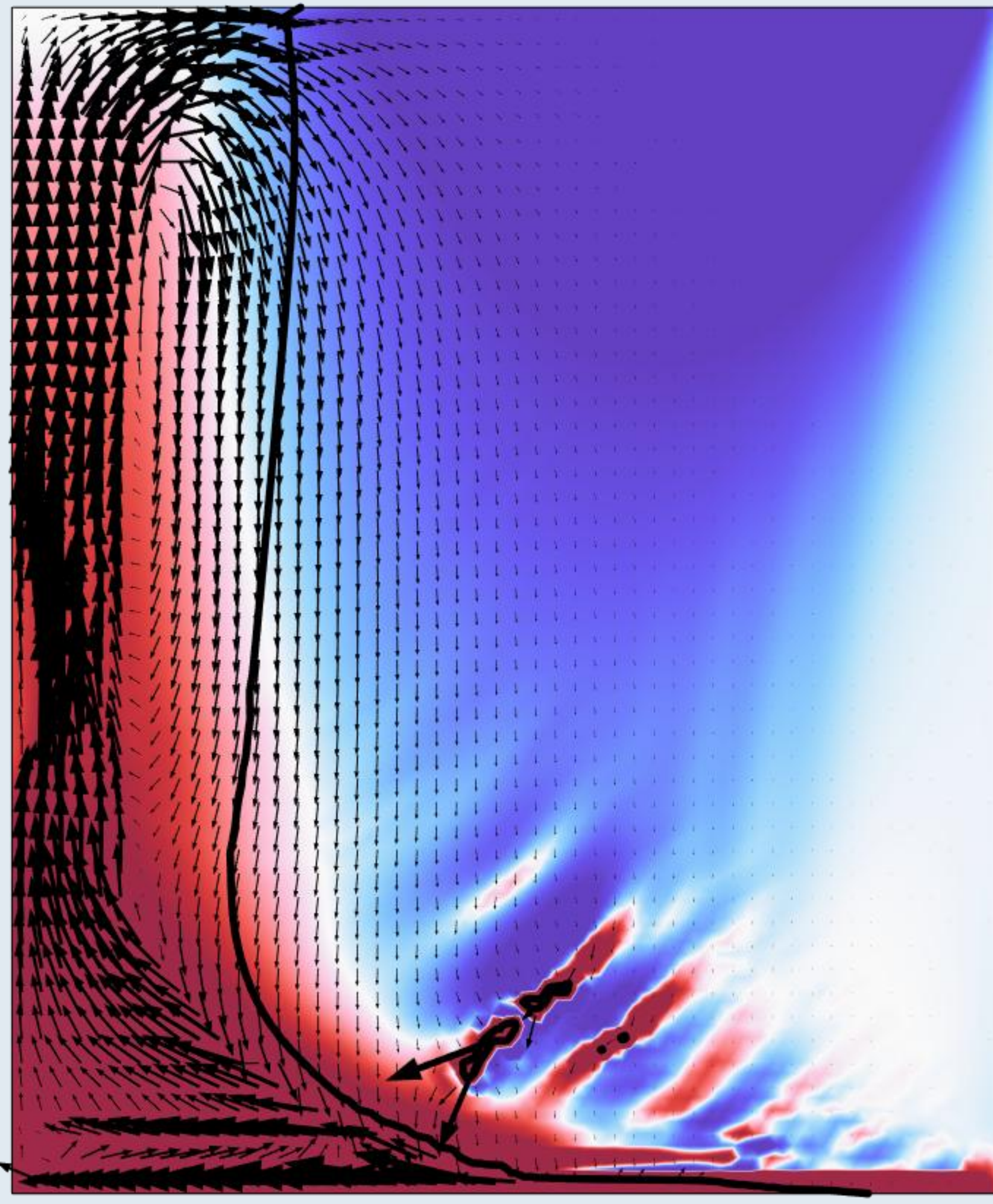




Benchmarking COMSOL Multiphysics® for Predicting Macrosegregation in Binary Alloy Solidification

Assessing COMSOL Multiphysics® as a predictive tool for macrosegregation in binary alloy solidification, benchmarked against independent numerical solutions.

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Abstract

Macrosegregation, defined as chemical heterogeneity at the casting scale, remains a major challenge in solidification modeling, driven by strongly coupled heat transfer, solute transport, and thermosolutal convection, and marked by a well-known instability producing oblique "channel" segregates. This work implements a 2D columnar solidification benchmark [1], using an enthalpy-based finite-element

formulation, and evaluates its predictive capability through mesh/time-step convergence studies and a parametric analysis of the cooling rate. Results for two binary alloys (Pb-18wt%Sn and Sn-10wt%Pb) show consistent qualitative and quantitative agreement with four independent benchmark codes, confirming COMSOL Multiphysics® as a reliable tool for macrosegregation prediction

Methodology

The volume-averaged conservation equations (mass, Brinkman momentum, energy, solute) are solved under thermodynamic equilibrium (lever rule, see Figure 1), using an enthalpy formulation solved jointly with temperature in a weak finite-element sense to avoid spurious oscillations at the phase-change front.

