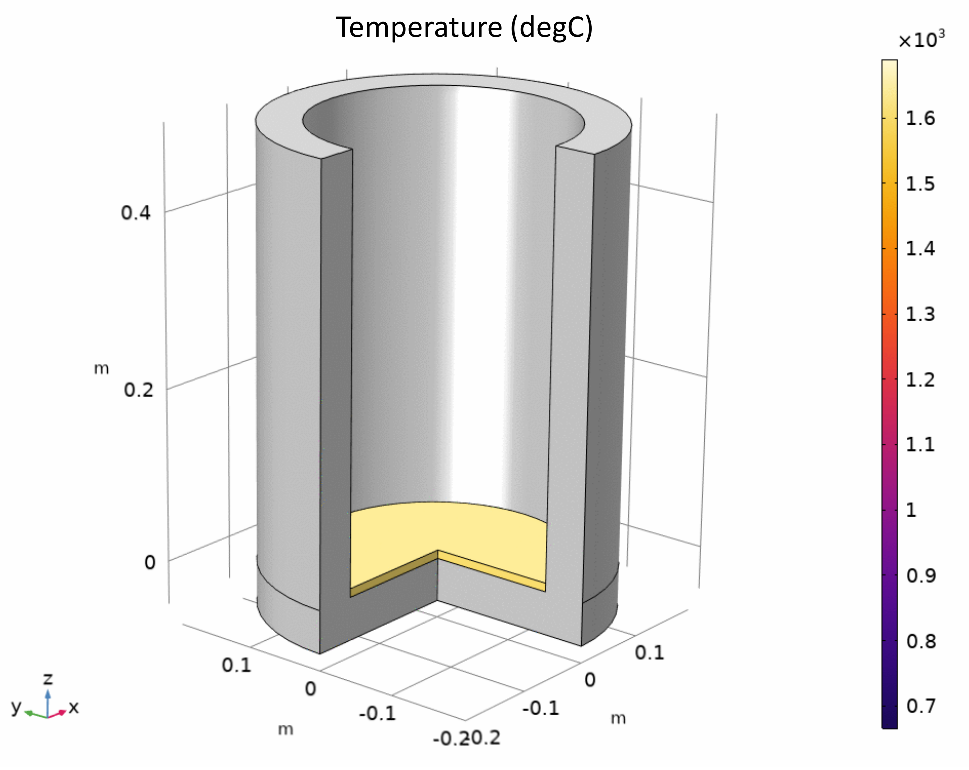
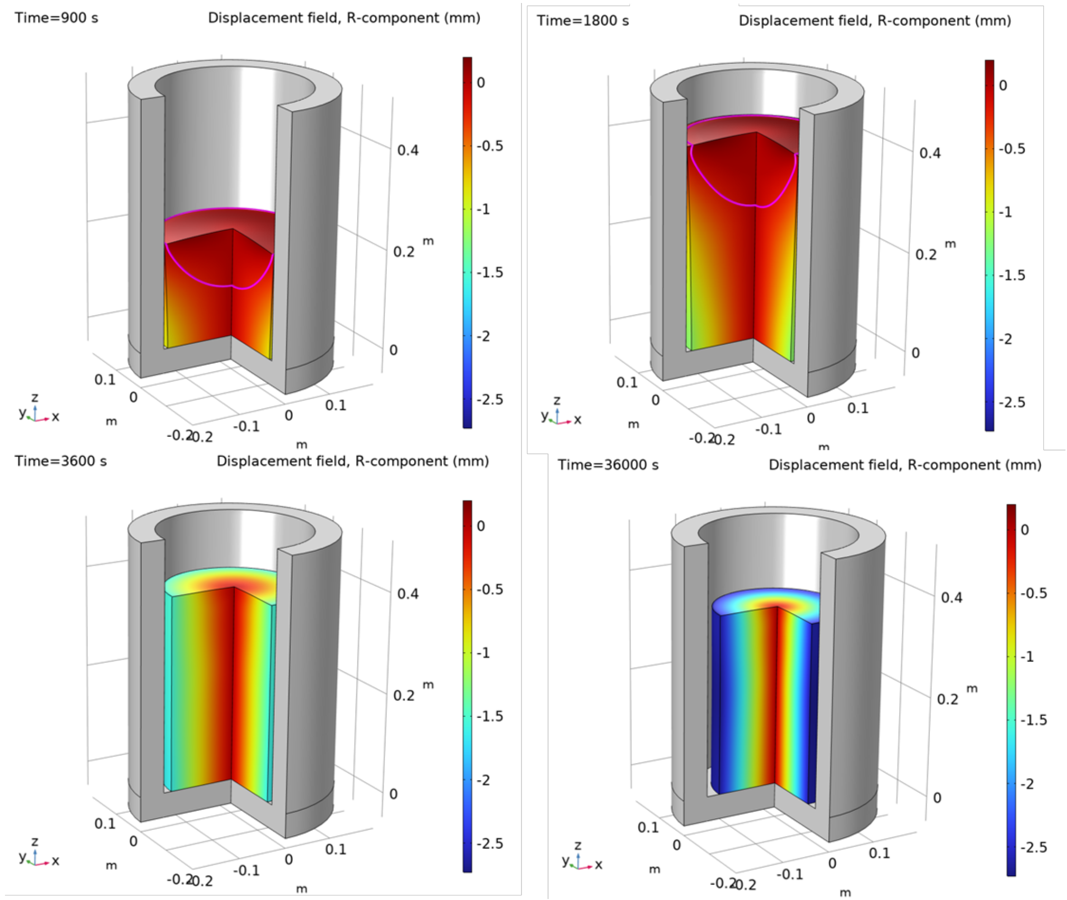
Results

