A partitioned solution algorithm for fluid flow and stress-strain computations applied to continuous casting

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Abstract. Continuous casting is currently the main industrial process for steel production. Since long time, industries search for efficient simulation methods, by which macrosegregation and deformation induced cracks can be predicted. As a first step this requires achieving concurrent simulation of fluid flow and stress-strain. Therefore, a partitioned solution algorithm is developed for such simulation with application to continuous casting. Liquid flow induced by natural convection or filling step, solidification shrinkage as well as thermally induced deformation of solid phase are accounted for.

1. Introduction
When modelling the continuous casting process, one of the critical issues is to concurrently achieve simulation of fluid flow in the liquid region, stress-strain analysis in the solidified region and solute transportation. For industry, it is of crucial importance to predict the macrosegregation phenomena and deformation related defects in order to optimize cast products. Therefore, the first and most important step of this solidification modelling issue is to achieve a concomitant computation of fluid flow and stress-strain, i.e. the full mechanical problem.

In the present work, a partitioned two-step solution algorithm is proposed. In one time increment, the momentum and mass conservation equations are solved twice. The first one is solid-oriented, performed with an arbitrary high liquid viscosity. From this first solution are deduced, the velocity and pressure field in the solidified regions and its associated stress-strain fields. The second solution is fluid-oriented, resuming to the Navier-Stokes equations, giving access to the liquid velocity and pressure field in the liquid regions. In addition, an arbitrary Lagrangian-Eulerian (ALE) formulation is necessary for a non-stationary simulation of the continuous casting process, in which the Lagrangian treatment applies to solid regions while the Eulerian treatment applies to liquid regions. The volume averaging methodology and the Darcy’s law are used to model the interactions between solid and liquid phases in the mushy zone. All conservation equations are formulated in the framework of the level set method in order to track the metal/gas interface. The current algorithm is coupled with an existing non-linear energy solver to calculate the temperature field [1]. Finally, application to a quasi 2D continuous casting case test is presented and discussed.
2. Numerical model

2.1. Level set method

The level set method was initially proposed by Osher and Sethian [2] to capture moving interfaces. In the present work, the metal/gas interface \( \Gamma \) is represented by the zero-isovalue of the signed distance function \( \varphi(\mathbf{x}, t) \), with \( \mathbf{x} \) a point of domain \( \Omega \) at time \( t \). Noting \( \Omega^M \) and \( \Omega^G \), two subdomains of \( \Omega \) representing respectively the metal and gas subdomains, the smoothed Heaviside function \( \mathcal{H}^M \) is then introduced, indicating the belonging of the metal subdomain with respect to the interface:

\[
\mathcal{H}^M(\varphi) = \begin{cases} 
0 & \text{if } \varphi < -\varepsilon \\
1 & \text{if } \varphi > \varepsilon \\
\frac{1}{2} \left( 1 + \frac{\varphi}{\varepsilon} + \frac{1}{\pi} \sin \left( \frac{\pi \varphi}{\varepsilon} \right) \right) & \text{if } -\varepsilon \leq \varphi \leq \varepsilon
\end{cases}
\]

(1)

where \( \varepsilon \) is the half thickness of a transition zone artificially distinguishing the subdomains. Respectively denoting \( \psi^M \) and \( \psi^G \) the physical property relative to the metal and gas subdomains, the mixed property \( \bar{\psi} \) is given by:

\[
\bar{\psi} = \mathcal{H}^M \psi^M + (1 - \mathcal{H}^M) \psi^G
\]

(2)

Thus, over the thickness \([-\varepsilon, \varepsilon]\) around the interface \( \Gamma \), a smooth and continuous transition of properties is defined.

