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# A partitioned solution algorithm for concurrent computation of stress-strain and fluid flow in continuous casting process

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**Abstract:** Control of macrosegregation phenomena and deformation related defects is a main issue in steel continuous casting. Numerical simulation could help industrial engineers to master these defects. However, as a first step, it is essential to achieve a concurrent computation of fluid flow in the bulk liquid and stress-strain evolution in the already solidified regions. With this aim in view, a new specific partitioned solver has been developed to model the liquid flow, essentially induced by the inlet jet distributed by the submerged nozzle, as well as the thermal deformation of the solid shell. The solver procedure allows simulating the transient regime, up to convergence to the steady-state regime. For this purpose, the computational finite element mesh moves and grows continuously. Within this evolving mesh, three different zones are defined: the solid shell as a pure Lagrangian zone, the liquid nozzle region as a pure Eulerian zone, and an intermediate Eulerian-Lagrangian zone. Conservation equations (energy, mass, and momentum) are solved in a general arbitrary Lagrangian-Eulerian framework, with a level-set formulation to track the free surface evolution at the meniscus. The article is composed of two parts. In the first part, the model is detailed with the resolution steps involved in the coupled resolution approach. In the second part, a simple verification test case is firstly proposed, followed by a more relevant and practical application to model an industrial pilot continuous casting process.

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## 30 **1 Introduction**

31 Continuous casting (CC) is likely the most important steel casting process due to its productivity and  
32 cost-efficiency. It is also a very sophisticated process as it involves numerous complex physical  
33 phenomena. Supported by the rapid development of computational capacities during the last decades,  
34 numerical modeling plays a more and more important role in the understanding and future developments  
35 of the CC process for steel companies. CC modeling consists principally in at least four physical  
36 phenomena: heat transfer, fluid flow, solid deformation, and solute transfer.

37 In the literature, most existing numerical models addressing CC can be classified into two categories. In  
38 the first category, the focus is set on thermo-fluid analyses, ignoring the other two aspects. The approach  
39 is essentially focused on what is named the primary cooling zone, that is the mold region where liquid  
40 steel is delivered at high speed by a submerged entry nozzle. With these models, industrial issues related  
41 to fluid flow can be investigated. Influence of process parameters such as the nozzle holes orientation,  
42 casting speed and mold width, on fluid flow patterns was successfully predicted.<sup>[1, 2]</sup> Heat convection  
43 and other fluid flow related transport phenomena, for e.g. motion of argon gas bubbles and non-metallic  
44 inclusions, can be modeled.<sup>[3, 4]</sup> Complex phenomena, such as interactions between fluid flow, slag  
45 infiltration and mold oscillations are also considered.<sup>[5]</sup> It is important to note that thermo-fluid  
46 simulation codes may give access to macrosegregation simulation by complementing the thermo-fluid  
47 solver with an additional solver for transport of chemical species.<sup>[6, 7]</sup> By contrast, in the second category,  
48 numerical models focus on solid deformation. The main investigated industrial issues are still in primary  
49 cooling: mold distortion and crack formation in solidified zones. But numerical codes for solid  
50 mechanics also permit studying the deformation of the solid shell during secondary cooling, with defects  
51 such as bulging between support rolls and associated crack formation.<sup>[8-10]</sup>

52 Following the presentation of these two categories - fluid flow and solid deformation - let us focus now  
53 on the interest in coupling the two approaches in the context of CC modeling:

- 54 • First, the deformation of the solid shell in primary cooling may modify significantly the thermal  
55 contact between the solid shell and the metallic mold, through the opening of a gas gap. This  
56 gap appearance decreases drastically the heat exchange coefficient characterizing the heat flow  
57 at product/mold interface. It is then easy to understand that an accurate simulation of the  
58 solidification process in the mold region must take into account such changes in thermal  
59 boundary conditions.
- 60 • Second, the prediction of the deformation and stress build-up in the solid shell in primary  
61 cooling is generally addressed by use of solid structural codes (such as Abaqus for instance).  
62 However, when proceeding this way, the influence of liquid convection loops in the mold region,  
63 with localized critical zones such as those directly impacted by the hot nozzle jet, cannot be  
64 taken into account. Hence, the prediction of cracking occurrence in the thin solid shell cannot  
65 be accurate and reliable.

66 • Third, in secondary cooling, the interactions between the solid deformation and the  
67 subsequently induced fluid flow in the mushy zone have been proven to have a dominant effect  
68 on the formation of the central macrosegregation.<sup>[11]</sup> Therefore, an algorithm allowing the  
69 concurrent computation of stress-strain and fluid-flow is essential for a successful modeling of  
70 such a phenomenon and furthermore to provide a more accurate model of solidification.

71 Regarding this coupling perspective, Thomas *et al.* have developed a strategy consisting in coupling  
72 several independent simulation codes together: one code for fluid flow, a second one for shell  
73 deformation.<sup>[12, 13]</sup> Zapulla *et al.* applied this approach to the simulation of the CC of stainless steel  
74 slabs,<sup>[12]</sup> while Koric *et al.* applied it to beam blanks CC.<sup>[13]</sup> It should be noted that such a coupling  
75 approach relies on a sophisticated interface engineering, in order to ensure the exchange of information  
76 between the different computational codes. This is all the more complex since this interface, namely the  
77 surface at solidus temperature, continuously evolve during the simulation. This might be also a possible  
78 source of robustness issues, or of efficiency loss in highly parallel computations. This is why the present  
79 approach is somewhat different, aiming at achieving such coupled solid/fluid resolutions in a unique  
80 computational code, and using a unique finite element mesh.

81 The coupled problem, as described above, can be seen as a general fluid-structure interaction (FSI) issue.  
82 However, contrary to most FSI problems, the interaction considered here is between a very stiff structure  
83 on one hand (the solid shell), and a low viscosity fluid on the other hand (the liquid metal). As pointed  
84 out by Heil *et al.*,<sup>[14]</sup> the coupling effect between solid and fluid mechanics in a FSI problem can be  
85 characterized by a FSI index, defined as the ratio of the flow stress in the fluid and solid regions. It was  
86 proven that for problems with a low FSI index, such as in the present problem for continuous casting, a  
87 partitioned approach is more efficient than a monolithic approach. By partitioned approach, one should  
88 understand a staggered resolution scheme in which separate fluid and solid problems are solved and  
89 coupled, while a monolithic approach is for a unique resolution. The reason for the best performance of  
90 the partitioned approach lies in the fact that the monolithic approach is affected by a loss of numerical  
91 conditioning. Indeed, the spectrum of eigenvalues of the set of equations to be solved is too wide and  
92 dramatically affects the convergence speed of iterative solvers. More detailed analysis can be found in  
93 references [14] and [15].

94 Another characteristic feature of solid/liquid coupling in the context of solidification is the coexistence  
95 of solid and liquid phases in mushy zones, where temperature is in between the liquidus and the solidus  
96 (or eutectic) temperatures corresponding to the solidification interval. At the process scale, the interface  
97 between the two phases cannot be explicitly modeled. Instead, the liquid and solid phases have to be  
98 considered in a homogenized way within a mushy zone. In the literature, there are only a few numerical  
99 models which are capable of coupling fluid flow and solid deformation. They were developed only in  
100 recent years.<sup>[16-18]</sup> In those codes, fluid flow computation and stress-strain analysis are coupled and  
101 solved simultaneously within a single system of non-linear equations, expressing the momentum  
102 conservation equations relative to the solid and liquid phases, together with global mass conservation.

103 They are not affected by numerical conditioning problems because they focus essentially on the mushy  
104 zone deformation, without involving very stiff constitutive equations for solid metal. Such constitutive  
105 equations derive from generalized non-Newtonian fluid behavior models. Some interesting results were  
106 obtained with this approach. Koshikawa *et al.* studied the fluid flow and associated macrosegregation  
107 induced by the lateral punching of an ingot deformed upon solidification, a specific sollicitation aiming  
108 at mimicking soft reduction in CC.<sup>[11]</sup> Fachinotti *et al.*<sup>[16]</sup> and Rodrigues *et al.*<sup>[18]</sup> directly addressed the  
109 simulation of soft reduction in CC. However, this approach is not retained in the present work for two  
110 reasons: i) using such a behavior model for the solid, it is impossible to address the prediction of residual  
111 stress in solid metal (as this requires elastic-(visco)plastic constitutive models such as the one described  
112 in the work of Bellet and Thomas<sup>[19]</sup>), and ii) the computational cost is prohibitive. Actually, solving for  
113 the liquid and solid velocity fields in a unique set requires that 7 unknown values should be determined  
114 at each node or cell of the computational grid: the 3 components of the solid velocity, the 3 components  
115 of the liquid velocity plus a pressure unknown in case of a mixed velocity-pressure formulation. Hence,  
116 7 unknowns instead of 4 (3 velocity components plus a pressure) results in a dramatic increase of the  
117 computational time.

118 It is then clear that the partitioned approach is a good candidate to simulate FSI in CC. Similarly to the  
119 previous work aiming at simulating ingot casting,<sup>[15]</sup> special care has to be put to consider the mushy  
120 zone in each of the two solvers. This is especially true in CC, where the solid phase in the mushy zone  
121 is no more quasi-static, but moves at approximately the casting velocity. The global movement of the  
122 solid phase requires in turn an Arbitrary Lagrangian Eulerian (ALE) formulation. In the present work,  
123 a partitioned solution algorithm is then proposed for CC as an extension of the previous work done for  
124 ingot casting application.<sup>[15]</sup> The numerical model principally consists of two resolution steps performed  
125 at each time increment on the same computational domain: the first one, labeled STEP I, is a solid-  
126 oriented solution of the momentum and mass conservation equations, from which the stress-strain  
127 analysis is carried out in the regions partially or completely solidified. The second one, labeled STEP  
128 II, is a fluid-oriented solution of the momentum and mass conservation equations, giving access to the  
129 velocity and pressure fields in the fluid-containing zones, *i.e.* regions with liquid, mushy zone and gas.  
130 The volume averaging methodology and the Darcy's law are used to model the interactions between  
131 solid and liquid phases in the mushy zone. A characteristic feature of the present approach is that all  
132 conservation equations are formulated in the framework of a level set method in order to track the  
133 metal/gas interface. Another important point is that the partitioned algorithm is coupled with a non-  
134 linear energy solver to calculate the temperature field. As this solver was initially developed by Saad *et*  
135 *al.*<sup>[20]</sup> under a fixed solid phase hypothesis, it is also extended to consider the movement of the solid  
136 phase.

137 The paper is organized as follows. In Section 2 the algorithm is described with a special focus on the  
138 above-mentioned extensions. In Section 3, a verification of the extended approach is demonstrated  
139 through a simple case test. It is followed by a more relevant and practical application to an industrial  
140 pilot continuous casting process.

141

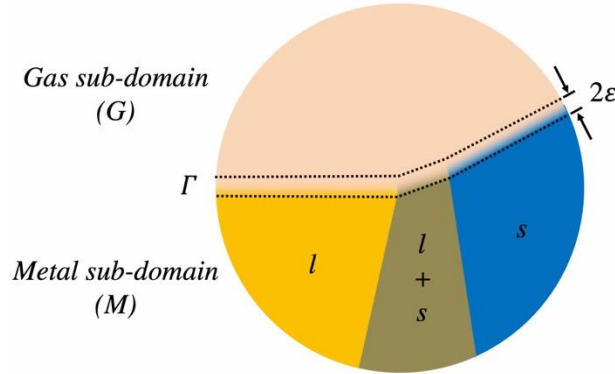
## 142 2 Model description

### 143 2.1 Level set method: short reminder and notations

144 A representative elementary volume (REV) of the simulation domain  $\Omega$  is composed of two sub-  
 145 domains, as schematized in **Fig. 1**. A gas-subdomain  $\Omega^G$  is defined above a metal sub-domain  $\Omega^M$ .  
 146 Three regions may be present in the metal sub-domain itself: a bulk liquid region,  $l$ , a fully solid region,  
 147  $s$ , and a mushy zone made of a mixture of the two former regions,  $l + s$ . The level set method is used to  
 148 explicitly model the evolution of the metal/gas boundary during the continuous casting process,  $\Gamma$ . More  
 149 precisely,  $\Gamma$  is represented by the zero-iso-value of the signed distance function  $\varphi(\mathbf{x}, t)$ , defined for any  
 150 point  $\mathbf{x}$  and time  $t$  in  $\Omega$ . The smoothed Heaviside function  $\mathcal{H}^M$  is defined based on  $\varphi(\mathbf{x}, t)$  as:

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

151 where  $\varepsilon$  is the half-thickness of the transition zone around the metal/gas boundary.



**Fig.1.** Schematic illustration of the simulation domain, including metal and gas sub-domains. The metal/gas boundary,  $\Gamma$ , is explicitly modeled through a diffusive level set transition zone, *i.e.* zone delimited by the two thick black dotted lines of thickness  $2\varepsilon$ .

