Avoiding segregation with *Code_Saturne*

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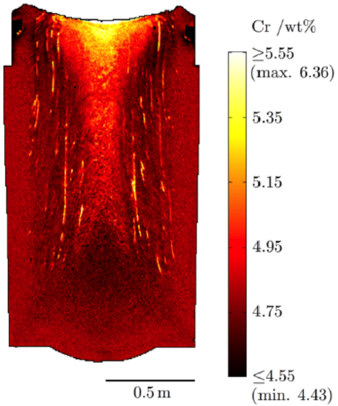
Introduction

- 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

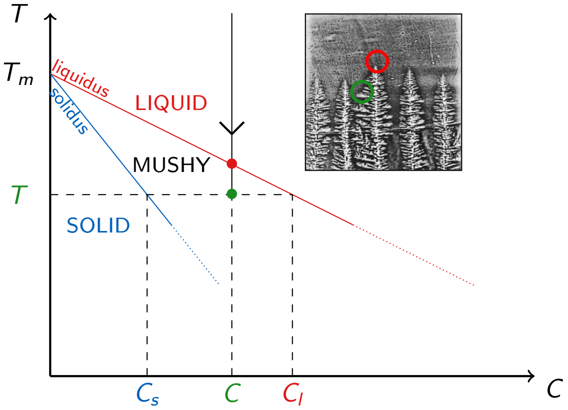


Need to understand the formation of segregations using experiments and simulations

Outline

Alloy solidification

Simplified phase diagram (binary alloy)



- The solid rejects enriched solute at the micro scale (**microsegregation**)
  - $C_s < C_l$
- Lever rule hypothesis: perfect diffusion in the solid close to the solid-liquid interface
  - $C_s = k_p C_l$

Alloy solidification

Segregations: main concepts

Microsegregations
($\sim 100\mu m$)

+

Relative motion between solid and liquid phase

(a) **Thermo-solutal convection** (b) Solid grain movement

(c) Solidification shrinkage (d) Deformation of the solid network

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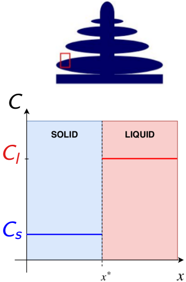
- **Mesosegregations** ($\sim cm$)
- **Macrosegregations** ($\sim m$)



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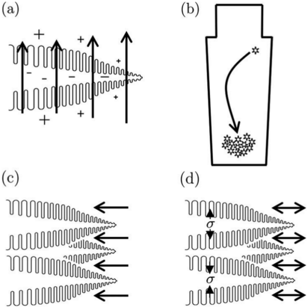

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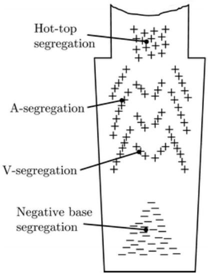

Mixture model for solidification

General approach

Following Bennon and Incropera[1] approach:

- Define a Representative Elementary Volume (REV) and volume fraction:

$$\begin{cases} \text{V: Volume of the REV (scale} \sim 1\, mm) \\ V_k\text{: Volume of phase } k \text{ in V} \\ g_k\text{: Volume fraction of phase } k \text{ in V} \end{cases}$$

$$g_k = \frac{V_k}{V}$$

- Integrate conservation laws on the REV:

$$\partial_t \int_V (\rho_k \phi_k)\, dV_k + \int_A (\rho_k \phi_k \mathbf{u_k}).\mathbf{n}\, dA_k = -\int_A \mathbf{J}.\mathbf{n}\, dA_k + \int_V S_k\, dV_k$$

- Define mixture variables:

$$\Psi_m = g_l \Psi_l + g_s \Psi_s,$$

and sum integrated conservation laws on both phases.

[1] Bennon, W. D., and F. P. Incropera. "A continuum model for momentum, heat and species transport in binary solid-liquid phase change systems—I. Model formulation." International Journal of Heat and Mass Transfer 30.10 (1987): 2161-2170.

Mixture model for solidification

Hypothesis and closure laws

- Thermodynamic equilibrium between liquid and solid phase:
  - Temperature, density
  - Thermal conductivity, specific heat, diffusion coefficient

- Hypothesis for momentum conservation:
  - Newtonian fluid
  - Boussinesq approximation: constant density except in the buoyancy term

$$\rho_b = \rho_{ref}(1 - \beta_T(T - T_{ref}) - \beta_C(C_l - C_{ref}))$$

  - Darcy law in the mushy zone: drag force accounting for porosity

$$\mathbf{F} = -\frac{\mu}{K(g_l)}\,\mathbf{u_m} \quad \text{with} \quad K(g_l) = \frac{\lambda_2^2}{180}\frac{g_l^3}{(1-g_l)^2}$$