2.2. Solid-oriented solution

In the solid-oriented solution, the approach proposed elsewhere is applied [3]. In addition with the level set formulation, the following momentum and mass conservation equations are solved using a finite element method:

\[
\begin{align*}
\nabla \cdot \mathbf{\hat{s}} - \nabla p + \hat{\rho} \mathbf{g} &= 0 \\
\nabla \cdot \mathbf{v} &= \mathcal{H}^M (H(T_C - T) \text{tr}(\dot{\varepsilon}_{el}) + \text{tr}(\dot{\varepsilon}_{th}))
\end{align*}
\]

(3)

where \( \mathbf{\hat{s}} \) and \( \hat{\rho} \) are respectively the mixed stress tensor and the density in domain \( \Omega \), defined in Table 1. \( \mathbf{s}^M, \langle \rho \rangle^M \) are respectively the stress tensor and average density in the metal subdomain. \( \mathbf{s}^G, \rho^G \) are the stress tensor and density in the gas subdomain. \( p \) is the pressure and \( \mathbf{g} \) is the constant gravity vector. In this solid oriented resolution, the average density in metal is assumed to be the intrinsic density of solid \( \rho^S \) in the entire metal subdomain, to approximate the thermally induced solid deformation without solidification shrinkage effect.

\[
\begin{array}{|c|c|}
\hline
\text{Notation} & \text{Definition} \\
\hline
\mathbf{\hat{s}} & \mathcal{H}^M \mathbf{s}^M + (1 - \mathcal{H}^M) \mathbf{s}^G \\
\hat{\rho} & \mathcal{H}^M \langle \rho \rangle^M + (1 - \mathcal{H}^M) \rho^G \\
\hline
\end{array}
\]

Table 1. Mixing properties in the solid-oriented solution.

\( \dot{\varepsilon}_{el} \) and \( \dot{\varepsilon}_{th} \) are respectively the elastic part and thermal part of the strain rate tensor \( \dot{\varepsilon} \). \( H(T_C - T) \) is the standard Heaviside function, taken for the temperature difference \( (T_C - T) \). It is introduced as an indicator relative to the use of the thermo-elastic-viscoplastic (TEVP) constitutive model for elements with average temperature lower than the critical transition temperature \( T_C \). Otherwise the thermo-viscoplastic (TVP) model is used for temperature higher than \( T_C \). The corresponding relationships between the the von Mises equivalent stress, \( \bar{\sigma} \), the generalized plastic strain, \( \bar{\varepsilon} \), and the equivalent strain rate, \( \dot{\bar{\varepsilon}} \), is given by:

\[
\begin{align*}
\bar{\sigma} &= \sigma_Y + k(\sqrt{3})^{n+1} \dot{\varepsilon}^m \bar{\varepsilon}^n \quad (\text{TEVP}) \\
\bar{\sigma} &= k(\sqrt{3})^{n+1} \dot{\varepsilon}^m \quad (\text{TVP})
\end{align*}
\]

(4)
where \( n \) is the strain hardening coefficient, \( m \), the strain rate sensitivity, \( k \), the solid consistency and \( \sigma_y \), the yield stress.

In the present work \( T_C \) is taken below the solidus temperature to model the TEVP behaviour of material in the solid state; the TVP model is used for metal at high temperature, either in the solid state, mushy state or liquid state. At the critical transition temperature, the continuity of the flow stress is obtained by taking \( \sigma_y(T_C) = 0 \) and \( n(T_C) = 0 \). Note that the mushy zone is considered as a homogenized non-Newtonian fluid, in which the strain rate sensitivity is continuously increasing with the liquid fraction and eventually with a pure Newtonian behaviour in the fully liquid state. In addition, in order to prevent numerical instabilities due to the huge difference between solid consistency and liquid viscosity, the liquid viscosity is artificially augmented for the solid-oriented solution (typically \( 1 \) to \( 100 \, \text{Pa} \cdot \text{s} \) instead of nominal value \( 5 \times 10^{-3} \, \text{Pa} \cdot \text{s} \)). In addition, the gas is taken as an incompressible Newtonian fluid in the gas subdomain.

Finally, a velocity-pressure solution is performed, the nodal velocity and pressure fields obtained from this first step being denoted \((v_i, p_i)\) as solution of Eq. (3).

