Three dimensional simulation of macrosegregation in steel billets by a meshless method

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Abstract. There is a continuously developing need for benchmarking of solidification simulations - from the theoretical as well as from the applied points of view. The history of related benchmarking shows differences of the results between different numerical methods, and differences in comparison with the experiments when solving even quite simple solidification situations. The present benchmark test proposes a three dimensional version of the recently developed two dimensional solidification benchmark of the continuous casting with turbulent fluid flow and solidification with macrosegregation. The macroscopic transport equations for mass, momentum, energy, species, turbulent kinetic energy and dissipation rate are considered. Turbulent effects are incorporated through the solution of a low-Re turbulence model. The solidification system is treated by the mixture-continuum model, where the mushy zone is modeled as a Darcy porous media with Kozeny-Karman permeability relation and columnar solid phase moving with the casting velocity. The Fe-C binary phase diagram and the lever rule microsegregation model are used to obtain the carbon segregation in the billet. The transport equations are solved by our newly developed and efficient meshless numerical technique, based on local collocation with radial basis functions and fractional step velocity-pressure coupling. The presented results represent first simulations of a three-dimensional solidification problem by a meshless method.

1. Introduction

Continuous casting [1] is the most common process in the production of steel. The process starts by pouring the molten metal into the water cooled mold, where cooling intensity is high enough to solidify steel around the inner surface of the mold and generates the solid shell with molten metal in the center of strand. After several minutes, the strand is pulled into the secondary cooling system, which contains water spray systems with much smaller cooling intensity as in the water channels in the mold, and rollers, which support and guide the strand up to the end of the casting machine. The quality of the casted product (round or square billets, blooms or slabs) depends mainly on the process parameters in the mold region, where complex physical phenomena occur. The liquid metal, poured with a high velocity from the submerged entry nozzle (SEM) into the mold, produces turbulent flow with several re-circulating zones. Large heat fluxes, extracted from the mold, are a consequence of very high flow rates of the cooling water in the mold channels. It is impossible to measure temperature, velocity field and macrosegregation [2] inside the strand due to the very high
temperatures of steel and inaccessibility of the region during the process. The numerical models [3, 4] help us to better understand the casting behavior and to further improve and optimize the process, particularly in such experimentally sophisticated situations. Various numerical methods have already been used to simulate the described spectra of problems [5, 6, 7, 8, 9]. However, until now, there is a lack of benchmark tests that would enable verification of numerical methods for solving transport phenomena in continuous casting of steel in an ordered way. We recently tried to fill this gap with proposing a first such benchmark [10, 11]. In these papers, the two dimensional turbulent heat transfer, fluid flow, and species transfer solidification discussion in [12] is upgraded to three dimensions. The main aim of the test is to get new reference results and to be able to further compare the results of different numerical methods for the same physical model. The presented physical model considers turbulent fluid flow and macrosegregation of carbon steel. Turbulent flow is modeled by the two-equation eddy-viscosity model with the low-Re corrections. The numerical results are shown for the case with lever microsegregation model of 0.55 wt%C steel. The novel meshless Local Radial Basis Function Collocation Method (LRBFCM) is employed for solving the coupled system of six partial differential equations in three dimension. The main aim of the test is to get new reference results and to be able to further compare the results of different numerical methods for the same physical model. The presented physical model considers turbulent fluid flow and macrosegregation of carbon steel. Turbulent flow is modeled by the two-equation eddy-viscosity model with the low-Re corrections. The numerical results are shown for the case with lever microsegregation model of 0.55 wt%C steel. The novel meshless Local Radial Basis Function Collocation Method (LRBFCM) is employed for solving the coupled system of six partial differential equations in three dimension. The objective of the present paper is to produce a first reference numerical solution of the given problem. LRBFC was first developed in [13] for diffusion problems, to convection diffusion problems in [14], and to driven cavity and natural convection problems in [15, 16]. The turbulence was tackled in [17, 18]. The melting benchmark [19] was successfully solved in [20] and the macrosegregation benchmark [3] in [21, 22]. The magneto-hydrodynamic effects were tackled in [23] for natural convection in a cavity and in [24] for backward facing step situation.