  - Crossed-terms neglected compared to porosity contribution
  - Motionless solid phase:

$$\mathbf{u_s} = 0 \text{ so that } \mathbf{u_m} = g_l \mathbf{u_l}$$

Mixture model for solidification

Balance equations

4-equation mixture model (binary alloy)

- Momentum equation

$$\begin{cases} \partial_t(\rho \mathbf{u}) + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla(p) + \mathrm{div}(\mu \nabla \mathbf{u}) + \rho_b(T, C)\mathbf{g} - \dfrac{\mu}{K(g_l)}\,\mathbf{u} \\ \mathrm{div}(\mathbf{u}) = 0 \end{cases}$$

- Heat equation

$$\rho c_p \partial_t T + \rho c_p \mathrm{div}(T\mathbf{u}) = \mathrm{div}(\lambda \nabla T) - \partial_t(\rho L g_l)$$

- Solute transport equation

$$\partial_t(\rho C) + \mathrm{div}(\rho C_l \mathbf{u}) = \mathrm{div}(\rho D \nabla C)$$

- 8 unknowns: $(\mathbf{u}, p, T, g_s, g_l, C_s, C_l, C)$, L: latent heat

- 4 additional equations:
  - Definition
    - $g_s + g_l = 1$
    - $C = g_s C_s + g_l C_l$
  - Closure laws
    - $T = T_m + m_l C_l$
    - $C_s = k_p C_l$

Numerical scheme

Overview

General loop

1. Solve scalar equations (C, T)
2. Update (g_l, C_l) following the phase diagram
   - ⋆ In the mushy zone: $g_l(T, C) = 1 - \frac{1}{1-k_p}\frac{T-T_l(C)}{T-T_m}$, $C_l(T) = \frac{T-T_m}{m_l}$.
3. Solve mass and momentum conservation $(\mathbf{Q} = \rho\mathbf{u}, \mathbf{u}, P)$

Discrete settings

- SIMPLEC algorithm with sub-loops (PISO-like) on steps 1-3 with updated buoyant scalars
- Spatial: First-order upwind scheme
- Time: (mostly) Implicit Euler scheme

Additional features:

- Ensure equilibrium between hydrostatic pressure gradient and external forces (*iphydr=1*)
- Kill mass fluxes linked with solid cells (*iporous=3*)

Numerical scheme

Details for time discretization: sub-loop k of iteration n (implicit terms)

1. Solve scalar equations:

$$\begin{cases} \rho \dfrac{C^{n+1,k} - C^n}{\Delta t} + \mathrm{div}(C_l^{n+1,k-1}\,\mathbf{Q}^{n+1,k-1}) = \mathrm{div}(\rho D \nabla C^{n+1,k}), \\ \rho c_p \dfrac{T^{n+1,k} - T^n}{\Delta t} + c_p\,\mathrm{div}(T^{n+1,k}\,\mathbf{Q}^{n+1,k-1}) = \mathrm{div}(\lambda \nabla T^{n+1,k}) - s_T^{n+1,k/k-1}, \end{cases}$$

with:

$$s_T^{n+1,k/k-1} = \left.\frac{\partial(\rho g_l L)}{\partial T}\right|_{n+1,k-1} \frac{T^{n+1,k} - T^n}{\Delta t} + \left.\frac{\partial(\rho g_l L)}{\partial C}\right|_{n+1,k-1} \frac{C^{n+1,k} - C^n}{\Delta t}.$$

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3 -1 Velocity prediction:

$$\rho \frac{\widetilde{\mathbf{u}}^k - u^n}{\Delta t} + \mathrm{div}(\widetilde{\mathbf{u}}^k \otimes \mathbf{Q}^{n+1,k-1}) = \mathrm{div}(\mu \nabla \widetilde{\mathbf{u}}^k) - \nabla p^{n+1,k-1} - \frac{\mu}{K^{n+1,k}} \widetilde{\mathbf{u}}^k + \rho_b^{n+1,k-1}(T, C)\mathbf{g}$$

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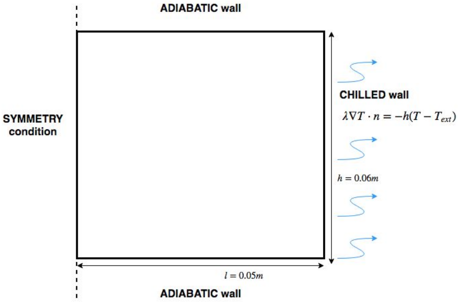
3-2 Pressure correction:

$$\begin{cases} \rho \dfrac{\mathbf{u}^{n+1,k} - \widetilde{\mathbf{u}}^k}{\Delta t} = -\nabla \Phi^k + \delta \rho_b^{n+1,k}, \\ \mathrm{div}(\mathbf{Q}^{n+1,k}) = 0. \end{cases} \qquad \text{with:} \qquad \begin{cases} \delta \rho_b^{n+1,k} = \rho_b^{n+1,k} - \rho_b^{n+1,k-1}, \\ P^{n+1,k} = P^{n+1,k-1} + \Phi^k. \end{cases}$$