152 Respectively denoting  $\psi^M$  and  $\psi^G$  the physical property  $\psi$  related to the metal and gas sub-domains,  
 153 the mixed property  $\hat{\psi}$  is given by:

$$\hat{\psi} = \mathcal{H}^M \psi^M + (1 - \mathcal{H}^M) \psi^G \quad (2)$$

154 Thus, over the thickness  $[-\varepsilon, \varepsilon]$  surrounding  $\Gamma$ , a smooth and continuous transition of properties is  
 155 defined. Note that the above-defined mixed property holds not only in the artificial transition zone  
 156 around the interface but also in the pure metal and gas sub-domains. Similarly, the mixed property  $\hat{\psi}^F$   
 157 associated with fluid, and being related to the liquid regions of the metal sub-domain and the gas sub-  
 158 domain, can be defined by the following expression:

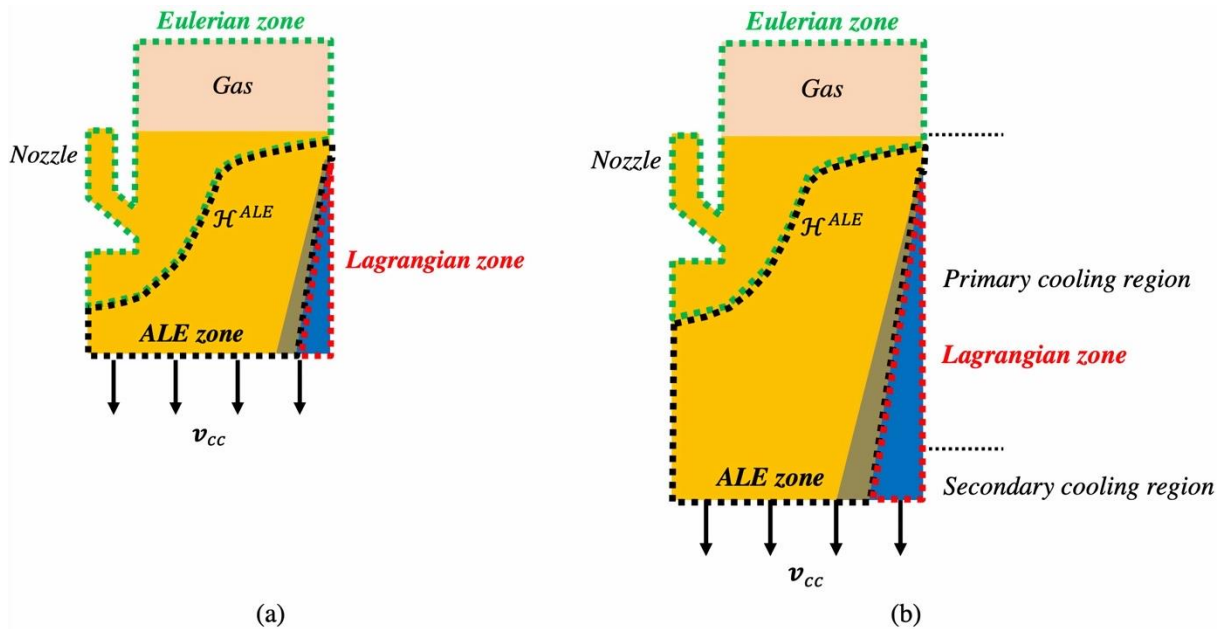
$$\hat{\psi}^F = \mathcal{H}^M \psi^l + (1 - \mathcal{H}^M) \psi^G \quad (3)$$

159 where  $\psi^l$  refers to the intrinsic property associated with the liquid phase in the metal sub-domain.

160

## 161 2.2 Moving mesh, and ALE formulation

162 The model of CC hereafter presented considers transient regimes. It aims at simulating non-steady states  
163 of the process thus requiring a continuously growing computational domain. The mold that characterizes  
164 the CC machine is of internal rectangular section. Its length defines the primary cooling region. The  
165 mold itself is not directly modeled. Instead, initial and boundary conditions of the simulation domain  $\Omega$   
166 are defined to account for its role in the solidification process. Initially,  $\Omega$  encompasses a metal  
167 sub-domain  $\Omega^M$  in the primary cooling region (i.e., in the mold), plus the above located gas sub-domain  
168  $\Omega^G$ . During the simulation,  $\Omega^M$  grows in the casting direction at the velocity defined by the withdrawal  
169 speed,  $v_{cc}$ , progressively filling the whole primary cooling region, and then the secondary cooling zone  
170 underneath the mold.



**Fig.2.** Schematics of the computational domain at (a) an early stage of the process when the metal is still fully located in the mold region and (b) at a later stage when the metal occupies the full mold region and has entered the secondary cooling region. Typical dimensions are: width 0.5 to 1 m (for half of the product, as represented here), thickness 150 to 250 mm, height of the mold (primary cooling region) 600 to 800 mm, thickness of solid shell at mold exit 10 to 15 mm.

171 In this context, as explained hereafter, an evolving and constantly growing mesh is required. **Fig. 2**  
172 illustrates the evolution of the computational domain  $\Omega$  at two different stages of the simulation,  
173 respectively at an early stage (a) and at a later stage (b). At the top of the simulation domain, in  $\Omega^G$   
174 as well as in the neighborhood of the nozzle, a constant Eulerian zone is predefined where the mesh is  
175 fixed. The dimensions of this Eulerian zone are defined at the beginning of the simulation and kept  
176 unchanged all along the calculation. Its contour is drawn with thick green dotted lines in **Fig. 2**. In the  
177 solidified shell, a convenient and accurate approach consists in having a mesh following the  
178 displacement of the solid material. Indeed, the behavior of the solid material is elastic-viscoplastic, and

179 thus of memory type. As it will be seen below, the solution of incremental elasto-viscoplasticity is based  
 180 on total (or particle) time derivatives, which are extremely difficult to calculate accurately when using  
 181 a non-Lagrangian mesh (*i.e.* a mesh that would not evolve at the same speed as the material). For this  
 182 reason, a Lagrangian zone is defined, *i.e.* zone delimited by the contour using thick red dotted lines, as  
 183 shown in **Fig. 2**, corresponding to the fully solidified regions in the metal sub-domain. Unlike the  
 184 Eulerian zone, this Lagrangian zone keeps increasing during the simulation as it moves at material speed  
 185 in the solid shell (Lagrangian approach). Note that the bottom boundary of the simulation domain grows  
 186 at the casting speed with a vertical downward velocity,  $\mathbf{v}_{cc}$ . The rest of the computational domain is  
 187 defined as an ALE zone, including the mushy zone and a part of the bulk liquid zone. The ALE zone is  
 188 delimited by the thick black dotted contour in **Fig. 2**. Like the Lagrangian zone, this zone keeps  
 189 increasing due to the imposed extraction speed of the machine which is prescribed along the bottom  
 190 surface. The mesh movement in this zone is rather arbitrary.

191 In the context of this work, the transition between the ALE zone (mobile mesh) and the Eulerian zone  
 192 (fixed mesh) is achieved through the use of a Heaviside function,  $\mathcal{H}^{ALE}$ . This Heaviside function is  
 193 defined over the interface between the ALE and Eulerian zones, *i.e.* the coincident line of the thick  
 194 dotted green and black lines shown in **Fig. 2**. This Heaviside function, varying between 0 in the Eulerian  
 195 zone and 1 in the ALE zone, is smoothed over a certain thickness around the surface defined by  $\mathcal{H}^{ALE} =$   
 196 0.5, that is the interface between the two zones. This allows a smooth and progressive evolution of the  
 197 mesh dimensions that avoids excessive distortions. It should be mentioned that the location of this  
 198 interface is rather arbitrary: it depends on the definition of the Eulerian zone. Nonetheless, once this  
 199 interface is defined, it is kept unchanged over the whole simulation domain, and during the whole  
 200 simulation, as well as the associated Heaviside function defined above. The strategy to force a smooth  
 201 transition of the mesh evolution at the boundary between ALE and Lagrangian zones will be detailed in  
 202 the next section. As a summary, the simulation considers an evolving computational domain, with a  
 203 moving mesh composed of three regions:

- 204 • a fixed mesh in the gas and the nozzle neighborhood (Eulerian approach),
- 205 • a mesh moving at material speed in the solid shell (Lagrangian approach),
- 206 • a mesh having an arbitrary velocity in between.

207 The mesh velocity will be denoted  $\mathbf{v}_{msh}$  in the sequel, the use of a moving mesh in turn inducing the  
 208 use of an ALE formulation to take into account  $\mathbf{v}_{msh}$  in the discretization of conservation equations. In  
 209 ALE, the relationship between the partial time derivative of any physical quantity  $\psi$  with respect to the  
 210 moving mesh,  $\partial_{msh}\psi/\partial t$  (often named grid derivative), and the total time derivative  $d\psi/dt$ , is resumed  
 211 in the following equation:

$$\frac{\partial_{msh}\psi}{\partial t} = \frac{d\psi}{dt} - (\mathbf{v} - \mathbf{v}_{msh}) \cdot \nabla\psi \quad (4)$$

212 where  $\mathbf{v}$  represents the material velocity field. Note that in the case of a pure Eulerian framework,  
 213  $\mathbf{v}_{msh} \equiv 0$  and  $\partial_{msh}\psi/\partial t = \partial\psi/\partial t$ . The relationship between the partial and total derivatives of  $\psi$  is



214 then retrieved:  $d\psi/dt = \partial\psi/\partial t + \mathbf{v} \cdot \nabla\psi$ . In a pure Lagrangian framework,  $\mathbf{v}_{msh} \equiv \mathbf{v}$ , and Eq. (4)  
 215 simply expresses that  $\partial_{msh}\psi/\partial t = d\psi/dt$ . Finally, substituting the classical relationship  $d\psi/dt =$   
 216  $\partial\psi/\partial t + \mathbf{v} \cdot \nabla\psi$  into Eq. (4), an alternative relation is obtained:

$$\frac{\partial_{msh}\psi}{\partial t} = \frac{\partial\psi}{\partial t} + \mathbf{v}_{msh} \cdot \nabla\psi \quad (5)$$

217 Hence, this allows for an easy adaptation and discretization of conservation equations in ALE. First, in  
 218 Lagrangian regions, it will be seen in Section 2.3 that only total derivatives are required. We have then  
 219  $d\psi/dt \equiv \partial_{msh}\psi/\partial t$ , and the discretization is achieved by means of nodal finite differences:  
 220  $(\psi_n^{t+\Delta t} - \psi_n^t)/\Delta t$ , where  $n$  denotes a node of the moving mesh. Second, in all other regions (metal in  
 221 mushy or liquid state, gas)  $\mathbf{v}_{msh}$  is different from the material velocity, and possibly null. Besides, it  
 222 will be seen in Sections 2.3 and 2.4 that the constitutive model is of no-memory type (viscoplastic or  
 223 Newtonian behavior), and that conservation equations require only partial time derivatives  $\partial\psi/\partial t$ . They  
 224 will be replaced by  $\partial_{msh}\psi/\partial t - \mathbf{v}_{msh} \cdot \nabla\psi$ , according to Eq. (5). The time grid derivatives will be  
 225 discretized by means of nodal finite differences:  $(\psi_n^{t+\Delta t} - \psi_n^t)/\Delta t$ , where  $n$  denotes a node of the  
 226 moving mesh.

227

### 228 **2.3 STEP I: stress-strain analysis**

229 As already mentioned above, the two resolution steps are successively performed at each time increment.  
 230 An important point is that they are operated on the same computational mesh covering the entire domain  
 231  $\Omega$ . Hence, STEP I is not operated on the “solid” only; STEP II is not operated on the “liquid” only.  
 232 Instead, both STEP I and STEP II are solved on  $\Omega$ .

233 The first resolution step is solid-oriented. This means that it essentially addresses the stress-strain  
 234 analysis in the solid regions and the mushy zone. The approach used was presented in detail in a previous  
 235 paper<sup>[15]</sup> and is briefly reminded here. The following momentum and mass conservation equations are  
 236 solved for the velocity field  $\mathbf{v}$  and the pressure field  $p$ , using a finite element method:

$$\begin{cases} \nabla \cdot \hat{\mathbf{s}} - \nabla p + \hat{\rho} \mathbf{g} = 0 \\ \nabla \cdot \mathbf{v} = \mathcal{H}^M (H(T_C - T) \text{tr}(\dot{\boldsymbol{\epsilon}}_{el}) + \text{tr}(\dot{\boldsymbol{\epsilon}}_{th})) \end{cases} \quad (6)$$

237 The tensor  $\hat{\mathbf{s}}$  and the scalar  $\hat{\rho}$  are respectively the mixed stress deviator and the mixed density in domain  
 238  $\Omega$ , as defined in Table 1. Vector  $\mathbf{g}$  is the constant gravity vector.

<i>Mixed property</i>	<i>Definition</i>
$\hat{\mathbf{s}}$	$\mathcal{H}^M \mathbf{s}^M + (1 - \mathcal{H}^M) \mathbf{s}^G$
$\hat{\rho}$	$\mathcal{H}^M \langle \rho \rangle^M + (1 - \mathcal{H}^M) \rho^G$

Table 1. Mixed properties between the metal and gas sub-domains in STEP I.

239  $\mathbf{s}^M$  and  $\langle \rho \rangle^M$  are respectively the stress tensor and average density in  $\Omega^M$ .  $\mathbf{s}^G$  and  $\rho^G$  are the stress tensor  
 240 and density in  $\Omega^G$ . The average metal density  $\langle \rho \rangle^M$  is defined as  $g^l \langle \rho \rangle^l + g^s \langle \rho \rangle^s$  where  $\langle \rho \rangle^l$  and  $\langle \rho \rangle^s$   
 241 are respectively the intrinsic density of the liquid and solid phases with  $g^l$  and  $g^s$  corresponding  
 242 respectively to the local volume fractions of the liquid and solid phases.

243  $H(T_C - T)$  is the standard Heaviside function, taken for the temperature difference  $(T_C - T)$ . It is  
 244 introduced as an indicator relative to the use of a thermo-elastic-viscoplastic (TEVP) constitutive model  
 245 for elements in the metal sub-domain with an average temperature lower than a certain critical transition  
 246 temperature  $T_C$ , while a thermo-viscoplastic (TVP) model is used for elements in the metal sub-domain  
 247 with a temperature higher than  $T_C$ .

