

SPLIT-SOLID-MODEL TO SIMULATE THE FORMATION OF SHRINKAGE CAVITIES AND MACROSEGREGATIONS IN STEEL CASTING

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Abstract

The final macrosegregation pattern in steel ingot castings is strongly influenced by the position of the last point to solidify, which in general is identical to the area of maximally enriched melt. The position of this point is very often determined by the development of the melt surface and the formation of shrinkage cavities during solidification.

The formation of deep shrinkage cavities of alloys with long solidification range is difficult to be modeled if the solid phases are assumed to be stationary. The present work introduces a model that splits the solid phases into a stationary and a mobile part without introducing new momentum equations for the mobile solid. The mobile solid is rather thermodynamically treated as solid, but hydrodynamically treated as liquid and thus included into the liquid momentum equations.

A 2D-CVM-model based on volume-averaging is used to predict the transient shape of the surface and the shrinkage cavity as well as their influence on the final solute distribution. The solute transport mechanisms are thermosolutal convection, diffusion in the liquid and feeding flow. Mushy zone flow is described by an isotropic permeability model. The moving surface is realized by implementing a volume-of-fluid (VOF) model modified for use with variable densities and solidification of the free surface. Phase transitions are calculated using a piecewise linear eutectic or peritectic phase diagram that considers one liquid and two solid phases.

Introduction

The task to predict the influence of a surface shrinkage cavity on the final macrosegregation pattern is extremely complex. Figure 1 shows some of the physical effects occurring during the solidification process of a steel casting with riser and which have been modeled in this work. The effect causing most of the trouble is shrinkage. While it is relatively easy to implement shrinkage terms inside the liquid, it becomes really difficult if the whole cast part including the moving free surface is described.

So far in macrosegregation simulations various methods have been used to treat the free surface. Sometimes the domain size is kept constant and a continuous fluid inlet is used [1,2]. Others keep the surface flat and decrease the size of the first surface cell row or move the surface by an average velocity [3]. There is huge number of works treating various aspects of the problem, like the formation of shrinkage cavities or the formation of macrosegregations by different flow phenomena. The present work tries to integrate as many aspects of the problem as possible and describes the formation of macrosegregations due to thermosolutal and shrinkage flow and how they are influenced by the development of the shrinkage cavity.