### 2.3. Fluid-oriented solution

The fluid-oriented solution takes the solid-oriented solution as an entry. While liquid is incompressible with a Newtonian behaviour, the formulation is extended to deal with a compressible formulation in the mushy zone. An effective two phase approach is used with a volume averaged method [4]. Solidification is assumed to take place with a purely columnar structure. Interactions between solid and liquid phases in the mushy zone are modelled by the Darcy’s law with a permeability coefficient \( K \) approximated by the Carman-Kozeny relationship [5]. The momentum and mass conservation equations relative to the liquid phase in the level set formulation are given by:

\[
\begin{equation}
\begin{aligned}
\rho^F \left( \frac{\partial v}{\partial t} (v - v_{msm}) + \frac{1}{\beta^F} (v - v_{msm}) p \right) - \nabla \cdot (\rho^F v) &= 0 \\
\nabla \cdot v &= -\frac{\kappa^M}{\rho^F} \frac{\partial}{\partial t} \left( \frac{\rho^F}{\rho} \left( g^I (\rho)^I + g^S (\rho)^S \right) + (v - v_{msm}) \cdot \nabla \rho + \nabla \cdot (g^S (\rho)^S v) \right)
\end{aligned}
\end{equation}
\]

(5)

with \( \rho^F, \beta^F, \beta^S, \beta^p, \mu^F, R^F \) corresponding respectively the mixing properties of fluid density, fluid fraction, averaged fluid stress tensor, averaged fluid density with Boussinesq approximation [1], averaged fluid viscosity and averaged fluid permeability coefficient between liquid and gas phases, defined in Table 2.

| Notation | Definition |
|----------|------------|
| \( \rho^F_0 \) | \( \mathcal{H}^M(\rho)^0_0 + (1 - \mathcal{H}^M)\rho^G \) |
| \( \beta^F \) | \( \mathcal{H}^M g^I + (1 - \mathcal{H}^M) \) |
| \( \beta^S \) | \( \mathcal{H}^M g^I (\rho)^I + (1 - \mathcal{H}^M) s^G \) |
| \( \beta^p \) | \( \mathcal{H}^M g^I (\rho)^I + (1 - \mathcal{H}^M) \rho^G \) |
| \( \mu^F \) | \( \mathcal{H}^M \mu^I + (1 - \mathcal{H}^M) \mu^G \) |
| \( R^F \) | \( \frac{2}{\lambda_2} \frac{g^F g^F}{(180(1 - g^F)^2)} \) |

| \( \rho^I_0, \rho^I_0, g^I, s^I, \mu^I, g^S, \rho^S, \lambda_2 \) | are respectively the intrinsic reference liquid density, intrinsic liquid density with Boussinesq approximation, liquid fraction, intrinsic liquid stress tensor, liquid viscosity, solid fraction, intrinsic solid density and the secondary dendrite spacing. \( \mu^G \) is the viscosity of gas,
assumed to be Newtonian and incompressible. \( \mathbf{v}_{msh} \) is the nodal mesh velocity field, computed with the following simplified algorithm:

\[
\mathbf{v}_{msh} = \begin{cases} 
0 & \text{in liquid} \\
\frac{g}{\rho} \mathbf{v}_l & \text{in mushy zone and at boundaries} \\
\mathbf{v}_l & \text{in solid zone}
\end{cases}
\]  

Let us note that the fluid-oriented solution does not need to be operated in the fully solid regions, in which the relevant information is already calculated in the first solid-oriented solution. A Dirichlet condition is thus applied for the fully solid regions, with values taken from the solid-oriented solution.

Finally, Eq. (5) is solved with a stabilized SUPG-PSPG finite element method [6]. The solution fields for nodal velocity and pressure deduced from this second step are denoted \((\mathbf{v}_l, p_l)\).