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\rho_0}{g_l} \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \frac{\mathbf{u}}{g_l} \right) = \nabla \cdot [-p\mathbf{I} + \mathbf{K}] - \frac{\mu_l}{\kappa} \mathbf{u} + \rho \mathbf{g}$$

$$\rho \frac{\partial \langle h \rangle}{\partial t} + \rho \mathbf{u} \cdot \nabla h_l + \nabla \cdot \mathbf{q} = 0$$

$$\frac{\partial \langle C \rangle}{\partial t} + \mathbf{u} \cdot \nabla C_l = 0$$

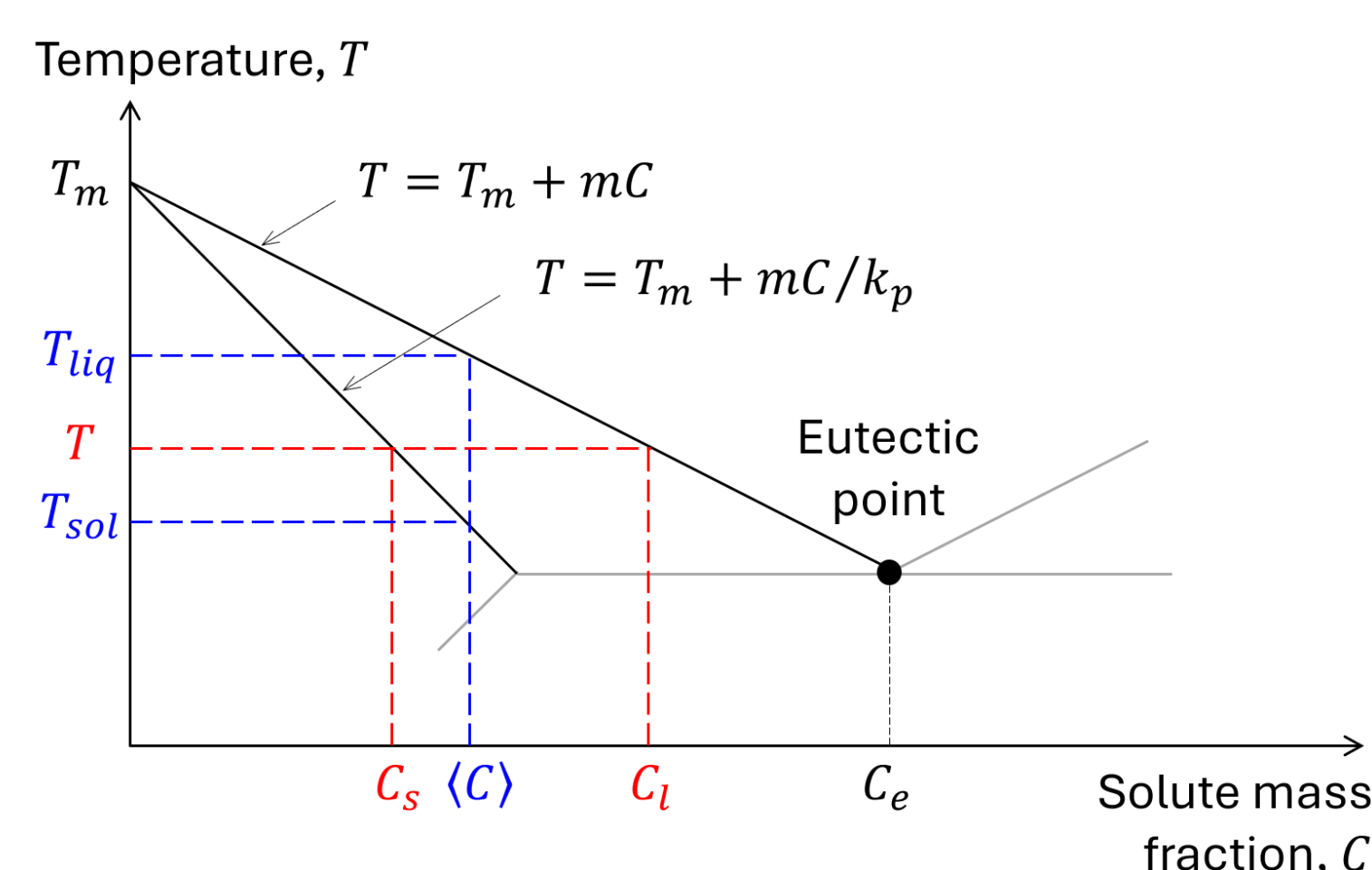


FIGURE 1. Simplified phase diagram

Results

Mesh and time-step convergence studies show that while the fine-scale structure of the segregated channels is highly sensitive to discretization (as found in [2]), the overall segregation pattern is robust even on coarse meshes. Comparison of the final macrosegregation maps for one of the two alloy cases against the four benchmark codes shows good qualitative agreement on the overall segregation pattern, with the main discrepancies concentrated in the fine channel structure. This confirms that COMSOL Multiphysics® provides reliable predictions for complex columnar solidification problems.