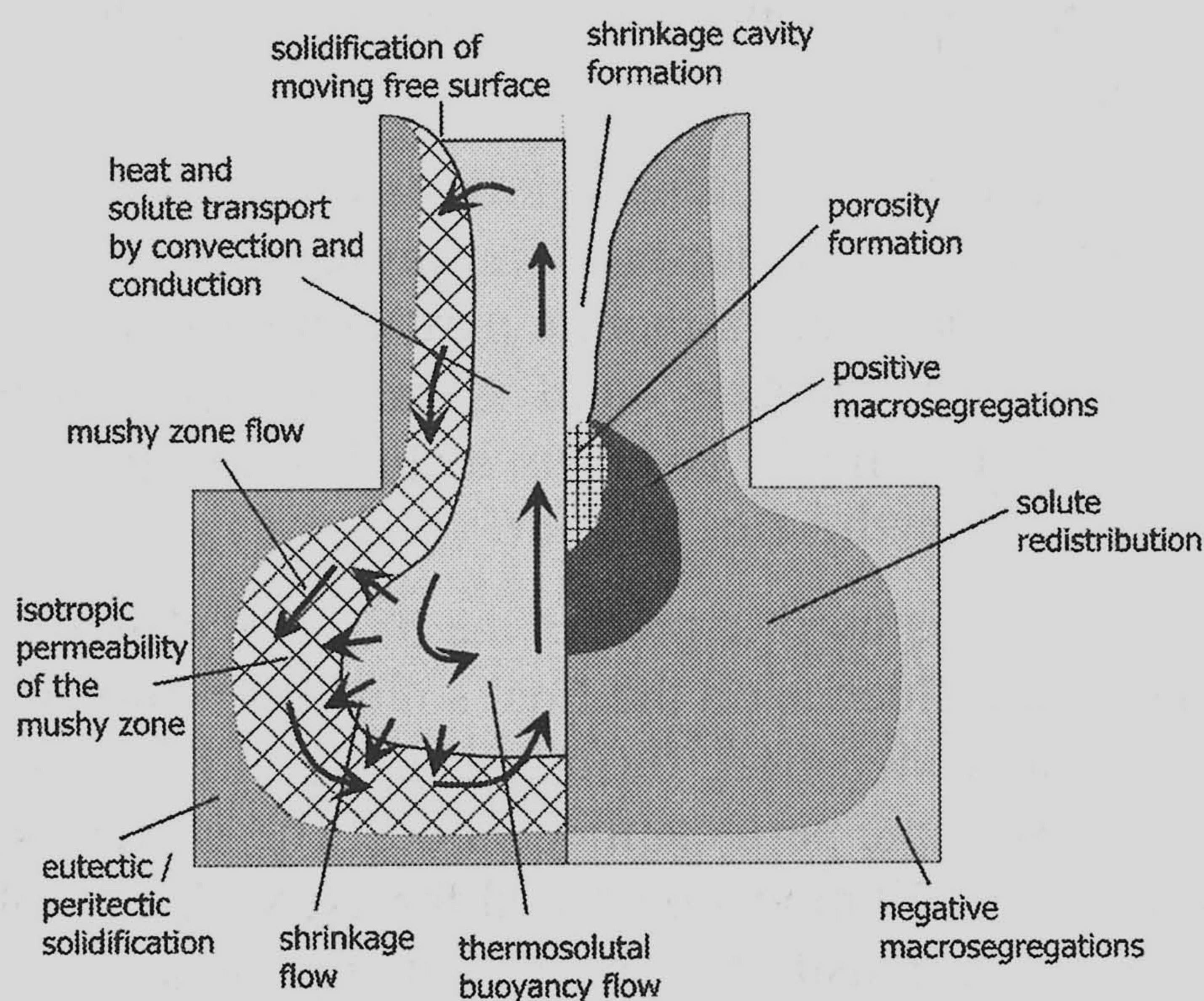


Figure 1: Physical effects that occur during the solidification process of a steel casting with riser and that have been implemented in the present model.

The present work introduces a number of new models:

- Modified VOF-model to describe the solidification of moving free surfaces with partial solidification of surface cells.
- *Split Solid Model* to describe the transport of equiaxed solid and to prevent premature solidification of the moving free surface
- Solidification algorithm to describe eutectic and peritectic solidification of binary alloys in systems with strong convective solute transport.
- Shrinkage porosity model that copes with areas cut off by freezing.

Together with differential equations for temperature, concentration in the liquid, pressure and velocities the models have been integrated to form a framework with complex interactions. In the present stage of development little effort has been put on the use of complicated physical models. The philosophy of the project was more to create a modular framework of simple models which in the future can be replaced by more sophisticated models without jeopardising the complex interactions.

Mathematical Model

One central idea of the model is the introduction of mobile solid fractions without introducing additional solid momentum equations. This is achieved by treating the mobile solid fraction

thermodynamically as solid, but hydrodynamically as liquid with solid density. This model will be called *Split Solid Model* (SSM).

Basic concept

The model considers eight “phases”:

liquid:	$q = l$	stationary solid γ - phase:	$q = \gamma \text{ dead}$
mobile solid δ - phase:	$q = \delta \text{ move}$	porosities:	$q = \text{pore}$
mobile solid γ - phase:	$q = \gamma \text{ move}$	obstacles:	$q = \text{obst}$
stationary solid δ - phase:	$q = \delta \text{ dead}$	void:	$q = \text{void}$

For each of these “phases” the following physical quantities have to be determined: x- and y-velocity u_q, v_q , temperature T_q , pressure p_q , concentration of solute C_q , and the volume fraction ε_q . This results in a total of 48 variables. This high number can be reduced by a number of assumptions. Thermal equilibrium between all phases and pressure equilibrium between all mobile phases and the porosities yields

$$T := T_q \quad p := p_l = p_{\delta \text{ move}} = p_{\gamma \text{ move}} = p_{\text{pore}} \quad p_{\delta \text{ dead}} = p_{\gamma \text{ dead}} = p_{\text{obst}} = 0 \quad (1)$$

For the velocity equations the assumptions of the SSM yield

$$\vec{v} := \vec{v}_{\delta \text{ move}} = \vec{v}_{\gamma \text{ move}} = \vec{v}_l \quad \vec{v}_{\delta \text{ dead}} = \vec{v}_{\gamma \text{ dead}} = \vec{v}_{\text{pore}} = \vec{v}_{\text{obst}} = \vec{v}_{\text{void}} = 0 \quad (2)$$

Mobile and stationary part of the same solid phase are assumed to be in solutal equilibrium:

$$C_\delta := C_{\delta \text{ move}} = C_{\delta \text{ dead}} \quad C_\gamma := C_{\gamma \text{ move}} = C_{\gamma \text{ dead}} \quad C_{\text{pore}} = C_{\text{obst}} = C_{\text{void}} = 0 \quad (3)$$