2.4. Solution algorithm

The partitioned solution algorithm for continuous casting is presented hereunder, decomposed in 6 successive stages in one time increment \( \Delta t \).
- 1st stage: Thermal solution. Energy conservation equation is solved, providing the temperature distribution in the metal and in the gas.
- 2nd stage: STEP I solid-oriented solution. The first folder of the momentum solution focuses on the stress-strain analysis in the solid region, with an augmented liquid viscosity and a continuity of solid density in the mushy and liquid regions.
- 3rd stage: STEP II fluid-oriented solution. The second folder of the momentum solution consists of the fluid flow computation in the liquid and mushy regions, with the correct value of the fluid viscosity including for solidification shrinkage.
- 4th stage: Mesh updating. The position of each mesh node is updated with the mesh velocity, following updating scheme: \( \mathbf{x}^{new} = \mathbf{x}^{old} + \Delta t \cdot \mathbf{v}_{msh} \).
- 5th stage: Metal/gas interface tracking. The updating of the level set function permits interface tracking. It is achieved by the convection-reinitialization scheme [7].
- 6th stage: Adaptive remeshing. The remeshing is guided by an error estimator of Hessian type, based on the interpolation error, which allows the adaptation of mesh to different fields [8].

3. Computational configuration

3.1. Model description

The partitioned algorithm is applied to a quasi-2D continuous casting application. The initial configuration is given in Figure 1a. A simple parallelepipedic geometry is considered. Heat is extracted from the metal through the lateral vertical surface. A flux is imposed at contact with the cold mould and a convection type expression at contact with water cooling. An insulation zone is artificially created in the present model, in order to make sure that the metal/gas surface at the meniscus with the vertical boundary is always in the liquid state. The metal is supposed to slide along the surrounding vertical surfaces and has a free surface boundary condition at the upper surface. Velocity is imposed for both the liquid inlet surface (horizontal velocity \( \mathbf{v}_{inlet} \)) and the bottom surface (vertical casting velocity \( \mathbf{v}_{cc} \)). The same mechanical boundary conditions are applied at both STEP I and STEP II. A symmetry plane is defined at the vertical right-hand surface, as well as the front and back surfaces, which makes the problem planar. The initial mesh is defined in Figure 1a. The material used in the simulation is a steel grade Fe – 0.4 wt.% C. Material and simulation parameters are given in Table 3. Thermal properties of gas (except the thermal conductivity) are approximated to those of the liquid phase in the metal subdomain. All other properties are given in the Appendix.

3.2. Results

Figure 2a illustrates the results corresponding to time \( t = 10 \) s. The zero-isovalue of the level set function is shown with the thick white line, representing the metal/gas interface. The blue and cyan lines
are respectively the solidus and liquidus isotherms. A solid shell has already formed due to primary mould cooling. The von Mises equivalent stress is shown, revealing a maximum value of 10 MPa. The fluid flow is concurrently computed, represented by coloured arrows: besides the inlet liquid flow, two vortices are created, one in upper liquid region, departing the metal/gas interface from an horizontal flat surface and another at the bottom position, slightly preventing the formation of the mushy zone due to heat transport. Figure 2b shows the concurrent results of the von Mises equivalent stress (left symmetry part) and the solid fraction (right symmetry part) at \( t = 100 \) s. The dotted white line represents the left-hand symmetry plane. The green line represents the exit of the mould cooling. Water sprays continuing to cool the metal, a solid region reaching a thickness of several centimetres has been formed with a maximum value of the equivalent stress of 11 MPa. Figure 2c shows the vertical stress profile 300 mm below the mould exit, at the middle of the slice thickness, as a function of the distance to the symmetry plane. Traction is formed at the cooling surface. As a consequence, a compression at inner place is observed.

