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Hybrid model of liquid metal flow and solidification

Hybrydowy model przepływu ciekłego metalu i krzepnięcia

Abstract

The article presents a hybrid model dedicated to simulations of liquid metal flow and its solidification. The developed solution is a key component of the developed integrated modelling concept, which combines the advantages of physical and computer simulations, while the concept itself is the foundation of a scientific workshop oriented at high-temperature processes (close to solidus lines). Examples of test simulation results are presented, indicating that the adopted model assumptions are correct.

Keywords: smoothed particle hydrodynamics (SPH), finite element method (FEM), extra-high temperatures, solidification, fluid flow

Streszczenie

W artykule przedstawiono hybrydowy model dedykowany symulacjom przepływu ciekłego metalu i krzepnięcia. Opracowane rozwiązanie jest kluczowym elementem rozwijanej koncpecji zintegrowanego modelowania łączącego zalety symulacji fizycznej i komputerowej, zaś sama koncepcja stanowi fundament warsztatu naukowego zorientowanego na procesy wysokotemperaturowe (bliskich linii solidus). Przedstawiono przykładowe wyniki symulacji testowych, wskazujących na poprawność przyjętych założeń modelowych.

Słowa kluczowe: metoda cząstek rozmytych, metoda elementów skończonych, ekstrawysokie temperatury, krzepnięcie, przepływ cieczy

1. Introduction

In particle methods, the fluid flow modelled, or the heat flow, is represented by a set of points. Each point has an assigned set of descriptors. These descriptors determine the point's properties in the model concerned (e.g. mass, temperature, thermal conductivity, location or speed). A point, together with its descriptors is called a particle. A set of particle descriptors depends on the model used in the simulation and may vary from a few to over ten components. Particle methods are a typical example of a problem related to interaction of a finite number of bodies. In the fluid flow, modelling interactions between particles are computed, and the results serve as the basis for tracking particle trajectory and speed. For phenomena coupled with thermal effects also, for instance, temperature changes are tracked. One of particle methods, widely used in issues involving fluid flow or modelling metal solidification processes, is known as the smoothed particle hydrodynamics (SPH). This method is opposite to methods that use meshes for discretisation of the area modelled (e.g. the finite element method). In meshfree methods, neither imposed restrictions nor any constraints limiting degrees of freedom within the system exist. Particles in these methods may move in any directions, and interactions between them only depend on their parameters and distances between them. Forces defined by the adopted interaction model act between each particle couple. Computer simulation is a sequence of iterations, where forces with which particles interact in each iteration are computed for each particle couple. Next, on the basis of the resultant force which has effect on the particle, acceleration of the particle in a given iteration is computed for each particle. This is the basis for computing a correction of particle velocity. The last step is computing a new particle position on the basis of the current position and computed velocity.

In this paper, the results of two test simulations are presented. They were carried out with a new generation 3D solver, included in the original simulation package DEFFEM. The main objective of the numerical tests was to check the implemented thermal solutions in the context of possibilities to simulate heat conduction or solidification processes. The developed model concept constitutes one of the foundations of the scientific workshop developed, focused on high-temperature processes. The term "high-temperature processes" defines two classes of issues, namely the processes of steel deformation modelling within a temperature range near the solidus line, and within a temperature range between the solidus and liquidus temperatures. Thus, the defined research and scientific area force alternative model solutions (which often have a complex nature) to be applied and developed. These solutions are dedicated to the analysis of the following, specific effects: mechanical, thermal, fluid mechanics, density changes or microstructure development. These issues are strictly related to the *soft-reduction* technology, or integrated strip casting and rolling processes. The modelling of effects occurring during both processes requires – due to its complexity – the use of solutions of many differential equations describing individual physical phenomena.

2. Hybrid model of liquid metal flow and solidification

The developed and implemented hybrid model combines advantages of the finite element method (FEM) and the smoothed particle hydrodynamics (SPH). The governing equations of fluids in the SPH method are based on the Navier-Stokes equations in the Lagrangian form. The main equations are given by [1, 2]:

$$\frac{d\rho}{d\tau} = -\rho\nabla\cdot v \tag{1}$$

$$\rho\frac{dv}{d\tau} = -\nabla p + \nabla\cdot\theta + \rho F \tag{2}$$

where: τ is time, v is velocity, p is pressure, F is external force, θ is a second-order tensor containing τ_{ij} stresses. Equation (1) is the continuity equation which describes the evolution of fluid density over time and Eq. (2) is the momentum equation which describes the acceleration of fluid medium. By employing the SPH interpolation given by:

$$\left\langle \nabla f\left(r_i\right)\right\rangle \approx \sum_{j=1}^{N}\frac{m_j}{\rho_j}f_j\nabla_i W\left(r_i - r_j, h\right) \tag{3}$$

to Eq. (1), the SPH representation of the continuity equation can be written as follows [1, 2]:

$$\frac{d\rho_i}{d\tau} = \sum_{j=1}^{N} m_j\left(v_i - v_j\right)\cdot\nabla_i W_{ij} \tag{4}$$

where: m_j and ρ_j are the mass and the density for particle j, respectively, W is the smoothing kernel, index j corresponds to any neighbouring particle of particle, i, f_j is the value of f for particle, j, N is the total number of particles, h is the smoothing length that defines the radius of influence around the current particle i. The momentum equation can be rewritten in the SPH formalism as:

$$\frac{dv_i}{d\tau} = -\sum_{j=1}^{N} m_j\left(\frac{p_j}{p_j^2} + \frac{p_i}{p_i^2} + \Pi_{ij}\right)\cdot\nabla_i W_{ij} + F \tag{5}$$