The 48 variables have been reduced to 15: $u, v, T, p, C_l, C_\gamma, C_\delta$, and the eight phase fraction variables ε_q . In the next sections the 15 equations are presented that are used to solve this problem. The quantities are volume-averaged following the model by [4]. To simplify the representation the following definitions are used:

$$\varepsilon_{\text{move/dead}} := \sum_{q=\text{move/dead}} \varepsilon_q \quad \text{where} \quad \text{move} = l, \delta \text{ move}, \gamma \text{ move} \quad \text{dead} = \delta \text{ dead}, \gamma \text{ dead}, \text{obst} \quad (4)$$

$$\rho_{\text{eff move/dead}} := \frac{\sum_{q=\text{move/dead}} (\varepsilon_q \rho_q)}{\varepsilon_{\text{move/dead}}} \quad C_{P \text{ eff move/dead}} := \frac{\sum_{q=\text{move/dead}} (\varepsilon_q \rho_q C_{Pq})}{\sum_{q=\text{move/dead}} (\varepsilon_q \rho_q)} \quad (5)$$

$$\varepsilon_{\text{mat}} = \sum_{q \neq \text{void}} \varepsilon_q \quad \lambda_{\text{eff}} = \frac{\sum_{q \neq \text{void}} (\lambda_q \varepsilon_q)}{\sum_{q \neq \text{void}} \varepsilon_q} \quad (6)$$

1. Continuity equation:

$$\sum_q \Gamma_q = \frac{\partial}{\partial t} (\varepsilon_{\text{move}} \rho_{\text{eff move}} + \varepsilon_{\text{dead}} \rho_{\text{eff dead}}) + \vec{\nabla} \cdot [\varepsilon_{\text{move}} \rho_{\text{eff move}} \vec{v}] = 0 \quad (7)$$

2. + 3. Momentum vector equation:

The equation has been developed using the assumption of a common constant effective viscosity μ_{eff} for all mobile phases. The complete equation is:

$$\begin{aligned} & \frac{\partial}{\partial t} \left[\varepsilon_{\text{move}} \rho_{\text{eff move}} \begin{pmatrix} u \\ v \end{pmatrix} \right] + \left(\vec{\nabla} \cdot \left[\varepsilon_{\text{move}} \rho_{\text{eff move}} \vec{v} \begin{pmatrix} u \\ v \end{pmatrix} \right] \right) = -\varepsilon_{\text{move}} \vec{\nabla} p \\ & + \left(\vec{\nabla} \cdot \left[\mu_{\text{eff move}} \varepsilon_{\text{move}} \vec{\nabla} u \right] \right) + \left(\vec{\nabla} \cdot \left[\mu_{\text{eff move}} \varepsilon_{\text{move}} \vec{\nabla} v \right] \right) + \frac{\partial}{\partial x} \left[\mu_{\text{eff move}} \left(\frac{\partial \varepsilon_{\text{move}}}{\partial x} \vec{v} + \vec{\nabla}(\varepsilon_{\text{move}} u) \right) \right] + \frac{\partial}{\partial y} \left[\mu_{\text{eff move}} \left(\frac{\partial \varepsilon_{\text{move}}}{\partial y} \vec{v} + \vec{\nabla}(\varepsilon_{\text{move}} v) \right) \right] \end{aligned}$$

$$+ \sum_{q=l, \delta \text{ move}, \gamma \text{ move}} \left[\varepsilon_q \left(\rho_q + \frac{\partial \rho_q}{\partial C} (C_q - C_{q \text{ ref}}) \right) \right] \bar{g} - \frac{\varepsilon_{\text{move}} \mu_{\text{eff}} (\varepsilon_{\delta \text{ dead}} + \varepsilon_{\gamma \text{ dead}})^2}{K_0 \varepsilon_{\text{move}}^2} \bar{v} \quad (8)$$

Consequence of the SSM is the presence of the mobile solid phases in all terms that are usually a function of liquid fraction only.

4. Energy equation:

The energy equation was developed from a mixed enthalpy equation considering enthalpies as linear functions of temperature, $h_q = h_{0q} + c_{Pq} (T - T_{0q})$. The complete equation is:

$$\frac{\partial \left[(\varepsilon_{\text{move}} \rho_{\text{eff move}} c_{P \text{ eff move}} + \varepsilon_{\text{dead}} \rho_{\text{eff dead}} c_{P \text{ eff dead}}) T \right]}{\partial t} + \bar{\nabla} \cdot (\varepsilon_{\text{move}} \rho_{\text{eff move}} c_{P \text{ eff move}} \bar{v} T - \varepsilon_{\text{mat}} \lambda_{\text{eff}} \bar{\nabla} T) \\ = \sum_{q \neq l} \left[\Lambda_q^* \frac{\partial (\varepsilon_q \rho_q)}{\partial t} \right] + \sum_{q=\delta \text{ move}, \gamma \text{ move}} [\Lambda_q^* \bar{\nabla} \cdot (\varepsilon_q \rho_q \bar{v})] + \sum_q (\varepsilon_q S_{\text{external } q}) \quad (9)$$

where $\Lambda_q^* = (h_{0l} - c_{Pl} T_{0l}) - (h_{0q} - c_{Pq} T_{0q}) = \text{const.}$ and $S_{\text{external } q}$ are external heat sources for phase q . Consequences of the SSM are the presence of the mobile solid phase fractions in the convective term and the new term on the right side of the equation that describes the transfer of latent heat by convection of mobile solid.