2. Governing equations

The system of equations, describing the coupled transport phenomena in the continuous casting of steel, is derived based on the mixture continuum formulation by Bennon and Incropera [25] and Reynolds time-averaging approach for modelling incompressible turbulent flow [26]. The time-averaged transport equations for mass, energy, momentum and solute conservation are

\[ \nabla \cdot \mathbf{u} = 0, \]

\[ \frac{\partial \mathbf{u}}{\partial t} + \rho \nabla \cdot (\mathbf{u} \mathbf{u}) = -\nabla P + \nabla \left[ 2(\mu + \mu_t) \mathbf{S} \right] - \frac{2}{3} \rho \nabla k - \mu_t \frac{K_0(1-f_s^2)}{f_s^3} (\mathbf{u} - \mathbf{u}_s) + \mathbf{F}_b, \]  \( \text{(2)} \)

\[ \rho \frac{\partial h}{\partial t} + \rho \nabla \cdot (\mathbf{u} h) = \nabla \cdot (\lambda \nabla T) + \rho \nabla \left[ f_s (h_l - h_s) (\mathbf{u} - \mathbf{u}_s) \right] + \nabla \cdot \left( f_t \frac{\mu}{\sigma_r} \nabla h_l \right), \]  \( \text{(3)} \)

\[ \rho \frac{\partial C}{\partial t} + \rho \nabla \cdot (\mathbf{u} C) = \nabla \cdot (f_s D_s \nabla C_s + f_t D_t \nabla C_t) + \rho \nabla \cdot \left[ (\mathbf{u} - \mathbf{u}_s) (C_l - C) \right] + \nabla \cdot \left( f_t \frac{\mu}{\sigma_c} \nabla C_l \right), \]  \( \text{(4)} \)

with \( \mathbf{u} \), \( P \), \( h \), \( T \) and \( C \) for velocity, pressure, enthalpy, temperature and solute concentration, respectively, and \( \rho \), \( \mu \), \( \mu_t \), \( f \), \( \lambda \), \( D \) are standing for density, molecular dynamic viscosity, turbulent dynamic viscosity, volume phase fraction, thermal conductivity, and diffusivity of the material. In above equations, subscripts \( L \) and \( S \) denote liquid and solid phase. \( \mathbf{S} \) stands for the strain-rate tensor. The fourth term on the right hand side of equation (2) represents the Darcy term, where \( K_0 \) is the morphology constant of the porous medium and \( \mathbf{u}_s \) is velocity of the solid phase. The fifth term on the right hand side of equation (2) represents the buoyancy forces, defined as

\[ \mathbf{F}_b = \rho \left[ \beta_T (T - T_{ref}) + \beta_C (C_l - C_{ref}) \right], \]  \( \text{(5)} \)
where $\beta_T$, $\beta_C$, $T_{ref}$ and $C_{ref}$ stand for thermal expansion coefficient, solute expansion coefficient, reference temperature and reference concentration, respectively. The turbulent dynamic viscosity is defined as $
u = \rho \mu_\mu f_\mu f_\mu^2/\varepsilon$, where $k$ and $\varepsilon$ are kinetic energy and dissipation rate, respectively. They are calculated by the following transport equations

$$
\rho \frac{\partial k}{\partial t} + \rho \mathbf{v} \cdot (\mathbf{u} k) = \nabla \cdot \left[ \left( \frac{\mu_s + \frac{\mu_t}{\sigma_s}}{\sigma_s} \right) \nabla k \right] + P_k - \rho \varepsilon + \rho D + \mu_L \frac{K_0 (1 - f_L^2)}{f_L^3} k ,
$$

(6)

$$
\rho \frac{\partial \varepsilon}{\partial t} + \rho \mathbf{v} \cdot (\mathbf{u} \varepsilon) = \nabla \cdot \left[ \left( \frac{\mu_s + \frac{\mu_t}{\sigma_s}}{\sigma_s} \right) \nabla \varepsilon \right] + \rho (c_{z_1} f_i - c_{z_2} f_i \varepsilon) \frac{\varepsilon}{k} + \rho E + \mu_L \frac{K_0 (1 - f_L^2)}{f_L^3} \varepsilon .
$$

(7)

In equations (3,4,6,7) $c_\mu$, $f_\mu$, $c_{z_1}$, $f_1$, $c_{z_2}$, $f_2$, $\sigma_t$, $\sigma_c$, $\sigma_k$ and $\sigma_\varepsilon$ are the closure coefficients, while $D$ and $E$ are additional source terms of the low-Reynolds turbulent model [26]. The constitutive temperature-enthalpy relationship $h_3$ and $h_e$ in equation (3) are defined as

$$
h_k = \int_{t_0}^t c_{ps} dT , \quad h_L = \int_{t_0}^T c_{ps} dT + \int_{t_0}^T c_{ps} dT + h_m = h_3 (T) + \int_{t_0}^T (c_{ps} - c_{ps}) dT + h_m ,
$$

(8,9)

respectively. The liquid fraction $f_L$, concentration of solute in liquid phase $C_L$, partition ratio $k_p$, and liquidus temperature $T_L$ are determined based on the level rule microsegregation model, i.e.

$$
f_L = 1 - \frac{1}{1 - k_p} \frac{T - T_L}{T - T_m} , \quad C_L = \frac{C}{1 + f_L (k_p - 1)} , \quad k_p = \frac{C_s}{C_e} , \quad T_L = T_m + (T_e - T_m) \frac{C}{C_e} ,
$$

(10,11,12,13)

where $T_m$, $T_e$ and $C_e$ are melting temperature, eutectic temperature and solute concentration in eutectic alloy, respectively. They are obtained from the phase diagram for the iron-carbon system.