248 Constitutive equations of the TEVP model, below  $T_C$ , are described hereafter as given in reference [10]:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}_{el} + \dot{\boldsymbol{\varepsilon}}_{vp} + \dot{\boldsymbol{\varepsilon}}_{th} \quad (7)$$

$$\dot{\boldsymbol{\varepsilon}}_{el} = \mathbf{E}^{-1} \dot{\boldsymbol{\sigma}} = \frac{1+\nu}{E} \dot{\boldsymbol{\sigma}} - \frac{\nu}{E} \text{tr}(\dot{\boldsymbol{\sigma}}) \mathbf{I} \quad (8)$$

$$\dot{\boldsymbol{\varepsilon}}_{vp} = \frac{\sqrt{3}}{2\bar{\sigma}} \left[ \frac{\bar{\sigma} - \sigma_Y}{\sqrt{3}K\bar{\varepsilon}^n} \right]_+^{\frac{1}{m}} \mathbf{s} \quad (9)$$

$$\dot{\boldsymbol{\varepsilon}}_{th} = -\frac{1}{3\rho} \frac{d\rho}{dt} \mathbf{I} \quad (10)$$

249 The strain rate tensor  $\dot{\boldsymbol{\varepsilon}}$  is split into an elastic part,  $\dot{\boldsymbol{\varepsilon}}_{el}$ , a viscoplastic part,  $\dot{\boldsymbol{\varepsilon}}_{vp}$ , and a thermal part,  $\dot{\boldsymbol{\varepsilon}}_{th}$   
 250 (Eq. (7)). The latter consists of the thermal expansion rate (Eq. (10)), with  $\rho$  the density. Eq. (8) yields  
 251 the hypoelastic Hooke's law where  $\mathbf{E}$  represents the elastic tensor depending on the Young's modulus  
 252  $E$ , and the Poisson's coefficient  $\nu$ .  $\dot{\boldsymbol{\sigma}}$  denotes the total time derivative of the stress tensor. Eq. (9) gives  
 253 the relation between the viscoplastic strain rate tensor and the stress deviator  $\mathbf{s}$ . It is reminded here that  
 254 the stress deviator is defined as  $\mathbf{s} = \boldsymbol{\sigma} - (1/3)\text{tr}(\boldsymbol{\sigma})\mathbf{I} = \boldsymbol{\sigma} + p\mathbf{I}$ , where  $\boldsymbol{\sigma}$  is the Cauchy stress tensor,  $p$   
 255 is the hydrostatic pressure, and  $\mathbf{I}$  is the identity tensor. Coefficient  $K$  is the viscoplastic consistency,  $\sigma_Y$   
 256 denotes the static yield stress below which no viscoplastic deformation occurs. The function  $[x]_+$  is  
 257 equal to 0 when  $x$  is negative and to the value  $x$  otherwise. Coefficients  $m$  and  $n$  denote the strain-rate  
 258 sensitivity coefficient, and the strain hardening coefficient, respectively. Finally, the corresponding  
 259 relationship between the von Mises stress,  $\bar{\sigma}$ , the generalized plastic strain,  $\bar{\varepsilon}$ , and the generalized strain  
 260 rate,  $\dot{\bar{\varepsilon}}$ , is given by:

$$\bar{\sigma} = \sigma_Y + K(\sqrt{3})^{m+1} \dot{\bar{\varepsilon}}^m \bar{\varepsilon}^n \quad (11)$$

261 Constitutive equations of the TVP model, over  $T_C$ , are written as follows:

$$\dot{\boldsymbol{\varepsilon}} = \dot{\boldsymbol{\varepsilon}}_{vp} + \dot{\boldsymbol{\varepsilon}}_{th} \quad (12)$$

$$\dot{\boldsymbol{\varepsilon}}_{vp} = \frac{1}{2K} (\sqrt{3}\dot{\bar{\varepsilon}})^{1-m} \mathbf{s} \quad (13)$$

$$\dot{\boldsymbol{\varepsilon}}_{th} = -\frac{1}{3\rho} \frac{d\rho}{dt} \mathbf{I} \quad (14)$$

262 The strain rate tensor  $\dot{\boldsymbol{\varepsilon}}$  is split into a viscoplastic part,  $\dot{\boldsymbol{\varepsilon}}_{vp}$ , and a thermal part,  $\dot{\boldsymbol{\varepsilon}}_{th}$  (Eq. (12)). Eq. (13)  
 263 is the classical constitutive law for a generalized non-Newtonian fluid. It relates the viscoplastic strain  
 264 rate  $\dot{\boldsymbol{\varepsilon}}_{vp}$  to the stress deviator  $\boldsymbol{s}$ , in which the strain-rate sensitivity  $m$  continuously increases with the  
 265 liquid fraction in the mushy zone. The Newtonian behavior, which is assumed to be the behavior law  
 266 for the liquid metal above its liquidus temperature,  $T_L$ , as well as for the gas, is obtained for  $m = 1$ . In  
 267 this case, the viscoplastic consistency  $K$  is simply the dynamic viscosity of the fluid (liquid metal or  
 268 gas). Finally, the corresponding relationship between the von Mises stress  $\bar{\sigma}$  and the generalized strain  
 269 rate  $\dot{\boldsymbol{\varepsilon}}$  is the following one:

$$\bar{\sigma} = K(\sqrt{3})^{m+1} \dot{\boldsymbol{\varepsilon}}^m \quad (15)$$

270 In the present work,  $T_C$  is taken exactly as the solidus temperature to model the TEVP behavior of steel  
 271 in a fully solid state; the TVP model is used for metal either in the mushy state or liquid state. At this  
 272 critical transition temperature, the continuity of the flow stress is obtained by taking  $\sigma_Y(T_C) = 0$  and  
 273  $n(T_C) = 0$ .

#### 274 Specific points of STEP I resolution

275 Two important characteristic features deserve attention:

- 276 • First, in order to prevent numerical instabilities due to the huge difference between solid consistency  
 277 and liquid or gas viscosities, the values of these latter properties are artificially augmented. The  
 278 liquid viscosity is typically set to 1 Pa · s, which is about 200 times the nominal value for liquid  
 279 steel for instance. The gas is considered as an incompressible Newtonian fluid in the gas sub-domain,  
 280 also with a viscosity typically set to 1 Pa · s. It is important to note that these simplifications have  
 281 no significant impact on the main focus of STEP I, which is the calculation of stress and strain in  
 282 already solidified regions during CC.
- 283 • A second important point in STEP I is the treatment of solidification shrinkage and liquid expansion.  
 284 Usually, when performing the solid-oriented resolution step alone, without STEP II, like in  
 285 reference [19], the thermal dilatation of both liquid and solid phases, are taken into consideration,  
 286 together with the solidification shrinkage. However, when adding STEP II to STEP I, another  
 287 strategy has been found more efficient. Keeping in mind that the focus of STEP I is the stress-strain  
 288 analysis in already solidified regions, only the solid thermal expansion is taken into account below  
 289  $T_L$  (considering  $\langle \rho \rangle^s = f(T)$  as an input). Especially, in the mushy zone, we are essentially  
 290 interested in the intrinsic velocity of the solid phase (*i.e.* the movement of the columnar dendritic  
 291 structure). Such a numerical approximation appears to be a simple but efficient way to achieve the  
 292 computation of a velocity field approaching the intrinsic velocity of the solid phase. In addition,  
 293 over  $T_L$ , the material is considered incompressible:  $\langle \rho \rangle^M \equiv \langle \rho \rangle^s(T_L)$ . Hence, in Eq. (12), the thermal

294 part of the strain rate tensor,  $\dot{\boldsymbol{\epsilon}}_{th}$ , is constantly null. The treatment of solidification shrinkage and  
 295 liquid expansion is done in STEP II and explained in the next Section.

296 Finally, a velocity-pressure resolution of the weak form of Eq. (6) is performed on  $\Omega$ . The velocity and  
 297 pressure fields resulting from this first step are denoted  $(\mathbf{v}_I, p_I)$ .

298

## 299 2.4 STEP II: fluid flow computation

300 In this second fluid-oriented resolution step, the solution from the previous STEP I is taken as an entry.  
 301 The objective of this second step resolution is to calculate the fluid flow in liquid and mushy regions,  
 302 taking into account the motion of the solid phase, as deduced from STEP I. In order to consider liquid  
 303 flow through the permeable solid phase in the mushy zone, an effective two-phase approach is used with  
 304 a volume-averaged method.<sup>[21]</sup> Solidification is assumed to take place with a purely columnar structure.  
 305 Interactions between solid and liquid phases in the mushy zone are modeled by the Darcy's law with a  
 306 permeability coefficient  $\kappa$  approximated by the Carman-Kozeny relationship.<sup>[22]</sup> Although the liquid is  
 307 considered as incompressible with a Newtonian behavior, a compressible formulation is used to deal  
 308 with solidification shrinkage in the mushy zone and thermal dilatation of the liquid phase. It is also  
 309 important to mention that in STEP II, contrary to STEP I, the nominal liquid viscosity is now used.

310 In a previous paper,<sup>[15]</sup> the conservation equations governing the fluid-oriented problem have been  
 311 established in the context of a level set formulation applied to a static mesh. As mentioned in Section  
 312 2.2, its extension to the context of a mobile mesh is achieved by replacing the partial time derivatives  
 313 by the grid derivatives according to Eq. (5). The conservation equations for STEP II are now expressed  
 314 with the ALE formulation:

$$\left\{ \begin{array}{l} \hat{\rho}_0^F \left( \frac{\partial_{msh} \mathbf{v}}{\partial t} + \frac{1}{\hat{g}^F} (\nabla \mathbf{v}) (\mathbf{v} - \hat{g}^F \mathbf{v}_{msh}) \right) - \nabla \cdot \hat{\mathbf{g}} \mathbf{s}^F + \hat{g}^F \nabla p - \hat{g} \hat{\rho}^F \mathbf{g} \\ \quad + \hat{g}^F \hat{\mu}^F (\hat{\kappa}^F)^{-1} (\mathbf{v} - \mathbf{v}_I) = 0 \\ \nabla \cdot \mathbf{v} = - \frac{\mathcal{H}^M}{\langle \rho \rangle^l} \left( \frac{\partial_{msh} \langle \rho \rangle^M}{\partial t} + \mathbf{v} \cdot \nabla \langle \rho \rangle^l - \mathbf{v}_{msh} \cdot \nabla \langle \rho \rangle^M + \nabla \cdot (g^s \langle \rho \rangle^s \mathbf{v}_I) \right) \end{array} \right. \quad (16)$$

315 where the unknowns are the average fluid velocity,  $\mathbf{v} = \mathcal{H}^M g^l \langle \mathbf{v} \rangle^l + (1 - \mathcal{H}^M) \langle \mathbf{v} \rangle^G$ , and the pressure,  
 316  $p$ . Notations  $\hat{\rho}_0^F$ ,  $\hat{g}^F$ ,  $\hat{\mathbf{g}} \mathbf{s}^F$ ,  $\hat{g} \hat{\rho}^F$ ,  $\hat{\mu}^F$ ,  $\hat{\kappa}^F$  correspond respectively to the mixing properties of the fluid  
 317 density, the fluid fraction, the averaged fluid stress deviator, the averaged fluid density with temperature  
 318 dependence, the fluid viscosity and the fluid permeability. These variables are defined in Table 2.

<i>Mixed property</i>	<i>Definition</i>
$\hat{g}^F$	$\mathcal{H}^M g^l + (1 - \mathcal{H}^M)$
$\hat{\rho}_0^F$	$\mathcal{H}^M \langle \rho \rangle_0^l + (1 - \mathcal{H}^M) \rho^G$
$\widehat{\rho}^F$	$\mathcal{H}^M g^l \langle \rho \rangle^l + (1 - \mathcal{H}^M) \rho^G$
	with $\langle \rho \rangle^l = \langle \rho \rangle_0^l \left( 1 - \beta_T^l (T - T_L) \right)$
$\widehat{g\mathbf{s}}^F$	$\mathcal{H}^M g^l \langle \mathbf{s} \rangle^l + (1 - \mathcal{H}^M) \mathbf{s}^G$
$\hat{\mu}^F$	$\mathcal{H}^M \mu^l + (1 - \mathcal{H}^M) \mu^G$
$\hat{\kappa}^F$	$\lambda_2^2 \hat{g}^{F3} / (180(1 - \hat{g}^F)^2)$

Table 2. Mixed properties between the liquid regions of the metal sub-domain and the gas sub-domain in STEP II.

319  $\langle \rho \rangle_0^l, \langle \rho \rangle^l, \beta_T^l, \langle \mathbf{s} \rangle^l, \mu^l, \lambda_2$  are respectively the intrinsic reference liquid density at  $T_L$ , the intrinsic liquid  
320 density depending linearly from the temperature, the dilatation coefficient of the liquid, the intrinsic  
321 liquid stress tensor, the liquid viscosity, and the secondary dendrite arm spacing.  $\mu^G$  is the viscosity of  
322 the gas, assumed to be Newtonian and incompressible.

323 In the fully solid regions, there is actually no need to operate a STEP II resolution: all relevant  
324 information (velocity field, updated values of the generalized viscoplastic deformation, deviatoric stress  
325 tensor, and pressure) has been already calculated in the first solid-oriented resolution step. However, in  
326 the present approach, STEP II is operated on the whole domain  $\Omega$ , but with a Dirichlet condition applied  
327 to the fully solid regions: for nodes with their nodal liquid fraction  $g^l$  equal to zero,  $\mathbf{v}_{II}$  is imposed equal  
328 to  $\mathbf{v}_I$ . Finally, Eq. (16) is solved with a stabilized SUPG-PSPG finite element method.<sup>[23]</sup> The velocity  
329 and pressure fields resulting from this second step are denoted  $(\mathbf{v}_{II}, p_{II})$ .