5. + 6. + 7. Concentration conservation equations

The model uses the lever-rule, i.e. it assumes complete solutal equilibrium inside each phase and uses equilibrium phase diagrams. This leads to solid concentration equations

$$C_\delta = \kappa_\delta C_l \quad C_\gamma = \kappa_\gamma C_l \quad (10)$$

The liquid concentration equation was developed from a volume-averaged mixture concentration equation:

$$\frac{\partial}{\partial t} (\varepsilon_l \rho_l C_l) + \bar{\nabla} \cdot (\varepsilon_l \rho_l \bar{v} C_l) = \bar{\nabla} \cdot (\varepsilon_l \rho_l \tilde{D}_l \bar{\nabla} C_l)$$

$$+ \sum_{q=\delta, \gamma} \left\{ - \frac{\partial}{\partial t} [(\varepsilon_{q \text{ move}} + \varepsilon_{q \text{ dead}}) \rho_q C_q] - \bar{\nabla} \cdot (\varepsilon_{q \text{ move}} \rho_q \bar{v} C_q) + \bar{\nabla} \cdot (\varepsilon_{q \text{ dead}} \rho_q \tilde{D}_{q \text{ dead}} \bar{\nabla} C_q) \right\} \quad (11)$$

Main consequence of the SSM is the convective term on the right side of the equation that accounts for the solute transport by mobile solid. There is no diffusive term for the mobile solid phases because they are assumed not to be in contact.

There are still eight equations necessary to be able to determine the eight phase fractions.

8. + 9. Sum over all phases and constant obstacle phase

Of course the sum over all phases must be 1:

$$\varepsilon_l = 1 - \varepsilon_{\delta \text{ move}} - \varepsilon_{\gamma \text{ move}} - \varepsilon_{\delta \text{ dead}} - \varepsilon_{\gamma \text{ dead}} - \varepsilon_{\text{obst}} - \varepsilon_{\text{pore}} - \varepsilon_{\text{void}} \quad (12)$$

and the fraction of obstacle phase is constant and results from the initial conditions:

$$\varepsilon_{\text{obst}} = \text{const.} \quad (13)$$

10. VOF equation for solidifying free surfaces

The well known VOF equation with partial cell treatment, [5], has been extended to the case of solidification (time dependent obstacles) and time dependent liquid densities. These modifications allow to use the equation to describe complex interactions of shrinkage flow and the solidification of moving free surfaces.

$$\frac{\partial}{\partial t} (\varepsilon_{open} \rho_{eff\ open} F_{move}) + \vec{\nabla} \cdot (\varepsilon_{open} \rho_{eff\ open} \vec{v}_l F_{move}) = -F_{move} \frac{\partial}{\partial t} (\varepsilon_{closed} \rho_{eff\ closed}) \quad (14)$$

where

$$F_{move} := \frac{\varepsilon_{move}}{\varepsilon_{open}} \quad (15)$$

11. Shrinkage Porosity Model

The fraction of porosities is determined by the fact that the pressure drop that drives liquid through the mushy zone is limited by a minimal pressure that is defined by the point where nucleating gas pores become stable. As a first very simple model vapour pressure of the alloy is assumed to be this minimal pressure.

$$p_{min} = p_{vapour} \quad (16)$$

12.+13. Solidification model

For reasons of simplicity two additional phase fractions are defined. As mobile and stationary solid are thermodynamically treated as one single phase

$$\varepsilon_{\delta} := \varepsilon_{\delta\ move} + \varepsilon_{\delta\ dead} \quad \varepsilon_{\gamma} := \varepsilon_{\gamma\ move} + \varepsilon_{\gamma\ dead} \quad (17)$$

To determine the all over solid fractions a concept is used that has been described in [6]. One of the two equations is obtained from the phase diagram:

$$T(C_l^i) = T_{liquidus} \quad (18)$$

Unfortunately this equation does not contain any of the phase fractions in demand, whereas the temperature and liquid concentration equations do:

$$T = T(\varepsilon_{\delta}, \varepsilon_{\gamma}) \quad C_l^i = C_l^i(\varepsilon_{\delta}, \varepsilon_{\gamma}) \quad (19)$$