### 3. Solution procedure

Our solution procedure is based on the novel meshless technique that follows the following steps. We seek the solution of the equations for the velocity, pressure, temperature, concentration, turbulent kinetic energy, and dissipation at time $t + t_0$ by assuming known fields $u$, $p$, $T$, $C$, $k$, and $\varepsilon$ at time $t_0$ and known boundary conditions at time $t > t_0$. The coupled set of mass conservation equation (1) and momentum conservation equations (2) are solved by the fractional step method [27], where the continuity of the mass (1) is considered by constructing the pressure Poisson’s equation. The governing equations are discretized by using the explicit time discretization. This leads to the following algorithm, summarized through the following 7 steps: (I) The intermediate velocity components are calculated without the pressure gradient, (II) the pressure Poisson equation is treated, (III) the velocity components are corrected by the pressure gradient, (IV), after the solution of the velocity field, the transport equation (3) for energy is solved, (V) the temperature field is calculated from the enthalpy field, calculated in previous step, using the inverse of the constitutive temperature-enthalpy relationships (8,9), i.e. $T = T(h)$, (VI) species concentration (4), turbulent kinetic energy (6) and dissipation rate (7) fields are calculated, and finally (VII) the turbulent viscosity, solute concentrations (11,12) and liquidus temperature (13), are updated for each node and the solution is set ready for the next time step. All derivatives of the transport equations are calculated by the LRBFCM [12], where the collocation is made locally on overlapped sub-domains. On each sub-domain, the scalar function $\Phi$ (standing for temperature, species concentration, velocity components, pressure, turbulent kinetic energy, and turbulent dissipation rate) is represented over a set of (in general) non-
equally spaced nodes $p_i; n = 1, 2, \ldots, N$ in the following way $\Phi(p) \approx \sum_{k=1}^{K} \psi_k(p) \alpha_k$, $\psi_k(p) = \left[r_i^2 + c^2\right]^{1/2}$, where $\psi_k$ stands for the multi-quadric radial basis shape functions [28], $\alpha_k$ for the coefficients of the shape functions, $K$ the number of the shape functions, $c$ the shape parameter, and $r_i$ the radial distance between two points in the sub-domain. The detailed procedure of calculating the derivatives with the LRBFCM can be found in [3]. Seven subdomain nodes are used in three dimensions.

4. Description of CC case

Geometry: The geometry represents a simplified 3D model of the continuous casting process. The geometry of the simplified casting machine is shown in figure 1. A billet with a square cross-section is assumed. The computational domain represents a quarter of the longitudinal section of the billet with length 1.15 m, shown in figure 2. The dimensions of the casting geometry are billet width $a_b = 0.18$ m, diameter of the SEN $d = 0.035$ m and mold height $l_m = 0.8$ m, respectively.

Material properties: Generally, the material properties of steel are temperature dependent. However, in this work, constant values are used for each phase. They are given in table 1.

| $\rho$ (kg/m$^3$) | $\xi_p$ (J/kg K) | $\lambda$ (W/m K) | $\mu$ (kg/m s) | $T_{\text{liq}}$ (K) | $T_{\text{sol}}$ (K) | $h_m$ (J/kg) | $K_0$ (W/m K) | $k_p$ (l) |
|-------------------|-------------------|-------------------|-----------------|---------------------|---------------------|--------------|---------------|-----------|
| 7200              | 700               | 30                | 0.006           | 1760                | 1680                | 250000       | 1.6 x 10$^7$ | 0.48      |

$D_s$ (m$^2$/s) $D_t$ (m$^2$/s) $\beta_{T}$ (K$^{-1}$) $\beta_{C}$ (l)