Hebditch and Hunt benchamrk

Configuration



- 2D configuration proposed for benchmark[2]
  - Binary alloy Pb-Sn
  - Same solidification model but different numerical methods

Group	Software	Scheme	Mesh	Time step (s)
IJL	SOLID (FV)	Upwind	192x232	5.10^{-3}
CEMEF	R2SOL (FE)	SUPG	46502 nodes	5.10^{-3}
EPM-SIMAP	FLUENT (FV)	2^{nd} order upwind	200x240	5.10^{-3}
TREFLE	THETIS (FV)	TVD	268x324	1.10^{-3}
IJL	OpenFOAM (FV)	Upwind or Quick	200x240	5.10^{-3}
EDF R&D	*Code_Saturne* (FV)	Upwind	200x240	1.10^{-3}

[2] H. Combeau et al. "Analysis of a numerical benchmark for columnar solidification of binary alloys." IOP Conference Series: Materials Science and Engineering. Vol. 33(1). IOP Publishing, 2012.

Hebditch and Hunt benchmark

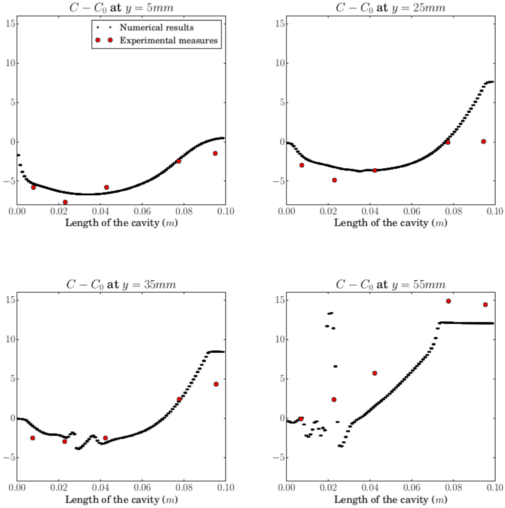
Results with *Code_Saturne*. Left: concentration, Right: liquid volume fraction.

Play/Pause Media Caption

Hebditch and Hunt benchmark

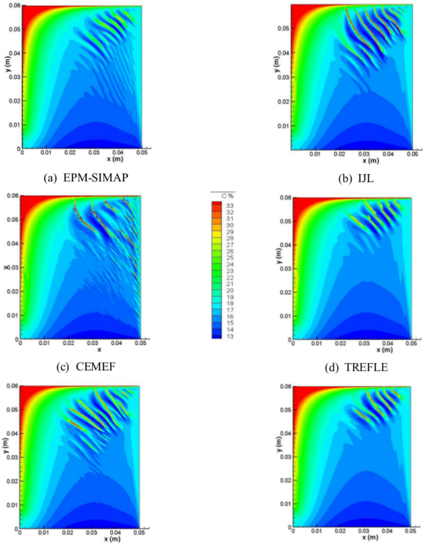
Results with *Code_Saturne*. Experimental validation (similar configuration).

- Segegration profiles on four lines

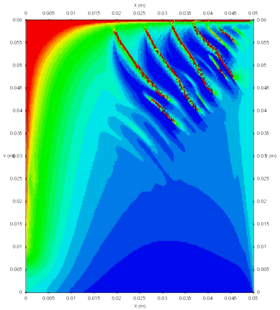


Hebditch and Hunt benchmark

Comparison with 5 other codes: segregation map



(a) EPM-SIMAP (b) IJL (c) CEMEF (d) TREFLE (e) IJL OpenFOAM upwind (f) IJL OpenFOAM QUICK



Code_Saturne

- Qualitatively OK
- Strong influence of the numerical method for segregated channels
- Difficulties to get reference solutions with solidification models

Conclusion and perspectives

Conclusion

- A mixture model for alloy solidification has been implemented in *Code_Saturne*
- A PISO-like approach has been proposed to solve efficiently the couplings
- Numerical tests have been successfully performed on academical configurations

Further work

- Industrial test cases:
  - Comparison with experimental data on thermal and concentration fields
  - Collaboration with EDF R&D China
- Modelling: multi-components alloys, microsegregations model, grain movement
- Numerics: improving convergence with a better treatment of the penalization term