But as they are already used to calculate the temperature and liquid concentration respectively, they give no additional information about the phase fractions. The missing equation is obtained from the conditions arising from the current solidification type. Four different types are considered:

- *primary δ -solidification* : Only liquid and δ -solid is present $\rightarrow \varepsilon_{\gamma} = 0$ (20)

- *primary γ -solidification* : Only liquid and γ -solid is present $\rightarrow \varepsilon_{\delta} = 0$ (21)

- *Solid state transformation δ/γ* : No liquid is present $\rightarrow \varepsilon_{\gamma} = 1 - \varepsilon_{\delta}$ (22)

- *eutectic / peritectic solidification* : Liquid, δ -solid and γ -solid is present, The missing equation arises from the condition, that the solidification is linked to the eutectic / peritectic plateau. $\rightarrow T(\varepsilon_{\delta}, \varepsilon_{\gamma}) = T_{eut/peri}$ (23)

14.+15. Split Solid Model

The last two equations determine how the solid that forms is split into the mobile and stationary part. The SSM has been developed to prevent small amounts of stationary solid forming close to the free surface in early stages of solidification from blocking the further surface movement and the formation of a deep shrinkage cavity. For small all over solid fractions ($\varepsilon_{\delta} + \varepsilon_{\gamma}$) all solid is mobile, for high solid fractions all solid is stationary. For solid fractions of $\varepsilon_{0\ mv\ dd} \pm \frac{1}{2} \Delta\varepsilon_{mv\ dd}$ (cf. figure 2) the fraction of mobile solid varies smoothly from all mobile to all stationary. δ - and γ -solid are both split up into mobile part and stationary part in the same way.

Split solid equations. These rules lead to the following set of equations:

$$\varepsilon_{\delta\ move} = SSF(\varepsilon_{\delta} + \varepsilon_{\gamma}) \cdot \varepsilon_{\delta} \quad (24)$$

$$\varepsilon_{\gamma\ move} = SSF(\varepsilon_{\delta} + \varepsilon_{\gamma}) \cdot \varepsilon_{\gamma} \quad (25)$$

The *Split Solid Function* (SSF) can be chosen in different ways. So far three function types have been tested, figure 2. For the present calculations the sinus type function was used.