1.6 x 10$^{-11}$ 1.0 x 10$^{-8}$ 1.0 x 10$^{-4}$ 4.0 x 10$^{-3}$

Boundary conditions: The boundary conditions for the velocity, temperature, turbulent kinetic energy, dissipation rate, and species concentration are set as follows.
Inlet: Constant values are prescribed for all variables: \( u_{\text{inlet,}x} = 0 \), \( u_{\text{inlet,}y} = \alpha u_{\text{cast}} / d_z \), \( k_{\text{inlet}} = 1.5 \left( I_x u_{\text{inlet,}y} \right)^2 \), \( \varepsilon_{\text{inlet}} = \frac{C_{\mu} k_{\text{inlet}}}{0.07 d_z} \), \( T_{\text{inlet}} = T_0 \), \( C_{\text{inlet}} = C_0 \), where \( u_{\text{cast}} \) is the casting velocity in the casting direction, and \( I_x \) is the turbulent intensity calculated from the following relation

\[
I_x = 0.16 \Re^{-1/8}, \quad \Re = \frac{\rho u_{\text{inlet,}y} d_z}{\mu}.
\]

Normal gradient of pressure is set to zero, i.e. \( \frac{\partial P}{\partial y} = 0 \).

Outlet: The pressure outlet is prescribed. The derivative in vertical direction of all other variables is set to zero

\[
P = 0, \quad \frac{\partial u_x}{\partial y} = 0, \quad \frac{\partial u_y}{\partial y} = 0, \quad \frac{\partial k}{\partial y} = 0, \quad \frac{\partial \varepsilon}{\partial y} = 0, \quad \frac{\partial T}{\partial y} = 0, \quad \frac{\partial C}{\partial y} = 0.
\]

Top surface (meniscus): At the meniscus, the symmetry boundary conditions are used (free surface flow). The normal derivative of all variables is set to zero, except the vertical velocity \( u_y \), which is set to zero.

Symmetry: The normal derivative of all variables is set to zero

\[
\frac{\partial P}{\partial n} = 0, \quad \frac{\partial u_x}{\partial n} = 0, \quad \frac{\partial u_y}{\partial n} = 0, \quad \frac{\partial k}{\partial n} = 0, \quad \frac{\partial \varepsilon}{\partial n} = 0, \quad \frac{\partial T}{\partial n} = 0, \quad \frac{\partial C}{\partial n} = 0.
\]

Moving walls: The walls with the solidified steel move with casting velocity along the casting direction. At the walls, where the liquid phase exists, the no-slip boundary conditions for the velocity are set. In the mold, the Robin boundary condition is used, with the surface heat transfer coefficient equal to 2000 Wm\(^{-2}\)K\(^{-1}\). Below the mold, at the secondary cooling system, the heat transfer coefficient is equal to 800 Wm\(^{-2}\)K\(^{-1}\). The normal derivative of the solute concentration is set to zero.

5. Numerical results

In this conference paper, the preliminary numerical results are obtained, without considering inverse segregation and shrinkage-induced flow. The low-Re turbulence model by Abe-Kondoh-Nagano (AKN) [29] is selected, where the normal distance in closure coefficients is calculated up to the wall. The simulation was performed on the node arrangement with 643891 non-uniformly positioned nodes. The steady-state solution shown in figures is approached by a false transient calculation using a fixed time-step of \( 7.5 \times 10^{-4} \) s. The following process parameters were used: \( u_{\text{cast}} = 1.1 \text{ m/min} \), \( T_0 = 1807 \text{ K} \) and \( C_0 = 0.55 \text{ wt\%} \).

Figure 3 represents the following fields: velocity magnitude, temperature and carbon concentration. The same fields at cross-section \( y = -0.8 \text{ m} \) are presented in figure 4. The liquid metal is pouring from the nozzle into the mold, where the flow is separated into upward and downward direction. In the upward direction, liquid flows around SEN up to the meniscus (top surface), and then turn into the mold wall. In the upper half of the mold, the flow in the mushy zone is oriented upward, which results in rejecting the carbon out from the mushy zone into the liquid pool. We get negative segregation in the mushy zone and positive segregation in the liquid pool.
Figure 3. Left: velocity magnitude field. Center: temperature field. Right: carbon segregation field.

Figure 4. Left: velocity magnitude field. Center: temperature field. Right: carbon segregation field.

6. Conclusions
This paper represents a continuation of numerical benchmarking [10] proposed for the continuous casting of steel. The geometry and material properties of the continuous casting process are simplified in order to enable straightforward performance comparisons with various numerical methods. In the paper, our in-house developed meshless numerical method, based on the local radial basis function collocation, is used to get the steady state solution of the turbulent fluid flow with heat transfer, solidification, and macrosegregation of carbon in three dimensions. A symmetric quarter of the billet was considered. The results were obtained without electromagnetic forces in the momentum equation, and with a lever microsegregation model. The benchmark will be further upgraded and adapted, based on the feedback from the colleges in the field of the numerical modelling of solidification processes. A journal paper with tabulated results of the related simulations, similar as [11], is underway. A web page of the benchmark results with systematically tabulated results of different numerical methods will be established, similar to [3].
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