Results

Thermo-Mechanical Results

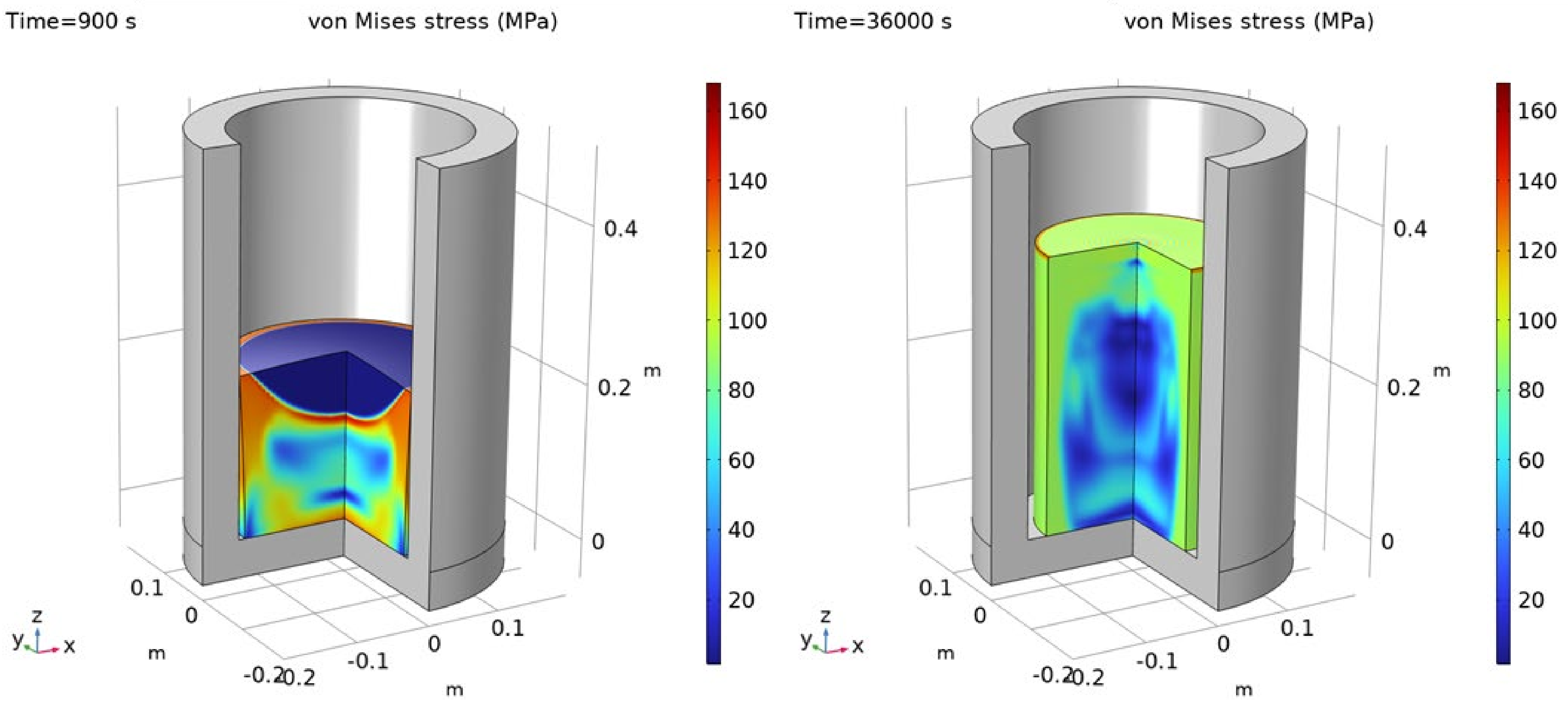




- Filling and Cooling phases can be studied
- Temperature field and thermal shrinkage are predicted