330

## 331 2.5 Coupled thermal resolution

332 A non-linear energy solver is coupled with the above STEP I and STEP II to provide the temperature  
333 field during the continuous casting process. The conventional energy conservation equation for  
334 solidification problems is given in Eq. (17), averaged over the REV in the metal sub-domain:<sup>[21]</sup>

$$\frac{\partial \langle \rho h \rangle^M}{\partial t} + \nabla \cdot \langle \rho h \mathbf{v} \rangle^M - \nabla \cdot (\langle k \rangle^M \nabla T) = 0 \quad (17)$$

335 where  $\langle \rho h \rangle^M = g^l \langle \rho \rangle^l \langle h \rangle^l + g^s \langle \rho \rangle^s \langle h \rangle^s$ ,  $\langle \rho h \mathbf{v} \rangle^M = g^l \langle \rho \rangle^l \langle h \rangle^l \langle \mathbf{v} \rangle^l + g^s \langle \rho \rangle^s \langle h \rangle^s \langle \mathbf{v} \rangle^s$  and  $\langle k \rangle^M =$   
336  $g^s \langle k \rangle^s + g^l \langle k \rangle^l$  with  $\langle h \rangle^l, \langle h \rangle^s, \langle k \rangle^l, \langle k \rangle^s, \langle \mathbf{v} \rangle^l$  and  $\langle \mathbf{v} \rangle^s$  corresponding respectively to the intrinsic  
337 specific enthalpy, the intrinsic heat conductivity and the intrinsic velocity relative to the liquid and solid  
338 phases, respectively. Based on the relationship given in Eq. (5), the ALE formulation of Eq. (17) is given  
339 by:

$$\frac{\partial_{msh}\langle\rho h\rangle^M}{\partial t} + \nabla \cdot \langle\rho h \mathbf{v}\rangle^M - \mathbf{v}_{msh} \cdot \nabla \langle\rho h\rangle^M - \nabla \cdot (\langle k\rangle^M \nabla T) = 0 \quad (18)$$

340 Developing the expressions of  $\langle\rho h \mathbf{v}\rangle^M$  and  $\langle\rho h\rangle^M$ , we obtain:

$$\begin{aligned} & \frac{\partial_{msh}\langle\rho h\rangle^M}{\partial t} + \nabla \cdot (g^l \langle\rho\rangle^l \langle h\rangle^l \langle \mathbf{v}\rangle^l) - \mathbf{v}_{msh} \cdot \nabla (g^l \langle\rho\rangle^l \langle h\rangle^l) \\ & + \nabla \cdot (g^s \langle\rho\rangle^s \langle h\rangle^s \langle \mathbf{v}\rangle^s) - \mathbf{v}_{msh} \cdot \nabla (g^s \langle\rho\rangle^s \langle h\rangle^s) - \nabla \cdot (\langle k\rangle^M \nabla T) = 0 \end{aligned} \quad (19)$$

341 Let's first consider the following term,  $\nabla \cdot (g^s \langle\rho\rangle^s \langle h\rangle^s \langle \mathbf{v}\rangle^s) - \mathbf{v}_{msh} \cdot \nabla (g^s \langle\rho\rangle^s \langle h\rangle^s)$  in Eq. (19). This  
 342 term represents the energy transport related to the solid phase. Assuming that the volume change of the  
 343 solid, due to elasticity and thermal dilatation, has a negligible impact on heat transfer, the solid phase is  
 344 thus assumed here to be intrinsically incompressible,  $\nabla \cdot \langle \mathbf{v}\rangle^s = 0$ . Therefore, the above term is  
 345 simplified into the following form,  $(\langle \mathbf{v}\rangle^s - \mathbf{v}_{msh}) \cdot \nabla (g^s \langle\rho\rangle^s \langle h\rangle^s)$ . Note that in the bulk liquid this term  
 346 is zero. Besides, the fully solidified regions are considered as Lagrangian in the present ALE framework.  
 347 Therefore, in fully solidified regions,  $\mathbf{v}_{msh} = \langle \mathbf{v}\rangle^s$  and this term also reduces to zero.

348 Finally, in the specific context of the present work, the mesh velocity  $\mathbf{v}_{msh}$  in the mushy zone is  
 349 proposed with the following explicit form:

$$\mathbf{v}_{msh} = g^l \mathbf{v}_{cc} + g^s \mathbf{v}_I \quad (20)$$

350 where  $\mathbf{v}_I$  is the solution field from the previous solid-oriented resolution step and  $\mathbf{v}_{cc}$  the constant  
 351 casting velocity of the CC machine. We remind that  $\mathbf{v}_I$  is designed to approach the intrinsic solid  
 352 velocity  $\langle \mathbf{v}\rangle^s$  in the previous solid-oriented resolution step. Besides, in continuous casting  $\langle \mathbf{v}\rangle^s$  in the  
 353 mushy zone is nearly  $\mathbf{v}_{cc}$  due to the continuity of the solid phase between the mushy zone and fully  
 354 solidified shell in contact with the molds. By consequence, the above-defined  $\mathbf{v}_{msh}$  keeps being a good  
 355 approximation of the intrinsic solid velocity  $\langle \mathbf{v}\rangle^s$  in the mushy zone. Therefore, this first energy  
 356 transport term related to the solid phase,  $(\langle \mathbf{v}\rangle^s - \mathbf{v}_{msh}) \cdot \nabla (g^s \langle\rho\rangle^s \langle h\rangle^s)$ , finally reduces to zero in the  
 357 whole metal sub-domain, including the bulk liquid, the mushy zone and the fully solidified regions, and  
 358 this term can be fully neglected from Eq. (19). In other words, the energy transport due to the motion of  
 359 the solid phase in the present model will be achieved through the mesh updating process within the ALE  
 360 framework. Finally, it is worth noting that the above-defined mesh velocity also holds in the fully  
 361 solidified regions, *i.e.*  $g^s = 1$  and  $\mathbf{v}_{msh}$  recovers the material speed in the solid shell,  $\mathbf{v}_I$ . A smooth  
 362 transition of mesh is thus ensured at the boundary of ALE and Lagrangian zones.

363 As stated above, the definition of the mesh velocity in the fully liquid zone is rather arbitrary and may  
 364 be different according to the specific configuration of each simulation. As explained in Section 2.2, a  
 365 pure Eulerian zone is usually defined with  $\mathbf{v}_{msh} = 0$  in regions where metal remains in a liquid state,  
 366 for e.g. regions near the nozzle entry. More intuitive details of such a definition will be given later in  
 367 application to the CC process. Indeed, an optimized mesh velocity would be better to prevent mesh  
 368 distortions, such as the algorithm described in the work of Bellet and Fachinotti,<sup>[10]</sup> where the mesh

369 velocity of a node in the liquid zone was defined roughly as the average velocity of its neighboring  
 370 nodes.

371 Considering now the second term  $\nabla \cdot (g^l \langle \rho \rangle^l \langle h \rangle^l \langle \mathbf{v} \rangle^l) - \mathbf{v}_{msh} \cdot \nabla (g^l \langle \rho \rangle^l \langle h \rangle^l)$  in Eq. (19), it represents  
 372 the energy transport related to the liquid phase. Assuming that the energy transfer due to the  
 373 solidification shrinkage and the thermal dilatation of the liquid phase is negligible, this term can be  
 374 approximated by  $g^l \langle \mathbf{v} \rangle^l \nabla (\langle \rho \rangle^l \langle h \rangle^l) - \mathbf{v}_{msh} \cdot \nabla (g^l \langle \rho \rangle^l \langle h \rangle^l)$ . We remind that  $\mathbf{v}_{II}$ , the solution from the  
 375 previous fluid-oriented resolution step, represents the averaged liquid velocity,  $g^l \langle \mathbf{v} \rangle^l$ , in the liquid and  
 376 mushy zones. In the meantime, it also tends to the solid velocity  $\mathbf{v}_I$  when approaching the end of the  
 377 mushy zone due to the Dirichlet condition applied to the fully solidified regions. Therefore, the  
 378 following approximation is proposed for the above energy transport term related to the liquid phase:

$$g^l \langle \mathbf{v} \rangle^l \cdot \nabla (\langle \rho \rangle^l \langle h \rangle^l) - \mathbf{v}_{msh} \cdot \nabla (g^l \langle \rho \rangle^l \langle h \rangle^l) = (\mathbf{v}_{II} - \mathbf{v}_{msh}) \cdot \nabla (\langle \rho \rangle^l \langle h \rangle^l) \quad (21)$$

379 Note that in the bulk liquid,  $\mathbf{v}_{II} = g^l \langle \mathbf{v} \rangle^l$ , the right-hand side (RHS) term of Eq. (21) recovers exactly  
 380 the left-hand-side (LHS) term of Eq. (21). In the fully solidified regions, the LHS term is zero as  $g^l = 0$   
 381 and RHS term is also zero as both  $\mathbf{v}_{II}$  and  $\mathbf{v}_{msh}$  equal to  $\mathbf{v}_I$ . Besides, in the mushy zone, Eq. (21)  
 382 remains a quite reasonable approximation, especially in regions with high liquid fraction where the  
 383 numerical solution  $\mathbf{v}_{II}$  corresponds nearly to  $g^l \langle \mathbf{v} \rangle^l$ . Finally, assuming that contribution of the gradient  
 384 of the liquid density is negligible in Eq. (21) and taking into consideration the enthalpy relationship  
 385 relative to the liquid phase, the above equation becomes:

$$(\mathbf{v}_{II} - \mathbf{v}_{msh}) \cdot \nabla (\langle \rho \rangle^l \langle h \rangle^l) = (\mathbf{v}_{II} - \mathbf{v}_{msh}) \cdot \langle \rho \rangle^l \langle C_p \rangle^l \nabla T \quad (22)$$

386 where  $\langle C_p \rangle^l$  is the intrinsic specific heat of the liquid phase defined by the liquid enthalpy  $\langle h \rangle^l =$   
 387  $\langle C_p \rangle^l T + L_f$  with constant latent heat of fusion  $L_f$ . Considering the above approximations made over  
 388 the energy transport term relative to both solid and liquid phases, the energy conservation equation in  
 389 the metal sub-domain for the CC process under the ALE framework is given by:

$$\frac{\partial_{msh} \langle \rho h \rangle^M}{\partial t} + (\mathbf{v}_{II} - \mathbf{v}_{msh}) \cdot \langle \rho \rangle^l \langle C_p \rangle^l \nabla T - \nabla \cdot (\langle k \rangle^M \nabla T) = 0 \quad (23)$$

390 Finally, the energy conservation equation is developed under a level set formulation and is given by:

$$\frac{\partial_{msh} \widehat{\rho h}}{\partial t} + (\mathbf{v}_{II} - \mathbf{v}_{msh}) \cdot \widehat{\rho C_p}^F \nabla T - \nabla \cdot (\widehat{k} \nabla T) = 0 \quad (24)$$

391 with  $\widehat{\rho h}$ ,  $\widehat{\rho C_p}$ ,  $\widehat{k}$  corresponding respectively to the mixing properties of the volumetric enthalpy, the  
 392 volumetric heat capacity and the heat conductivity between the metal and gas sub-domains, defined in  
 393 Table 3.

<i>Mixed property</i>	<i>Definition</i>
$\widehat{\rho h}$	$\mathcal{H}^M \langle \rho h \rangle^M + (1 - \mathcal{H}^M) \rho^G h^G$
$\widehat{\rho C_p}^F$	$\mathcal{H}^M \langle \rho \rangle^l \langle C_p \rangle^l + (1 - \mathcal{H}^M) \rho^G C_p^G$
$\widehat{k}$	$\mathcal{H}^M \langle k \rangle^M + (1 - \mathcal{H}^M) k^G$

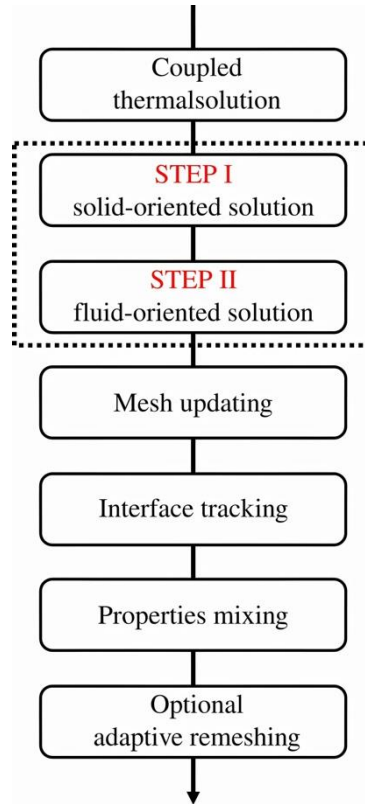
Table 3. Mixed properties between the metal and gas sub-domains in the coupled heat transfer step.