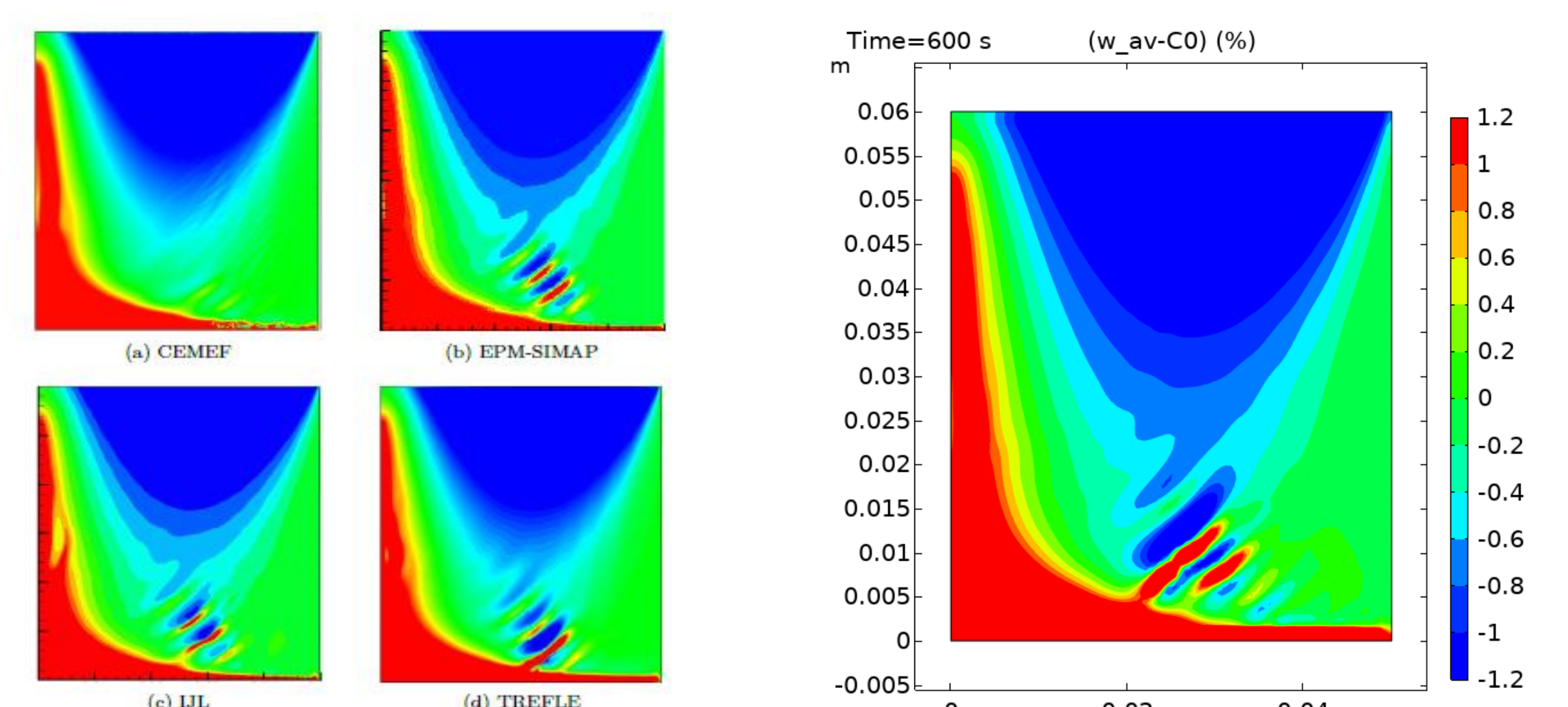


FIGURE 2. Case of Sn-10% Pb. Averaged solute mass fraction, $\langle C \rangle - C_0$ in %, at the end of solidification (t = 600 s) computed by different research groups (left) and the present model (right)

REFERENCES

1. M. Bellet et al., "Call for contributions to a numerical benchmark problem for 2D columnar solidification of binary alloys," *International Journal of Thermal Sciences*, vol. 48, no. 11, pp. 2013-2016, 2009.
2. H. Combeau et al., "A numerical benchmark on the prediction of macrosegregation in binary alloys," *Proceedings of frontiers in solidification science. Warrendale, USA: TMS2011*, 2011.