Results

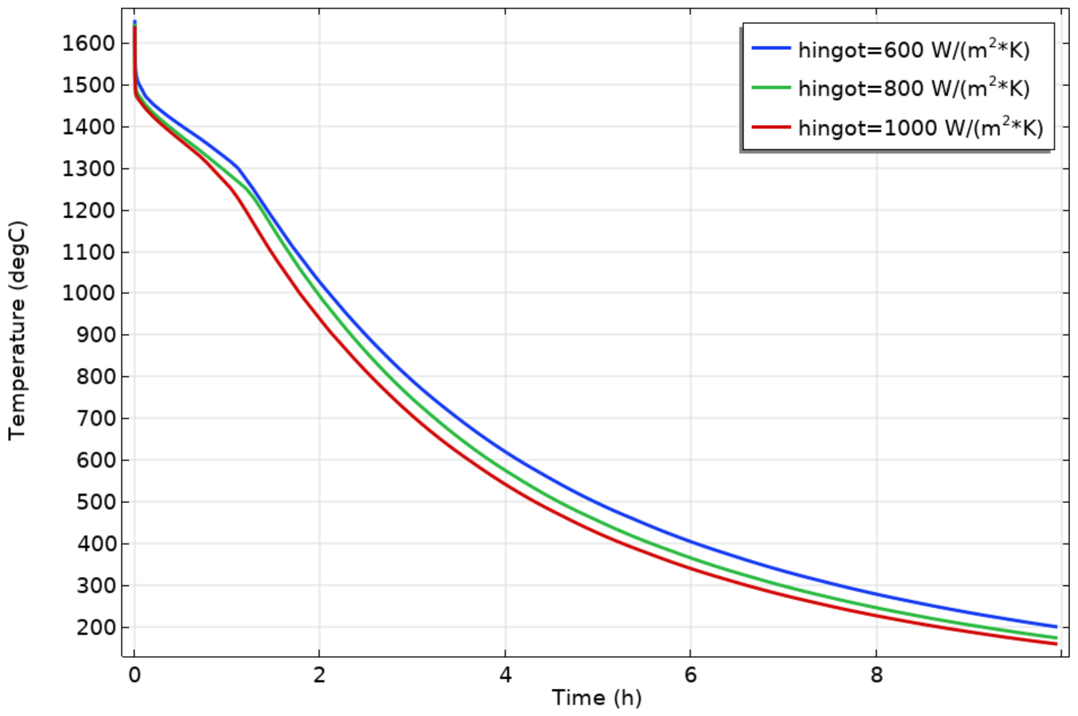
Thermo-Mechanical Results

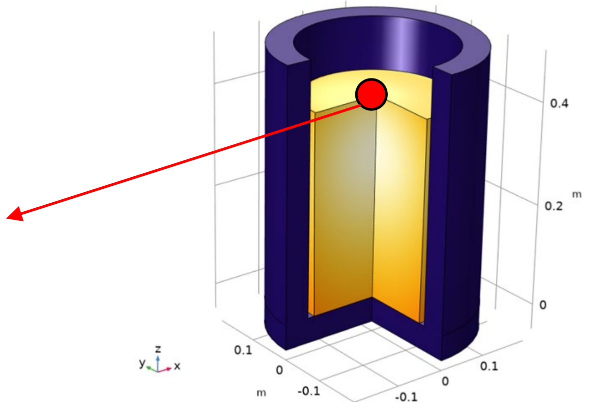


- Von Mises stress evolution → Residual deformation and stresses prediction

Results

Influence of Lateral Conductance

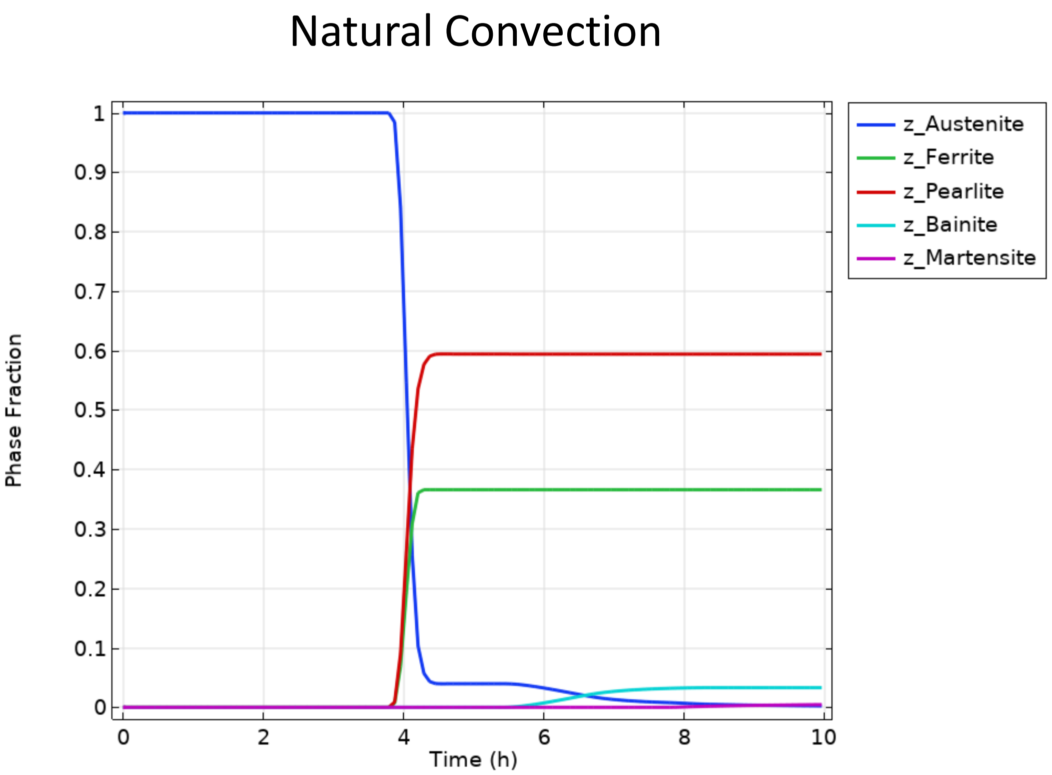


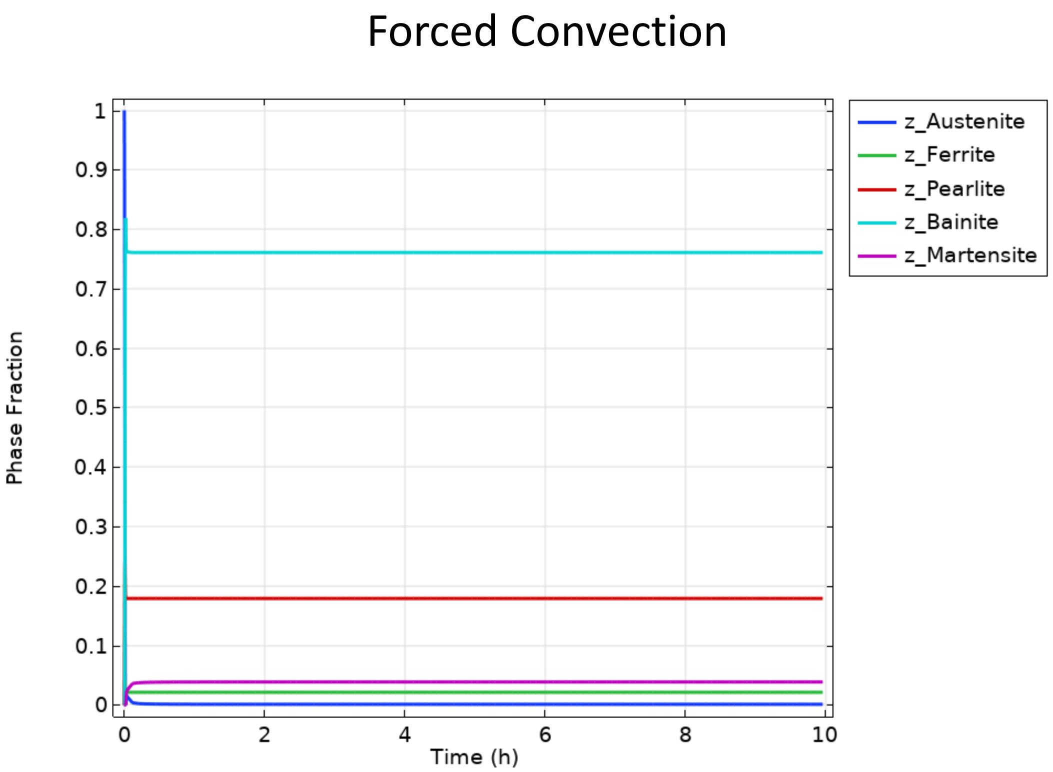