394 where  $h^G$ ,  $C_p^G$  and  $k^G$  are respectively the specific enthalpy, the specific heat and the heat conductivity  
395 of the gas. It is worth noting that Eq. (24) holds for both continuous and ingot casting processes.  
396 Especially, in a fully Eulerian framework where  $\mathbf{v}_{msh} = 0$ , Eq. (24) recovers the previous energy  
397 conservation equation developed for ingot casting processes under a fixed-solid hypothesis.<sup>[15]</sup>

398

## 399 2.6 Algorithm scheme

400 The algorithm scheme of the present partitioned solution algorithm for continuous casting is presented,  
401 considering that the two resolutions, STEP I and STEP II, and the coupled thermal resolution are  
402 performed once at each time increment  $\Delta t$ . The incremental resolution scheme is divided into 7 modules,  
403 as detailed hereunder in **Fig.3**:



**Fig.3.** Resolution scheme in a time increment



- 404 • *Coupled thermal solution.* The energy conservation equation is solved, giving access to the  
405 temperature distribution in the metal and gas sub-domains, and to the liquid metal fraction.
- 406 • *STEP I, solid-oriented solution.* The first folder of the mass and momentum conservation  
407 equations focuses on the stress-strain analysis in the already solidified regions, with an  
408 augmented liquid viscosity and a continuity of solid density in the mushy and liquid regions. It  
409 provides velocity and pressure fields on the whole domain:  $(\mathbf{v}_I, p_I)$ . However, only  $\mathbf{v}_I$  at nodes  
410 belonging to fully solid elements and in the mushy zone will be used in the follow-up of the  
411 resolution scheme. The stress tensor  $\boldsymbol{\sigma}$ , and the associated generalized plastic strain  $\bar{\epsilon}$  and strain  
412 rate  $\dot{\bar{\epsilon}}$ , are also deduced from this step.
- 413 • *STEP II fluid-oriented solution.* The second folder of the mass and momentum conservation  
414 equations consists of the fluid flow computation in the liquid and mushy regions, with a real  
415 liquid viscosity and including solidification shrinkage. It provides velocity and pressure fields  
416 on the whole domain:  $(\mathbf{v}_{II}, p_{II})$ . Note that at nodes belonging to fully solid elements,  $\mathbf{v}_{II}$  is  
417 imposed equal to  $\mathbf{v}_I$ .
- 418 • *Mesh updating.* The position of each mesh node is updated following an explicit scheme with  
419 the mesh velocity,  $\mathbf{v}_{msh}$ :

$$\mathbf{x}^{new} = \mathbf{x}^{old} + \Delta t \mathbf{v}_{msh} \quad (25)$$

420 It should be reminded that the energy transportation relative to the solid phase in the solid and  
421 mushy zones, is achieved through this mesh updating process under the present ALE framework.

- 422 • *Metal/gas interface tracking.* The updating of the level set function permits interface tracking.  
423 It is achieved by the convection-reinitialization scheme.<sup>[24]</sup> The advection velocity field  $\mathbf{v}$  is  
424 equal to the fluid velocity  $\mathbf{v}_{II}$  deduced from STEP II.
- 425 • *Mixing of material properties* according to the value of the updated level set function.
- 426 • *Possible adaptive remeshing* guided either by error estimation for different solution fields, as  
427 proposed by Coupez,<sup>[25]</sup> or more simply formulated based on signed level set distance function.

428

## 429 **3 Simulation results**

### 430 **3.1 Verification test case**

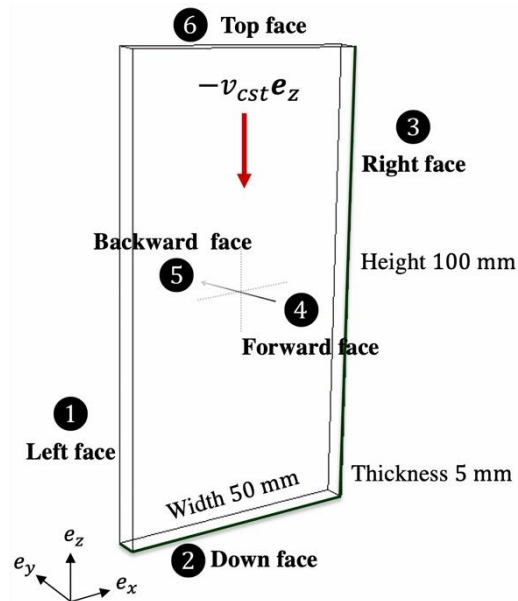
431 The objective of the test case detailed hereafter is to check the correct implementation and the  
432 performance of the above-proposed partitioned solution algorithm, including the new features  
433 introduced in the thermal solver, *i.e.* introduction of the solid movement, the energy transport relative  
434 to the solid phase and the mesh velocity. For this specific purpose, a simple solidification process  
435 configuration is studied, in which the gas sub-domain is neglected, as the new developments mainly

436 affect the metal sub-domain. Besides, the solid-oriented step is oversimplified: no effective stress-strain  
 437 analysis is performed. Only the velocity of the solid phase is imposed, its value being equal to the  
 438 constant casting speed of the machine.

439

### 440 3.1.1 Model description

441 The test case consists of the solidification of two identical 3D parallelepipedic ingots, under the same  
 442 heat boundary condition. The first ingot is fixed and serves as the reference simulation. Its solidification  
 443 is simulated using the previous algorithm developed for casting process.<sup>[15]</sup> The second ingot is entirely  
 444 submitted to a constant downward movement and is simulated with the algorithm presented above. For  
 445 simplicity, only the configuration of the moving ingot simulation is presented here as shown in **Fig.4**.  
 446  $v_{cst}$  denotes the value of the downward moving velocity. The initial mesh is isotropic, defined with a  
 447 uniform mesh size of 1 mm. A constant mesh velocity  $v_{msh}$  is defined over the whole ingot, oriented  
 448 downward and aligned on the vertical  $z$ -direction, with a module equal to  $v_{cst}$ . As the mesh velocity is  
 449 identical for all mesh nodes, the mesh will keep unchanged all along the simulation. Note that for the  
 450 reference simulation, the geometry and its discretization are the same as for the moving ingot at initial  
 451 state. Nonetheless, the value of mesh velocity is null and by consequence, a fixed mesh will be used for  
 452 the whole simulation.



**Fig.4.** Geometry of test case simulation of the moving ingot under solidification

453 Indeed, this moving simulation could be seen as a representation of a fixed slice of the metal product  
 454 for the CC process. Due to the symmetry of the system, only half of the slice is modeled. The six faces  
 455 of the ingot are numbered in order to clearly describe the boundary conditions. Note that the left face,  
 456 as well as the backward and forward faces, are defined as symmetry planes. In the following, the  
 457 associated thermal and mechanical boundary conditions, for the moving ingot simulation, are  
 458 summarized in Table 4.

Face position in Fig.4	Thermal boundary conditions	Mechanical boundary conditions	
		Fixed ingot (reference)	Moving ingot
① Left	Adiabatic	Sliding ( $\mathbf{v} \cdot \mathbf{e}_x = 0$ )	Sliding ( $\mathbf{v} \cdot \mathbf{e}_x = 0$ )
② Down	Flux by convection	Sticking ( $\mathbf{v} = \mathbf{0}$ )	Constant velocity ( $\mathbf{v} = -v_{cst}\mathbf{e}_z$ )
③ Right	Flux by convection	Sticking ( $\mathbf{v} = \mathbf{0}$ )	Constant velocity ( $\mathbf{v} = -v_{cst}\mathbf{e}_z$ )
④ Backward	Adiabatic	Sliding ( $\mathbf{v} \cdot \mathbf{e}_y = 0$ )	Sliding ( $\mathbf{v} \cdot \mathbf{e}_y = 0$ )
⑤ Forward	Adiabatic	Sliding ( $\mathbf{v} \cdot \mathbf{e}_y = 0$ )	Sliding ( $\mathbf{v} \cdot \mathbf{e}_y = 0$ )
⑥ Top	Adiabatic	Sticking ( $\mathbf{v} = \mathbf{0}$ )	Constant velocity ( $\mathbf{v} = -v_{cst}\mathbf{e}_z$ )

Table 4. Thermal and mechanical boundary conditions for the solidification test case

459 Heat is extracted from the metal through the right face and the bottom face using a convection-type  
460 expression for heat flux density,  $q_T = h_T(T - T_{ext})$ , where the heat transfer coefficient  $h_T$  and the  
461 external temperature  $T_{ext}$  are constant. The metal is supposed to slide along the surrounding faces  
462 except at the top, bottom and left faces, on which a constant velocity  $v_{cst}$  is imposed in the z-direction  
463  $\mathbf{e}_z$ . It should be reminded that the above-defined mechanical boundary condition is only applied in STEP  
464 II, as STEP I is over-simplified with solution  $\mathbf{v}_I$  predefined, equal to  $-v_{cst}\mathbf{e}_z$ , over the whole metal  
465 domain. Finally, note that for the reference simulation with fixed ingot, the energy boundary condition  
466 is the same as the above-detailed moving ingot simulation. For the mechanical boundary condition,  
467 sticking boundary condition is imposed on the top, bottom and left faces and all other faces are supposed  
468 to be purely sliding.

469 The initial temperature of the metal  $T_{ini}$  is chosen as the liquidus temperature  $T_L$ . Densities of the liquid  
470 and solid phases,  $\langle \rho \rangle^l$  and  $\langle \rho \rangle^s$ , are taken as constant and equal to the value at  $T_L$ ,  $\rho_L$ . Hence,  
471 solidification shrinkage is neglected and metal is assumed incompressible. Despite this assumption, in  
472 the momentum conservation equation relative to the liquid phase, the thermal convection in the liquid  
473 phase is taken into consideration by using the Boussinesq expression for the intrinsic liquid density:  
474  $\langle \rho \rangle^l = \rho_L (1 - \beta^l(T - T_L))$ , where  $\rho_L$  denotes the density of the liquid phase at the liquidus  
475 temperature and  $\beta^l$  the thermal dilatation coefficient of the liquid phase. In the specific context of this  
476 verification test case, the solidification path is considered in an oversimplified form, assuming that the  
477 volume fraction of the solid phase evolves linearly with temperature in the solidification interval.

478 The values of process, numerical, and material parameters used in this first test are summarized in Table  
479 5. Regarding material properties, they should be seen as representative of a carbon steel. As such, they  
480 are issued from different references and are simplified. For example, in this test, the thermal conductivity  
481 is assumed to be constant and equal for both the liquid and the solid phase. The latent heat of fusion is

482 also taken as constant. Nonetheless, two constant but different values are taken for the specific heat  
 483 capacity relative to liquid and solid phases.

Material parameters	Symbol	Value	Unit
Solidus temperature	$T_S$	1499	°C
Liquidus temperature	$T_L$	1552	°C
Densities	$\rho_L, \langle \rho \rangle^l, \langle \rho \rangle^s$	7060	$\text{kg} \cdot \text{m}^{-3}$
Thermal dilatation coefficient of liquid	$\beta^l$	$2.95 \times 10^{-4}$	$^{\circ}\text{C}^{-1}$
Secondary dendritic arm spacing	$\lambda_2$	$5 \times 10^{-4}$	m
Liquid viscosity	$\mu^l$	$4.2 \times 10^{-3}$	$\text{Pa} \cdot \text{s}$
Solid specific heat	$\langle C_p \rangle^s$	400	$\text{J} \cdot \text{kg}^{-1} \cdot ^{\circ}\text{C}^{-1}$
Liquid specific heat	$\langle C_p \rangle^l$	800	$\text{J} \cdot \text{kg}^{-1} \cdot ^{\circ}\text{C}^{-1}$
Thermal conductivity for solid and liquid phases	$\langle k \rangle^l, \langle k \rangle^s$	30	$\text{W} \cdot \text{m}^{-1} \cdot ^{\circ}\text{C}^{-1}$
Latent heat of fusion	$L_f$	$3.09 \times 10^5$	$\text{J} \cdot \text{kg}^{-1}$
Process and numerical parameters			
Initial temperature	$T_{ini}$	1552	°C
External temperature	$T_{ext}$	25	°C
Heat transfer coefficient	$h_T$	1000	$\text{W} \cdot \text{m}^{-2} \cdot ^{\circ}\text{C}^{-1}$
Downward moving velocity	$v_{cst}$	0.016167	$\text{m} \cdot \text{s}^{-1}$
Time step	$\Delta t$	0.1	s

Table 5. Values of material and numerical parameters used for the verification test case.

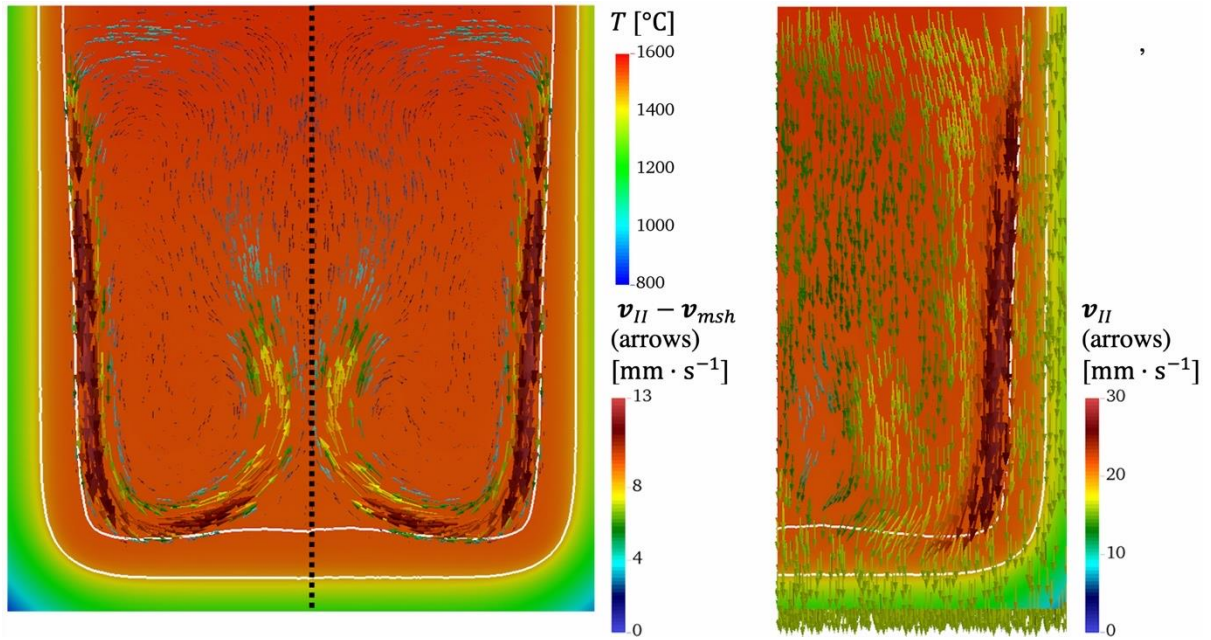
484

### 485 3.1.2 Results

486 **Fig. 5** illustrates the progress of the ingot solidification at time  $t = 40$  s. In **Fig. 5a**, results on the front  
 487 symmetry plane are shown, comparing the reference static ingot simulation (left half part of the figure)  
 488 and the moving ingot simulation (right half part). More precisely, the left part of **Fig. 5a** illustrates the  
 489 temperature field,  $T$ , and the fluid flow,  $\mathbf{v}_{II}$ , in the reference static ingot simulation. Note that the  
 490 velocity field can also be considered as  $\mathbf{v}_{II} - \mathbf{v}_{msh}$ , as  $\mathbf{v}_{msh}$  is indeed null in such a pure Eulerian  
 491 framework simulation. The right part of **Fig. 5a** describes the temperature field,  $T$ , and the relative fluid  
 492 flow,  $\mathbf{v}_{II} - \mathbf{v}_{msh}$ , for the moving ingot simulation in which  $\mathbf{v}_{msh} = -v_{cst} \mathbf{e}_z$  is imposed to the whole  
 493 computational mesh. It should be mentioned that the spatial positions of the two ingots are indeed  
 494 different, *i.e.* with a relative vertical distance difference. The two simulation results (separated by the  
 495 dotted black symmetric line) are put side by side in order to facilitate comparison.