| Parameters                                    | Symbol | Value | Unit       |
|----------------------------------------------|--------|-------|------------|
| Solidus temperature (nominal)                |        | 1452  | °C         |
| Liquidus temperature(nominal)                |        | 1505.5| °C         |
| Reference temperature                        |        | 1505.5| °C         |
| Reference liquid density                     | \( \langle \rho \rangle \) | 7036.5 | kg \cdot m\(^{-3}\) |
| Solid density                                | \( \rho^s \) | Tabulation | kg \cdot m\(^{-3}\) |
| Gas density                                  | \( \rho^G \) | 6900   | kg \cdot m\(^{-3}\) |
| Liquid thermal dilatation coefficient        |        | 8.96 \times 10^{-5} | K\(^{-1}\) |
| Secondary dendrite arm spacing               | \( \lambda_2 \) | 500    | \( \mu \)m |
| Gas viscosity                                | STEP I| \( \mu^G \) | \( 1 \times 10^{-1} \) Pa \cdot s |
|                                           | STEP II| \( \mu^G \) | \( 5 \times 10^{-3} \) Pa \cdot s |
| Liquid viscosity                             | STEP I| \( \mu^l \) | \( 1 \times 10^{-1} \) Pa \cdot s |
|                                           | STEP II| \( \mu^l \) | \( 5 \times 10^{-3} \) Pa \cdot s |
| Solid consistency                            |        | Tabulation | Pa \cdot s |
| Thermal conductivity in gas                  |        | 0.1    | W \cdot m\(^{-1}\) \cdot K\(^{-1}\) |
Thermal conductivity in metal & 30 W·m$^{-1}$·K$^{-1}$ \\
Initial temperature & 1535.5 °C \\
Critical temperature ($T_C$) & 1431 °C \\
External temperature & 20 °C \\
Time step ($\Delta t$) & 0.1 s \\
Casting velocity ($\nu_{CC}$) & 0.02667 m·s$^{-1}$ \\
Liquid inlet velocity ($\nu_{inlet}$) & 0.07068 m·s$^{-1}$ \\

| Table 3. Simulation and material parameters in the quasi-2D continuous casting test case. |

Figure 2. Snapshot of results (a) at time $t = 10$ s, showing (arrows, $\nu_{H}$) the fluid flow and ($\bar{\sigma}$) the von Mises equivalent stress (represented domain width 106 mm); (b) at time $t = 100$ s, the left symmetry part presents ($\bar{\sigma}$) the von-Mises equivalent stress and the right symmetry part presents ($g_s$) the solid fraction (represented domain width: 212 mm); (c) at time $t = 100$ s, vertical stress profile over the width from right-hand symmetry plan to the left-hand cooling surface 300 mm below the mould exit (green line).

4. Conclusions
An algorithm of concurrent simulation of fluid flow and stress-strain analysis for continuous casting is developed. The algorithm consists of a partitioned solution strategy, solving at one increment a solid-oriented solution and a fluid oriented solution. All solutions are formulated with the finite element method, using a level set tracking of the moving interface between the solidifying metal subdomain and the gas subdomain. This algorithm is tested in a quasi-2D continuous casting process. Simulation gives promising results, in which the fluid flow in the liquid and mushy regions and the equivalent stress formed in the solid regions are concomitantly computed.
The main perspectives of this work are twofold. Firstly, coupling of this algorithm with macrosegregation modelling for application to a 3D industrial casting process, requiring a more elaborated mesh velocity computation. Secondly, the algorithm could be coupled with equiaxed grain motion to give access to enhanced predictions of macrosegregation due to thermosolutal convection, shrinkage flow, transport of equiaxed grains [9] and thermomechanical deformation of solid and mushy regions.

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Appendix: Thermomechanical properties of steel Fe – 0.4 wt.% C

![Figure A1](image1.png)  
**Figure A1.** The liquid fraction in the solidification interval.

![Figure A2](image2.png)  
**Figure A2.** The solid density (until liquidus temperature) and the liquid density (until solidus temperature) as a function of temperature.
Figure A3. The solid consistency as a function of temperature.

Figure A4. The specific solid enthalpy and specific liquid enthalpy as a function of temperature.

Figure A5. The solid strain rate sensibility as a function of temperature.

Figure A6. The solid hardening coefficient as a function of temperature.

Figure A7. The Young modulus as a function of temperature.

Figure A8. The yield stress as a function of temperature.