- The knowledge of the contact conditions is important to predict precisely the temperature evolution of the ingot

Results

Influence of Cooling conditions – Temperature Evolution



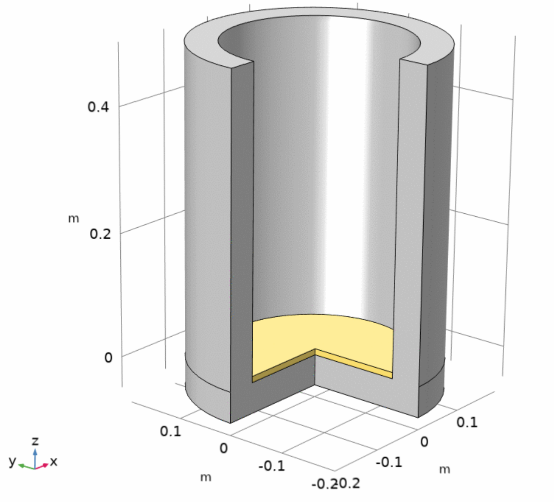


- For slow cooling (natural convection) **pearlite** is the final predominant phase
- For faster cooling condition (forced convection), **bainite** is the final predominant phase and **higher martensite** fraction

5 Conclusions

Conclusions

- Development of a thermo-metallo-mechanical model
- Numerical Validation of the model
- Improvement of lateral boundary condition modeling
- Prediction of residual deformation and resulting metallurgy
- Model usable for different applications and cooling conditions



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Thank you