496 It can be seen that, by eliminating the mesh velocity  $\mathbf{v}_{msh}$ , the same velocity field is found, which  
 497 corresponds in both simulations to the velocity induced by the thermal convection in the liquid phase.  
 498 Moreover, an identical temperature field is recovered in the moving ingot simulation compared to the  
 499 reference static ingot simulation. The liquidus and solidus isotherms, highlighted with white lines, are

500 perfectly connected on the (yz) symmetry plane. It is worth noting that in the moving ingot simulation,  
 501 energy transport relative to the solid phase is taken into consideration. The relative movement between  
 502 the solid and liquid phases is also considered. As shown in **Fig. 5b**, the velocity field  $\mathbf{v}_{II}$ , in the moving  
 503 simulation, is a mixture of the downward moving velocity and the thermal convection in the liquid phase.  
 504 It thus differs from the constant downward velocity,  $\mathbf{v}_I$ . Finally, note that as shown in **Fig. 5a**, the  
 505 amplitude of the fluid flow induced by convection is smaller than that of the constant downward  
 506 movement. This just fits in the fact for the presence of a global downward fluid flow is in **Fig. 5b**.



**Fig. 5.** Snapshot of solidification simulation showing (a) a comparison of the temperature field,  $T$ , and the relative fluid flow,  $\mathbf{v}_{II} - \mathbf{v}_{msh}$ , at time  $t = 40$  s, respectively in the reference static ingot simulation (left half part) and in the moving ingot simulation (right half part); (b) the velocity field  $\mathbf{v}_{II}$  associated with fluid flow in the moving ingot simulation. Liquidus and solidus isotherms are highlighted with white lines.

507

## 508 3.2 Application to continuous casting

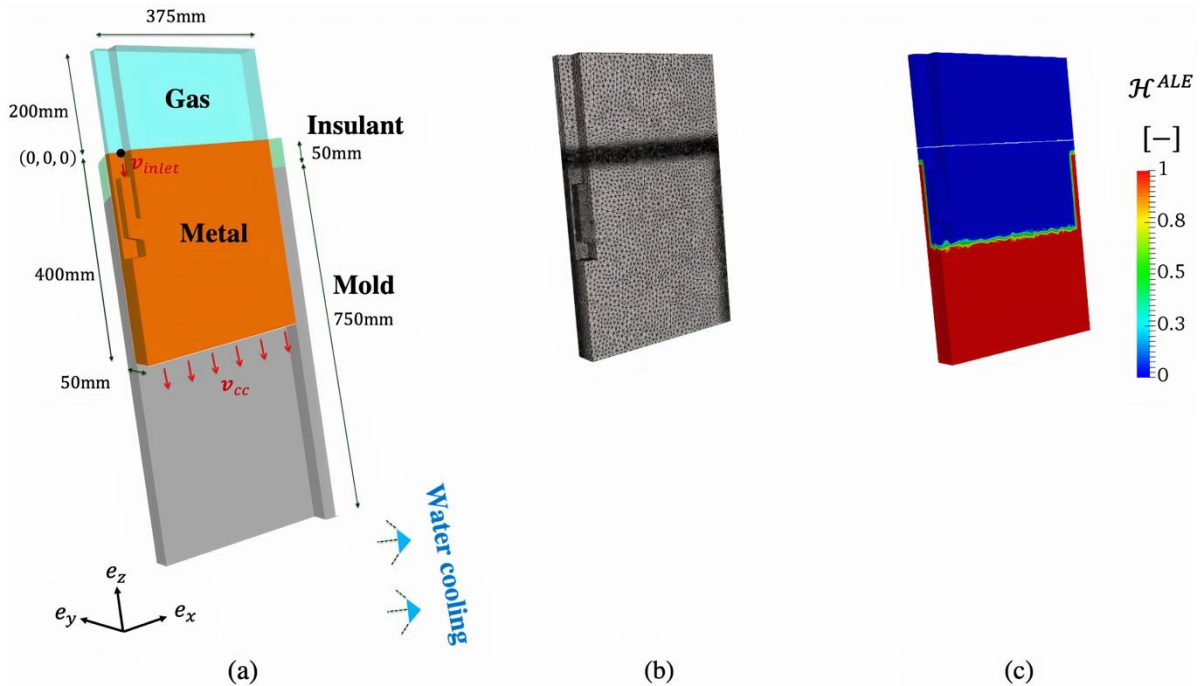
509 In this section, the application of the proposed two-step formulation to the simulation of an industrial  
 510 pilot CC process is proposed. This constitutes a preliminary step, for the present algorithm, before  
 511 addressing large and complex industrial CC processes. In particular, it intends to demonstrate its  
 512 capability to compute concurrently, in a quasi-industrial configuration, fluid flow and stress-strain in  
 513 the solid shell, in the mold region as well as in the secondary cooling zone.

514

### 515 3.2.1 Model description

516 The initial configuration of the model is given in **Fig. 6a**, with the consideration of a submerged entry  
 517 nozzle and the gas sub-domain. The cast product is a slab of thickness 100 mm and width 750 mm, the  
 518 primary cooling being operated by a mold of height 800 mm. Heat is extracted from the metal through  
 519 the lateral vertical surfaces (with normal  $\mathbf{e}_x$  and  $\mathbf{e}_y$ ). Constant flux is imposed along surfaces in contact

520 with the mold and a convection type expression is defined for flux associated with free surfaces located  
 521 below the mold exit in order to consider water cooling effect. It should be noticed that a small insulation  
 522 zone (50 mm) is imposed in the vicinity of the meniscus so as to always maintain a liquid-gas interface  
 523 in contact with the mold. The metal is supposed to slide vertically along the vertical surfaces. As  
 524 mentioned previously, although the mold is present in **Fig. 6a**, it is actually not explicitly modeled in  
 525 the simulation.



**Fig. 6.** Representation of (a) a schematic illustration of the 3D CC model at its initial configuration; (b) the associated initial mesh and (c) the constant Heaviside function,  $\mathcal{H}^{ALE}$ , defined in this simulation, assuring a smooth transition of mesh velocity between ALE and Eulerian zones.

526 A free velocity is considered on the upper surface of the simulation domain, allowing gas to flow in and  
 527 out freely. The surrounding faces of the entry nozzle are defined as sticking. The bottom surface of the  
 528 metal sub-domain is imposed with the constant vertical casting velocity  $v_{cc}$ . Moreover, another constant  
 529 vertical velocity  $v_{inlet}$  is imposed at the top surface of the entry nozzle, modeling the entry of the liquid  
 530 from the tundish to the mold region. The same mechanical boundary conditions as described above are  
 531 applied to both STEP I and STEP II, except for the surrounding vertical surfaces in contact with the  
 532 mold in STEP II. Along these surfaces, sticking boundary conditions are assumed, in order to reduce  
 533 numerical instabilities due to the presence of the intensive nozzle jet in contact with the mold.

534 Only a quarter of the full geometry is modeled considering the symmetry of the system. The initial mesh  
 535 is defined in **Fig. 6b**. Isotropic mesh with a constant mesh size of 10 mm is used over both the metal  
 536 and gas sub-domains except for two critical regions. First, in the 20 mm thick metal/gas transition zone,  
 537 the mesh is refined in an anisotropic manner with a mesh size of 1.5 mm in the vertical direction and 10  
 538 mm in the horizontal directions. An extra 20 mm thick transition zone is defined on each side of the  
 539 transition zone. This is done in order to ensure a smooth evolution of the mesh size between the transition  
 540 zone and the regions with isotropic coarse mesh size, thus reducing possible numerical instabilities due

541 to poor mesh quality in this critical region around the metal/gas boundary. Besides, for the metallic zone  
 542 in the vicinity of the mold, isotropic refined mesh is used, with a minimum mesh size of 4 mm, to ensure  
 543 a reliable stress-strain analysis in the very thin solid shell (on average, several centimeters thick in the  
 544 mold region). The number of mesh elements in the initial mesh as defined in **Fig. 6b** is about 640 000.  
 545 It is worth noting that the number of finite elements will keep increasing with a globally linear evolution  
 546 over time.

547 The related constant Heaviside function,  $\mathcal{H}^{ALE}$ , as introduced previously in Section 2.2, is shown in Fig.  
 548 6c. It is smoothed over a total thickness of 20 mm around the zero-isovalue, i.e. the green-colored line,  
 549 describing the boundary line between the ALE and Eulerian zones. Remind that it ensures the smooth  
 550 transition of the mesh velocity between these two zones. More precisely, the explicit definition of the  
 551 mesh velocity in the mushy and solid zones being given by Eq. (20), the mesh velocity over the whole  
 552 simulation domain writes  $\mathbf{v}_{msh} = \mathcal{H}^{ALE}(g^l \mathbf{v}_{cc} + g^s \mathbf{v}_I)$ .

553 The material properties are those of a 40CrMnMoS8-6 steel grade, as already documented in a previous  
 554 paper,<sup>[15]</sup> with several additional simplifications detailed below. Firstly, constant and equal densities are  
 555 taken for liquid and solid phases,  $\langle \rho \rangle^l = \langle \rho \rangle^s$  except in the momentum conservation equation of STEP  
 556 II where the density of the liquid phase follows the Boussinesq approximation,  $\langle \rho \rangle^l = \rho_L (1 -$   
 557  $\beta^l(T - T_L))$ , in order to model the thermal convection of the liquid phase. Besides, dilatation of the  
 558 solid phase is taken into consideration in the mass conservation equation of STEP I, such as  $\langle \rho \rangle^s =$   
 559  $\rho_S(1 - \beta^s(T - T_S))$  to allow a stress-strain analysis for the solid phase. Secondly, constant specific  
 560 heat is assumed for both solid and liquid phases. The latent heat of fusion is also taken as constant. Note  
 561 that the solidification path as well as the mechanical properties relative to the constitutive laws of solid  
 562 are kept as the same as in reference [15]. Finally, values of the material properties used together with  
 563 simulation parameters are summarized in Table 6. It should be mentioned that properties of the gas are  
 564 oversimplified in the current simulation in order to reduce possible numerical instabilities at the  
 565 metal/gas boundary. Nonetheless, these simplifications have almost no effect in the main focus of this  
 566 simulation, *i.e.* the concurrent fluid flow and stress-strain analyses in the metal sub-domain.

Material parameters	Symbol	Value	Unit
Solidus temperature	$T_S$	1431	°C
Liquidus temperature	$T_L$	1490.5	°C
Specific heat of solid and liquid	$\langle C_p \rangle^l, \langle C_p \rangle^s$	800	$J \cdot kg^{-1} \cdot ^\circ C^{-1}$
Specific heat of gas	$C_p^G$	1000	$J \cdot kg^{-1} \cdot ^\circ C^{-1}$
Latent heat of fusion	$L_f$	$2.4 \times 10^5$	$J \cdot kg^{-1}$
Metal density	$\rho_L, \rho_S, \langle \rho \rangle^l, \langle \rho \rangle^s$	7000	$kg \cdot m^{-3}$
Gas density	$\rho^G$	6000	$kg \cdot m^{-3}$
Thermal dilatation coefficient of liquid	$\beta^l$	$1 \times 10^{-4}$	$^\circ C^{-1}$
Thermal dilatation coefficient of solid	$\beta^s$	$1 \times 10^{-5}$	$^\circ C^{-1}$
Secondary dendrite arm spacing	$\lambda_2$	$5 \times 10^{-4}$	m
Gas viscosity	STEP I   STEP II $\mu^G$	1   $1 \times 10^{-1}$	$Pa \cdot s$
Liquid viscosity	STEP I   STEP II $\mu^l$	1   $5 \times 10^{-3}$	$Pa \cdot s$
Thermal conductivity in liquid	$\langle k \rangle^l$	30	$W \cdot m^{-1} \cdot ^\circ C^{-1}$
Thermal conductivity in solid	$\langle k \rangle^s$	30	$W \cdot m^{-1} \cdot ^\circ C^{-1}$
Thermal conductivity in gas	$k^G$	0.1	$W \cdot m^{-1} \cdot ^\circ C^{-1}$
Simulation parameters	Symbol	Value	Unit
Casting temperature		1520.5	°C
External temperature	$T_{ext}$	25	°C
Constant flux at narrow face		$8 \times 10^5$	$W \cdot m^{-2}$
Constant flux at wide face		$1.2 \times 10^6$	$W \cdot m^{-2}$
Heat transfer coefficient at narrow face		1100	$W \cdot m^{-2} \cdot ^\circ C^{-1}$
Heat transfer coefficient at wide face		150	$W \cdot m^{-2} \cdot ^\circ C^{-1}$
Time step	$\Delta t$	0.1	s
Casting velocity in the vertical direction	$\mathbf{v}_{cc} \cdot \mathbf{e}_z$	-0.015	$m \cdot s^{-1}$
Liquid inlet velocity in the vertical direction	$\mathbf{v}_{inlet} \cdot \mathbf{e}_z$	-0.88	$m \cdot s^{-1}$

Table 6. Simulation and material parameters in the 3D CC test case. Non-listed material properties can be found in Reference [15].