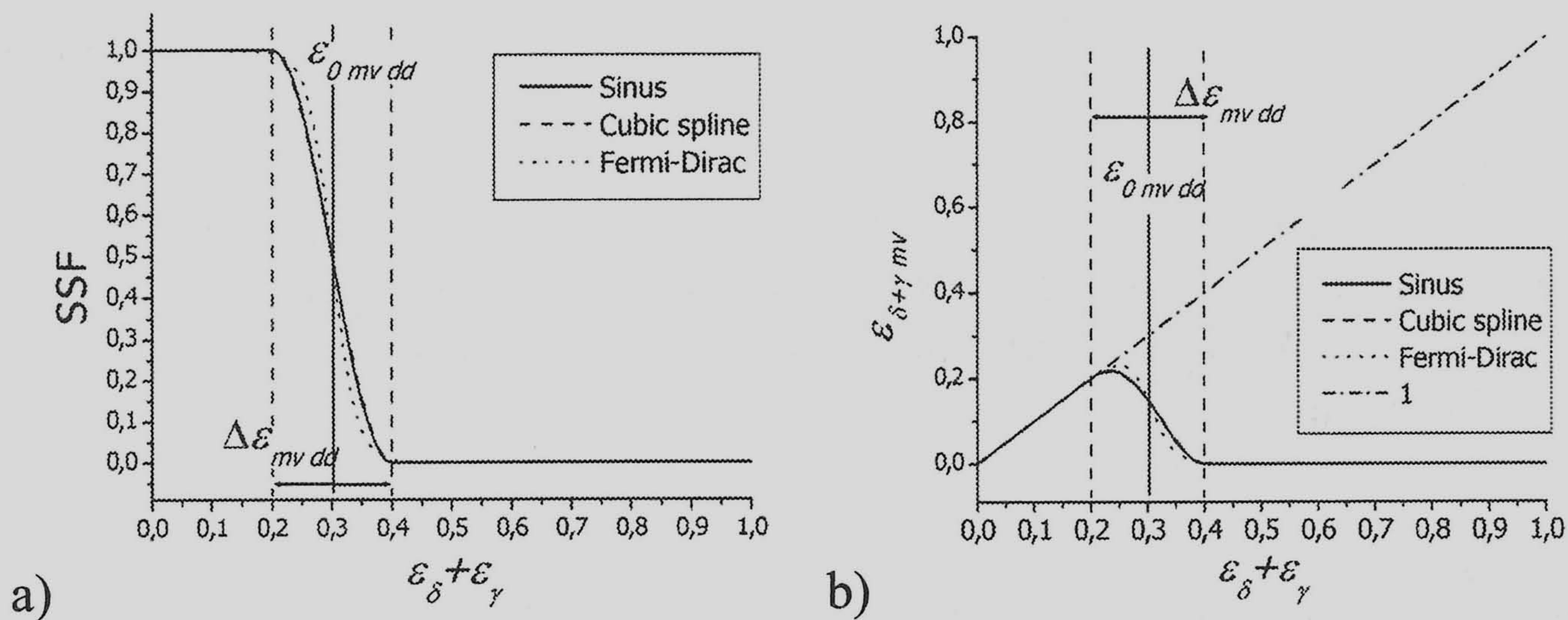


Figure 2: a) Comparison of three possible Split-Solid-Functions (SSF). b) Fraction of mobile solid as a function of total solid fraction for three types of SSF.

Columnar growth model. Close to mold walls or areas with high solid fraction solidification in many cases is not equiaxed but columnar. To describe this phenomenon a *columnar growth model* has been developed. So far this model switches off the split solid model if inside a radius $R_{columnar}$ there is either a solid wall or solid fractions above a limit $\epsilon_{columnar}$.

Numerical model

The numerical 2D CVM model uses a mixed explicit / implicit discretisation and the SIMPLER algorithm described in [7]. A sophisticated solidification algorithm has been developed that is suitable for the simulation of processes with strong convective solute transport and thus strong horizontal movements inside the binary phase diagram. The software has been parallelised using the shared memory standard OpenMP.

Numerical Set-up

A test calculation has been made to validate the model and to show the effect of the SSM. The simulation was compared to experimental results published in [8]. The cast part is a block of unalloyed steel GS60 with riser, cast in a sand mold with isolation at two ends, figure 3 a). The isolation is meant to create quasi 2D solidification conditions. Figure 3 b) shows the boundary conditions and initial configuration used for the calculation. Initial temperature was 1890 K. The simulation assumes a binary Fe0.42wt%C alloy. No porosity model was applied in this simulation. Table I shows the physical data of the FeC alloy system and some calculation parameters. Concentration dependent liquidus and solidus temperatures and segregation coefficients are taken on-line from the binary FeC equilibrium phase diagram.