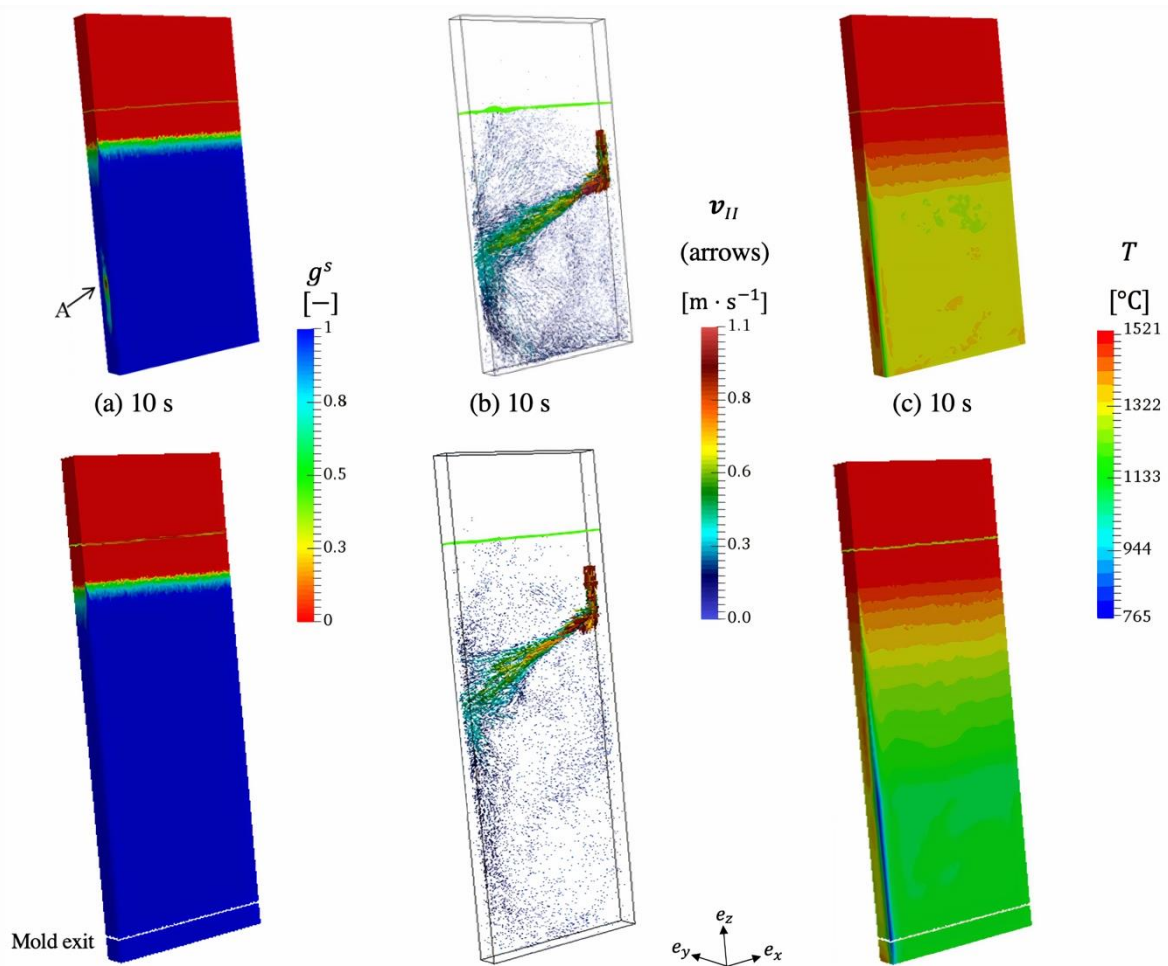
567

### 568 3.2.2 Results

569 **Fig. 7** illustrates the non-steady regime of the simulation through the distribution of solid fraction,  
570 velocity vectors and temperature, respectively at times  $t = 10$  s and  $t = 30$  s. The metal/gas boundary  
571 is represented by the green surface. As shown in **Fig. 7a**, after 10 s of solidification process, a solid shell  
572 has already formed along both the narrow and wide cooling faces. However, it is worth noting that on  
573 the narrow face, an unsolidified area is present with a slender oval shape (position A). The formation  
574 mechanism of this particular area is indeed a conjugate effect of the initial modeling configuration (the  
575 simulation is started with a metal sub-domain in fully liquid state) and of the impact from the hot nozzle



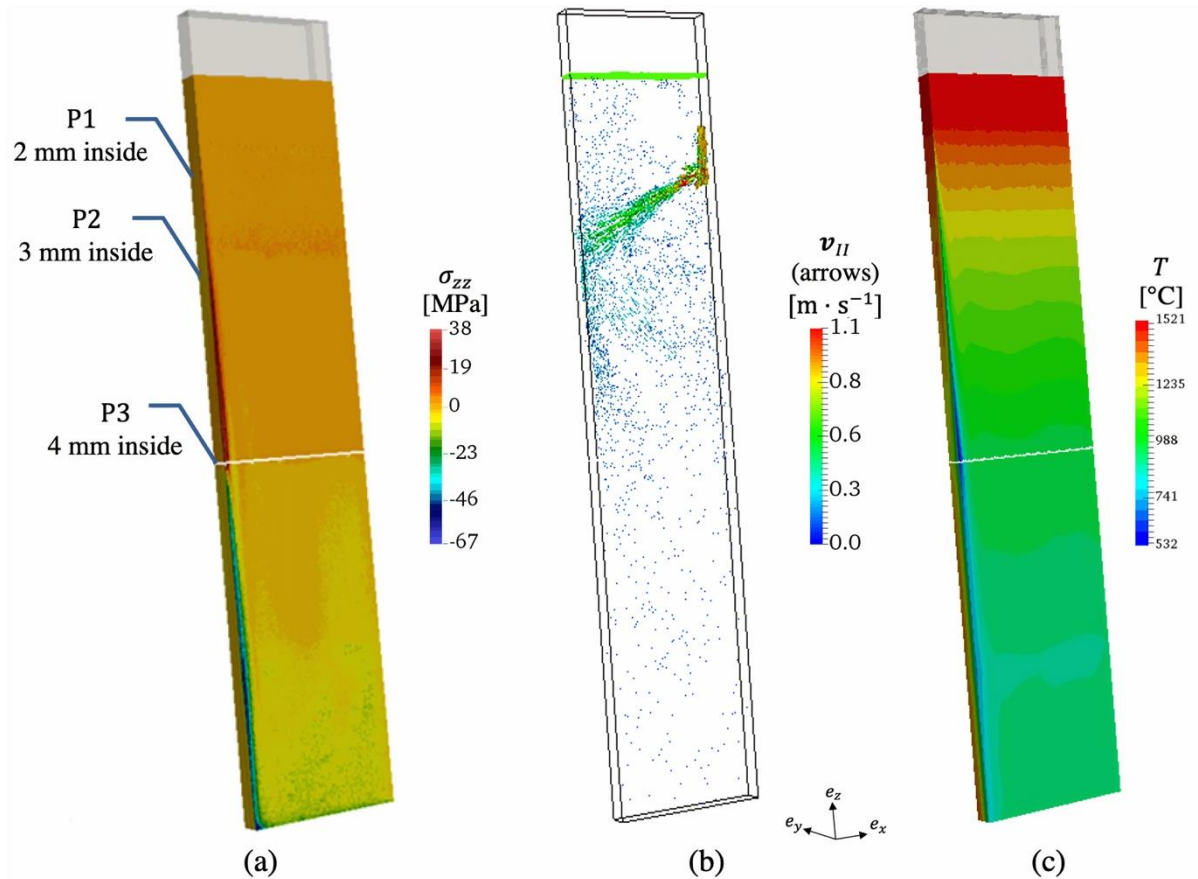
576 jet onto the mold region. More precisely, as shown in **Fig. 7b**, at time 10 s, a main intense flow can be  
 577 observed in the mold region due to the injected flow from the nozzle entry. This nozzle jet is split into  
 578 two vortices when it meets the narrow face, with one in the upward direction and another in the  
 579 downward direction. As it can be seen by comparing **Fig. 7a** and **Fig. 7b**, the unsolidified area labeled  
 580 A is located at the impingement zone of the main fluid flow on the narrow face. By consequence, starting  
 581 from a fully liquid state, this hot jet impingement delays the formation of the mushy zone, as well as the  
 582 solid shell, on this particular area, at an early stage of the solidification process. The temperature field,  
 583 at this time  $t = 10$  s, is shown in **Fig. 7c**. It can be seen that there is an impact of the fluid flow on the  
 584 solidification process. Especially on the narrow face, the temperature of the impingement zone remains  
 585 hottest, compared to its neighboring areas, with consequence on the distribution of the solid on the  
 586 narrow face already previously commented.



**Fig. 7.** Results for  $g^s$ ,  $v_{II}$  and  $T$  respectively at time  $t = 10$  s with (a) the distribution of solid fraction along the domain boundary, (b) the velocity vectors throughout the domain, (c) the temperature field along the product surface. The same fields at time  $t = 30$  s are shown on the bottom line: figures (d) to (f).

587 **Fig. 7d** shows the solid fraction at time  $t = 30$  s, when the metal sub-domain has just exited the mold  
 588 region (the mold exit is represented by the white line). It can be seen that the unsolidified area labeled  
 589 A in **Fig. 7a** has disappeared. This expresses the fact that the casting conditions are sustainable, without

590 major risk of liquid leakage at the exit of the mold. However, it is worth noting that, as shown in **Fig.**  
 591 **7e**, the direction and magnitude of the main fluid flow in the mold region are nearly the same as that at  
 592 time  $t = 10$  s. By consequence, the impingement area keeps being located approximately at position A.  
 593 Although the unsolidified area is no more present on the narrow cooling face at time  $t = 30$  s, the impact  
 594 of the fluid flow remains significant, and a permanent stabilized hot spot exists. **Fig. 7f** shows the  
 595 temperature field at time  $t = 30$  s. It can be seen that the solid shell in the impingement area, is hotter  
 596 than in the surrounding area.

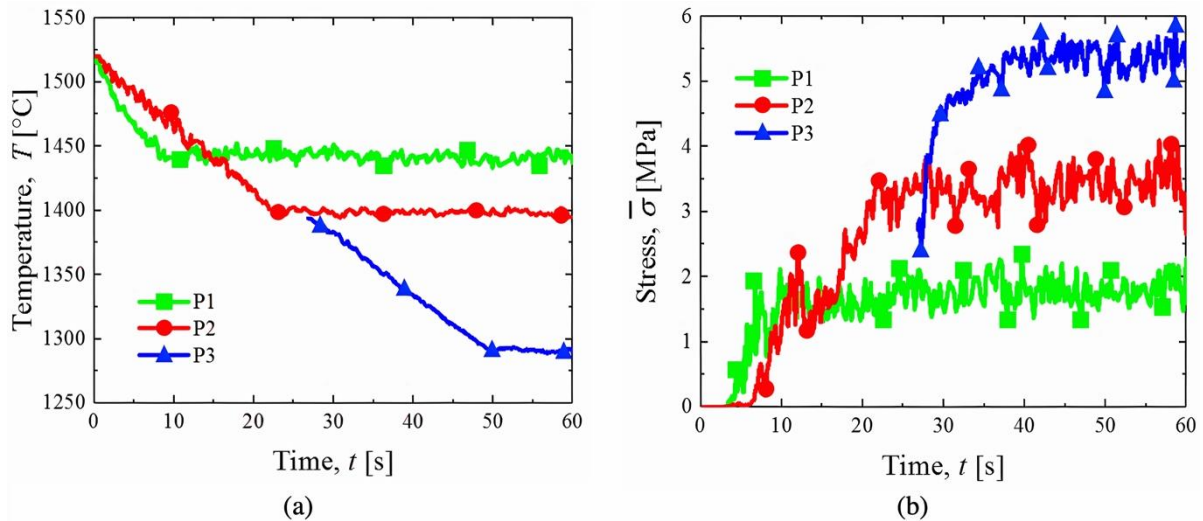


**Fig. 8.** Results at time  $t = 80$  s, showing (a)  $\sigma_{zz}$ , the longitudinal stress along the cooling faces with the white line representing the mold exit; (b) The fluid flow (arrows,  $v_{II}$ ) with the presence of the nozzle jet; (c) The temperature field along the cooling faces.

597 **Fig. 8** illustrates the results corresponding to time  $t = 80$  s. The longitudinal (vertical) stress component  
 598  $\sigma_{zz}$  along the external cooling faces of the product is shown in **Fig. 8a**, revealing that the solid shell is  
 599 under traction within the mold region, in particular along the edge, while in compression after the mold  
 600 exit, with maximum values reaching respectively 38 MPa and -67 MPa. The fluid flow is concurrently  
 601 computed, represented by colored arrows in **Fig. 8b**. The length and color of arrows are related to the  
 602 vector magnitude. It can be seen that the fluid flow is intensive in the mold region and slows down when  
 603 reaching the mold exit. **Fig. 8c** shows the temperature field over the two cooling faces. Because heat  
 604 extraction in secondary cooling is much lower than in the mold region, a minimum of temperature along  
 605 the edge is found at the mold exit (here 532  $^{\circ}C$ ). It is worth noting that the extra-cooling along the edge  
 606 of the product is indeed overestimated with respect to the real industrial process. This is because the

607 formation of an air gap between the product and the mold is not under consideration in the present model.  
 608 The presence of such an air gap has an important influence on heat extraction in the vicinity of the corner,  
 609 i.e. slowing down the cooling process and thus resulting in higher values of temperature in this region  
 610 than calculated here.<sup>[26]</sup>

611 It is then interesting to investigate when the steady-state regime is reached in the present non-steady  
 612 simulation. For this specific purpose, three fixed observation points are defined at positions  $(x, y, z) =$   
 613  $(373, 0, -200)$ ,  $(372, 0, -400)$  and  $(371, 0, -800)$  with units in mm. They are respectively denoted as P1,  
 614 P2 and P3 and their locations can be seen in **Fig. 8a**. Remind that the  $(0, 0, 0)$  position is located at the  
 615 metal/gas nominal interface, at the intersection between the two vertical symmetry planes, as shown in  
 616 **Fig. 6a** (black dot). All three fixed positions are in the mold region, in the vicinity of the middle of the  
 617 narrow cooling face. Position P3 is located exactly in the transversal cross section at the mold exit, 4  
 618 mm deep in the thickness of the solid shell. Calculated evolutions of the temperature and the von Mises  
 619 stress at these predefined positions are recorded during 60 s and plotted in **Fig. 9**.



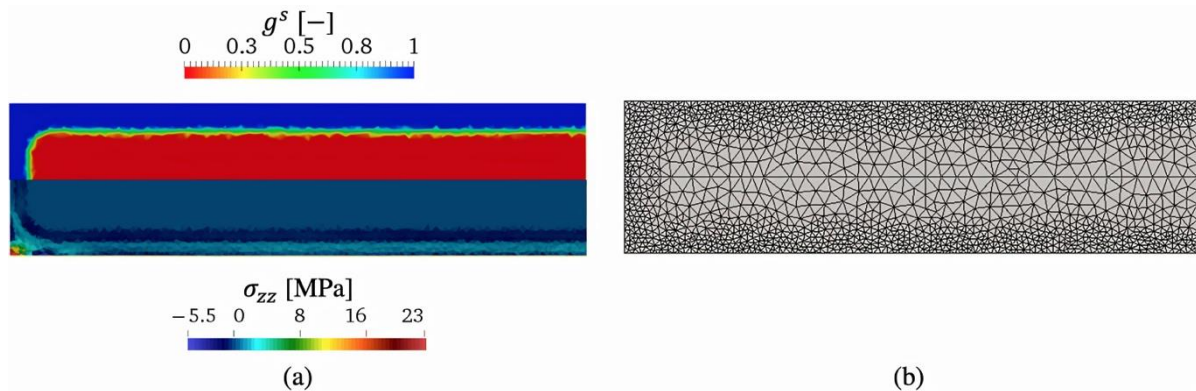
**Fig. 9.** Evolution of temperature  $T$  (left), and von Mises stress  $\bar{\sigma}$  (right) at three fixed locations P1, P2 and P3, defined in **Fig. 8a**.

620 It can be noted that for position P3, results are available only after about 25 s of simulation, as shown  
 621 by the blue colored lines in **Fig. 9**. This is because position P3 is outside the initial simulation domain,  
 622 as defined in **Fig. 6a**: it is then reached after a certain process time  $\Delta z/v_{cc} = 400/15 = 26.7$  s in the  
 623 present non-steady state approach. Conversely, the other two positions are located at the initial metal  
 624 sub-domain and thus results are available from the beginning.

625 It can be seen that the steady-state regime is reached within the entire mold region after about 50 s,  
 626 either from the thermal point of view (**Fig. 9a**) or from the mechanical point of view (**Fig. 9b**). As P3 is  
 627 the lower position in the mold it is also the last one to stabilize. After this position has been attained by  
 628 the growing computational mesh, it can be observed that it requires about 23 s to reach a steady state,  
 629 which is indeed a short process time, corresponding only to a casting length of 345 mm. Let us note  
 630 however that reaching the steady state would be longer if the heat transfer within the mold would be

631 considered in the simulation (instead of a constant imposed heat flux here). It is also interesting to note  
 632 that the mechanical steady-state regime is reached almost at the same time as the thermal steady-state  
 633 regime, for all three points. This is coherent with the boundary conditions prescribed along the cooling  
 634 faces, where only vertical displacement is allowed and the cooling faces cannot separate from the mold.  
 635 Thus, under this assumption, there is no coupling feedback from the mechanical simulation toward the  
 636 thermal simulation. Finally, one observes that steady state is in fact not perfect, all evolution curves  
 637 being affected by some perturbations. These perturbations are indeed inherent to the non-steady state  
 638 simulation. Actually, during the simulation, the mobile mesh passes by the different fixed positions. The  
 639 calculated value at a certain process time and for a selected position depends on the local spatial  
 640 interpolation which can be done at that precise moment. These fluctuations tend to increase with the  
 641 local mesh size, and with the local gradient of the interpolated solution fields. This is why fluctuations  
 642 are more visible for stress evolution (high gradients, see also hereunder) than for temperature evolution  
 643 (lower gradients).

644 **Fig. 10a** illustrates the solid fraction and the stress component in  $z$ -direction ( $\sigma_{zz}$ ) over the cross section  
 645 at mold exit, at time = 80 s, after the steady-state regime is achieved in the whole mold region.

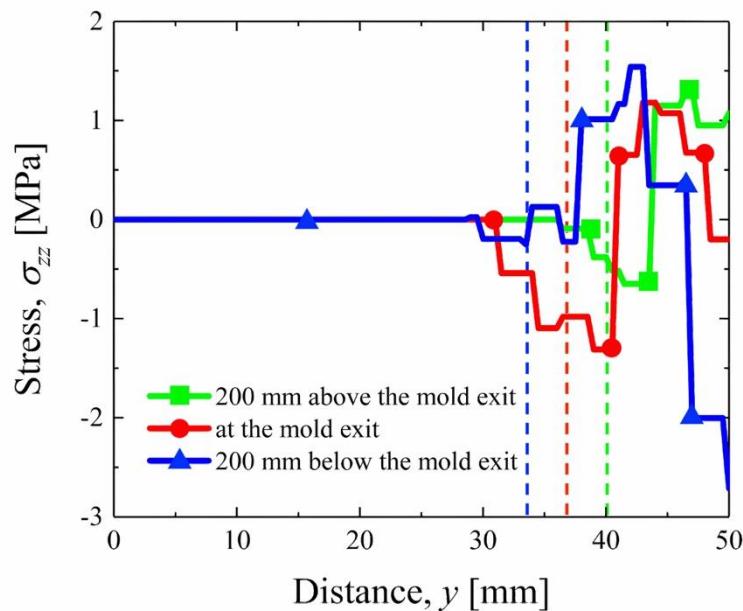


**Fig. 10.** (a) distribution of solid fraction  $g^s$  (top half of the figure), and of the stress component in the  $z$  direction  $\sigma_{zz}$  (bottom half of the figure) at time  $t = 80$  s in the transverse cross-section at mold exit; (b) section of the mesh over this cross-section in a 2D configuration.

646 First, it can be seen that a solid shell with thickness about 15 mm is formed on the wide cooling face.  
 647 Given the intensity of the extracted fluxes, of the order of  $1 \text{ MW m}^{-2}$ , this result is as expected. It  
 648 compares well, for instance, with experimental measurements published by Thomas *et al.*,<sup>[28]</sup> and with  
 649 associated numerical simulations performed by Pfeiler *et al.*,<sup>[29]</sup> based on similar casting conditions. The  
 650 slab format of the pilot machine studied here having a thin thickness, approximately one third of the  
 651 product is solidified at mold exit. It can also be seen that the corner of the cooling faces is submitted to  
 652 a high tensile stress, with a maximum value reaching 23 MPa, whereas the solidification front undergoes  
 653 smaller compression stress. Nonetheless, it should be mentioned that this maximum predicted value  
 654 might be unrealistic as the cooling faces are highly constrained (the velocity along faces is imposed to  
 655 be vertical). Finally, note that a simple remeshing strategy is adopted to ensure a correct implementation  
 656 of the above stress-strain analysis in such thin solid shell. **Fig. 10b** illustrates the corresponding  
 657 equivalent mesh over the whole cross-section. It is worth noting that the exact presentation of the mesh

658 in such a cross-section of the 3D geometry would be unintelligible. This is why an equivalent 2D mesh  
 659 has been drawn, with local size corresponding to the 3D mesh size. Being aware of this simplification,  
 660 it can be seen that the mesh is refined close to the cooling faces, providing a sufficient number of  
 661 elements to describe the stress gradient through the thickness of the solid shell.

662 In order to get a clearer insight of the stress developed in the solid shell, **Fig. 11** illustrates the stress  
 663 profiles,  $\sigma_{zz}$ , over the half-thickness of the product, at three different locations in the ( $yz$ ) symmetry  
 664 plane. These profiles are then perpendicular to the wide face, respectively at 200 mm above the mold  
 665 exit (green line, square symbols), at the mold exit (red line, dots) and 200 mm below the mold exit (blue  
 666 line, triangles). The  $y$  coordinate varies from 0 (central core of the product) to 50 mm (center of the  
 667 wide cooling face). The associated solidus position of each profile is represented by the dotted lines as  
 668 shown in **Fig. 11**.



**Fig. 11.**  $\sigma_{zz}$  stress profile through the thickness in the transverse symmetry plane at time 80 s, respectively at three different locations, 200 mm above the mold exit, at the mold exit and 200 mm below the mold exit. The dotted lines represent locations of the solidus, associated with each stress profile.

669 It can be seen that above the mold exit, the vertical stress along the wide cooling face (at  $y = 50$  mm in  
 670 **Fig. 11**) is tensile. Nonetheless, about half of the solid shell near the cooling face is still under  
 671 compression, expressing the necessary mechanical equilibrium along the vertical direction. At the mold  
 672 exit, the vertical stress on the wide cooling face starts to shift from tensile to slightly compressive, while  
 673 the vertical stress at the solidification front is still compressive. Below the mold exit, the vertical stress  
 674 along the wide cooling face becomes fully compressive, and by consequence, a global tensile stress is  
 675 obtained deeper in the solid shell. It is worth noting that for both three locations, the part of the mushy  
 676 zone with higher solid fractions, close to the solidus, is always submitted to a vertical compressive stress.  
 677 Finally, as expected, all vertical stresses recover to zero when they reach the fully liquid regions. Note



678 that both the evolution of the stress profile along the vertical direction and the stress level are in  
679 agreement with other simulation results obtained by either Risso *et al.*,<sup>[30]</sup> or Zappulla *et al.*,<sup>[31]</sup> for  
680 similar slab casting configurations.

681

## 682 **4 Conclusions**

683 A new partitioned solution algorithm has been developed to simulate steel CC processes, as an extension  
684 of a former two-step algorithm initially developed for ingot casting application.<sup>[15]</sup> This new algorithm  
685 allows a concurrent computation of fluid flow in the liquid and mushy regions, and stress-strain in the  
686 solid, in the context of a non-steady state simulation of CC processes. The algorithm consists of a  
687 partitioned solution strategy, to calculate, at each time increment, a solid-oriented solution, a fluid-  
688 oriented solution, and a coupled thermal solution. The three specific features of this new solution  
689 algorithm, which have been specially developed to simulate CC processes, are the followings:

- 690 • A global non-steady-state approach allows simulating the transient regime up to the convergence to  
691 the steady state regime. For this, the computational mesh continuously moves and grows, in  
692 accordance with the imposed extraction speed.
- 693 • This evolving mesh is partitioned in three regions: the solid shell, which is treated as a pure  
694 Lagrangian zone; the liquid nozzle region as a pure Eulerian zone; and an intermediate Eulerian-  
695 Lagrangian zone.
- 696 • The three solution steps (liquid-oriented mechanics, solid-oriented mechanics, and heat transfer),  
697 are performed sequentially for each time step on the same global mesh. For each solution step,  
698 conservation equations are solved in a general arbitrary Lagrangian-Eulerian (ALE) framework,  
699 with a level-set formulation to track the free surface evolution at the meniscus.

700 The correct implementation of this algorithm was firstly checked through a simple verification test case.  
701 It was then applied to a 3D pilot CC process. Simulation gave promising results, in which fluid flow in  
702 the bulk liquid or mushy zone and stress formed in the solid regions were concomitantly computed.

703 The main perspectives of this work are twofold. Firstly, coupling this new algorithm with  
704 macrosegregation modeling would allow demonstrating the influence of solid deformation on central  
705 macrosegregation in CC processes.<sup>[11]</sup> Secondly, the coupling with equiaxed grain motion would provide  
706 access to enhanced predictions of macrosegregation due to thermo-solutal convection, shrinkage flow  
707 and transport of equiaxed grains.<sup>[27]</sup>

708

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