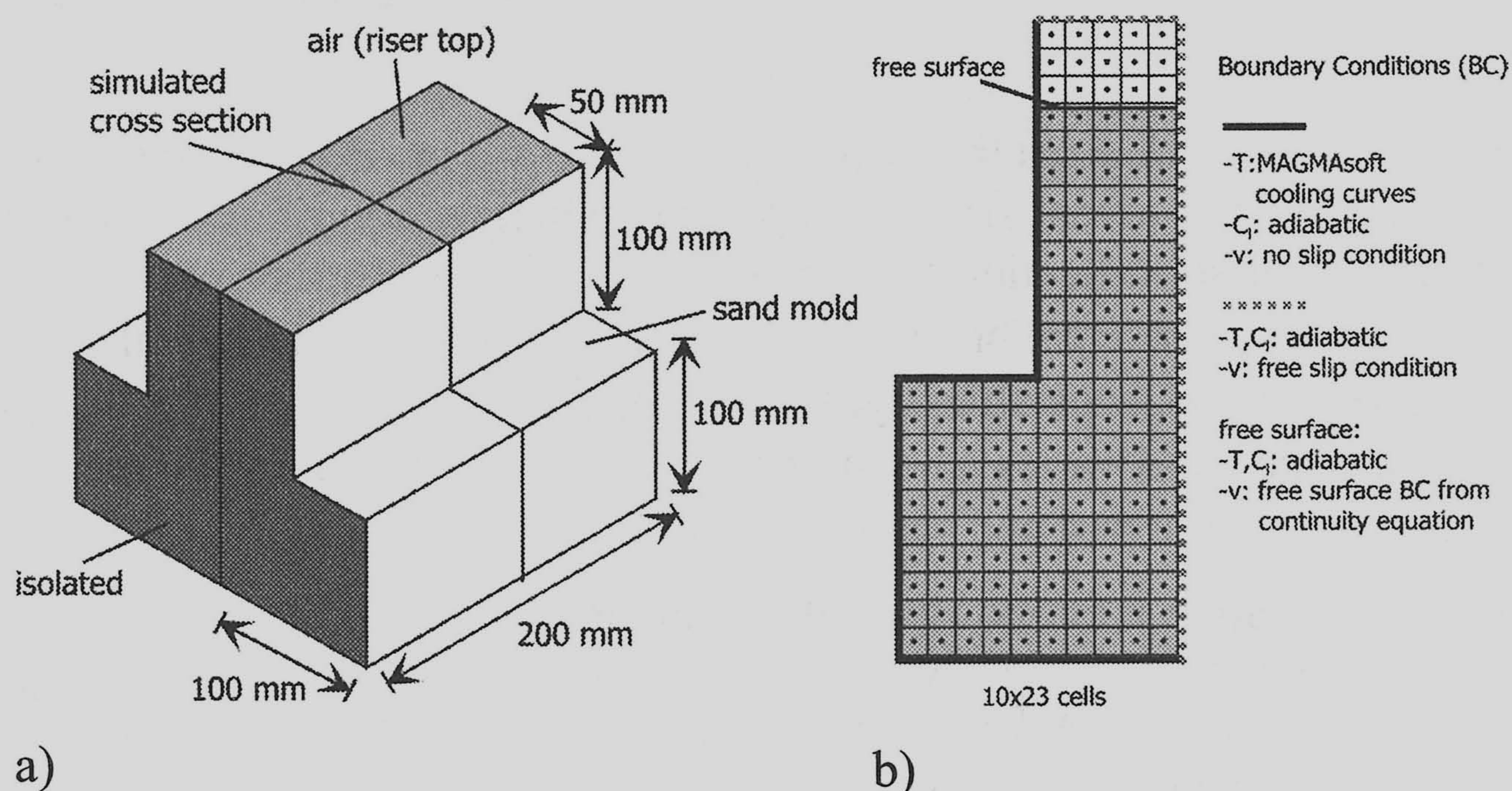


Figure 3: a) Geometry of cast part. The figure shows which faces of the ingot are in contact with the sand mold (white + bottom), isolation (dark grey) and air (light grey). b) Boundary conditions applied during the calculations.

Table I: Physical data of FeC alloy system and calculation parameters.

densities [kg/m ³]	$\rho_l(T) = 8547$ $- 0.835 \cdot T$	heat conductivities [W/(m·K)]	$\lambda_l = 27$
	$\rho_s = 8344$	permeability const.	$\lambda_s = 30$
heat capacities [J/(kg·K)]	$c_{pl} = 790$	latent heat $l_{\gamma/l\delta}$ [kJ/kg]	$\Lambda_{l\delta/l\gamma} = 275$
	$c_{p\delta} = 706$	Parameters of SSM	$\varepsilon_{0\,mv\,dd} = 0.3$
	$c_{p\gamma} = 675$		$\Delta\varepsilon_{mv\,dd} = 0.2$
dynamic viscosity [kg / (m·s)]	$\mu_{eff} = 6 \cdot 10^{-3}$		$R_{columnar} = 0.01$ m
			$\varepsilon_{columnar} = 0.6$

Results and Discussion

Figure 4 shows the simulation results and compares them to experimental results from [8], left half of figure 4 c). The right half always shows the calculated shape of the shrinkage cavity and the segregation pattern (deviation of carbon concentration from initial concentration) after a) 600 s, b) 1400 s) and c) 4620 s (cast part completely solidified). Both the shape of the shrinkage cavity and the final macrosegregations show promising accordances as well as large discrepancies. The depth of the cavity is comparable as well as the position of the last point to solidify.

The discrepancies can be explained by different arguments:

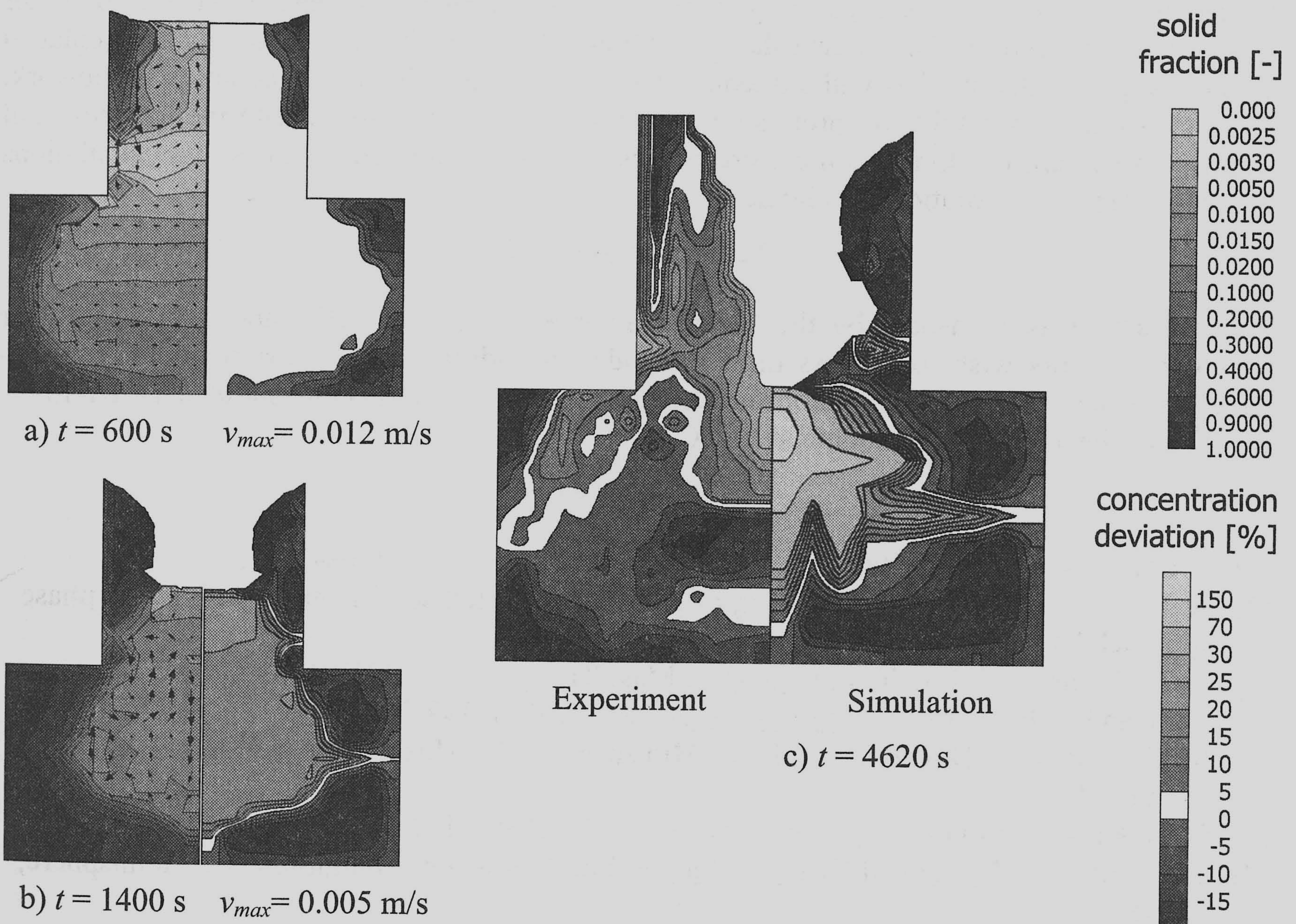


Figure 4: Simulation of steel ingot. Right: Carbon concentration deviation from initial concentration; Left: a) b) Solid fraction, velocities. c) Experimental carbon concentration deviation [8].

- The current model assumes constant solid density ρ_s . The choice of this density determines the amount and speed of shrinkage and by that the size and shape of the shrinkage cavity.
- The cooling has been realised by applying MAGMAsoft cooling curves as boundary conditions. The MAGMAsoft calculation did not consider fluid flow and convective heat transfer.
- A parameter study has to be done to investigate the influence of the parameters of the SSM and the columnar growth model on the shape of the shrinkage cavity.
- An anisotropic permeability model instead of the isotropic one used so far will have great influence on the final macrosegregation pattern.

The left half of figure 4 a) and b) shows the total fraction of solid and the velocity field. Figure 4 a) can help to understand the importance of the SSM. The area where significant fluid movement occurs, has solid fractions $< 0.2\%$. In this area all solid is mobile and the higher solid density leads to sedimentation. The solid fraction increases from about 0.0025 close to the surface up to about 0.1 at the bottom. In figure 4 b) the mobile solid fraction close to the surface reaches about 0.015. In a calculation without SSM these small amounts of solid would be stationary and would be sufficient to confuse the free surface algorithm. With SSM the mobile solid can just follow the surface movement. Observation of the transient velocity field showed that no stable convection cells occur. The flow is highly complex and transient and driven by the strong interaction between thermal and solutal convection, shrinkage flow and sedimentation of mobile solid.

Conclusions and Outlook

A 2D CVM model to simulate the formation of shrinkage cavities in steel castings and their influence on the final macrosegregation pattern has been presented. The realisation as a computer program was guided by the concept that the submodels are exchangeable and can be replaced by more sophisticated models without jeopardizing the functionality of the complex framework. The first simulation results are promising and show many accordances with the experimental results. To explain or eliminate the discrepancies extensive parameter studies and calculations with higher spatial resolution are planned.

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