The viscous force used in this implementation is the viscosity term which was introduced by Monaghan [1] and denoted ij Equation (5) shows that the change of the motion of a particle is due to the pressure field, viscosity and body forces acting on the fluid. An equation of state is required to calculate pressure in Eq. (5). The equation of state used in the presented model is a quasi-compressible form which is calculated by means of the density calculation from Eq. (4) and is given by [1]:

$$p = \beta\left[\left(\frac{\rho}{\rho_{ref}}\right)^{\gamma} - 1\right] \tag{6}$$

where: ρ_{ref} is the reference density, c is the speed of sound, β is the magnitude of pressure, γ=7 for liquid steel. The dynamic particle was selected as a definition of boundary conditions [3]. These kinds of particles have the same properties as fluid particles except that the equation of momentum is not solved for them.

Heat exchange between the particles occurs by considering heat conduction. The model of heat conduction is based on the enthalpy method which is given by:

$$\frac{dH}{d\tau} = \frac{1}{\rho}\nabla(\lambda\nabla T) \tag{7}$$

where: H is enthalpy, λ is thermal conductivity, and T is temperature. The SPH formulation of this equation is approximated by [4]:

$$\frac{dH_i}{d\tau} = \sum_j \frac{m_j}{\rho_i\rho_j}\frac{4\lambda_i\lambda_j}{(\lambda_i+\lambda_j)}(T_i - T_j)\frac{(r_i - r_j)\cdot\nabla_i W_{ij}}{(r_i - r_j)^2 + \eta^2} \tag{8}$$

where: η is a small parameter to prevent singularity when $(r_i - r_j)$ goes to zero. If the specific heats to be constant then the relationship between enthalpy and temperature can be written as [4]:

$$H = \begin{cases} c_{p\_s}T & ,T \le T_s \\ c_{p\_s}T_s + \dfrac{L}{(T_l - T_s)}(T - T_s) & ,T_s < T \le T_l \\ c_{p\_s}T_s + \left(\dfrac{L}{(T_l - T_s)}\right)(T_l - T_s) + c_{p\_l}(T - T_l) & ,T > T_l \end{cases} \tag{9}$$

The latent heat L describes the energy released by a particle to change the phase from liquid to solid. T_l and T_s : are the liquidus and solidus temperatures, respectively, and c_{p_l} and c_{p_s} are the specific heats in the liquid and solid phases, respectively. The temperature of each particle is then calculated by means of this relation in the temperature term [4]:

$$T_i = \begin{cases} \dfrac{H_i}{c_{p\_s}} & ,H_i \le H_s = c_{p\_s}T_s \\ T_s + \dfrac{H_i - H_s}{\left(\dfrac{L}{(T_l - T_s)}\right)} & ,H_s < H_i \le H_l = H_s + \left(\dfrac{L}{(T_l - T_s)}\right)(T_l - T_s) \\ T_l + \dfrac{H_i - H_l}{c_{p\_l}} & ,H_i > H_l \end{cases} \tag{10}$$

Phase transition (from liquid to solid) occurs when particle temperature is below the solidus temperature T_s. In the proposed solution, solid particles are modelled as a viscous pseudo fluid. It means that the behaviour of solid particles is like that of fluid particles but they move under very high viscosity. This approach is used to keep the forces acting on the solid particles and fluid particles.

The solution in the form of temperature field for the FEM model was searched by solving the Fourier equation, which in the general form can be written as follows:

$$\nabla^T(\lambda\nabla T)+\left(Q-c_p\rho\frac{\partial T}{\partial\tau}\right)=0 \tag{11}$$

where:
T – absolute temperature,
λ – thermal conductivity coefficient,
Q – heat generation rate for volume unit,
c_p – specific heat,
ρ – density,
τ – time.

The model coupling both domains (FE+SPH) is based upon a solution of coupling by fixing particles to the FE nodes.

3. Example results

As a part of test simulations, computing was carried out for two variants, focusing on the assessment of the implemented thermal solutions. C45 grade steel [5] is the material used in both simulations. Thermal properties (temperature dependent) necessary for the simulation were calculated by means of commercial JMatPro software [5]. The liquidus T_l and solidus T_s temperatures of the investigated steel are 1494.79°C and 1412.42°C, respectively. The first

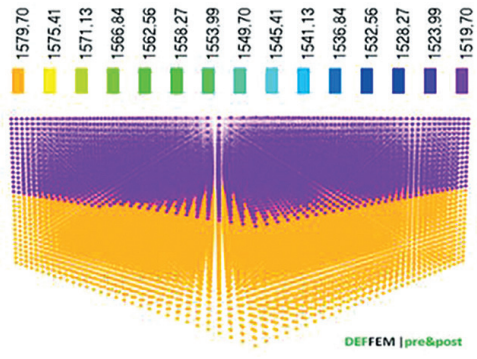

Fig. 1. Initial temperature of the computational domain

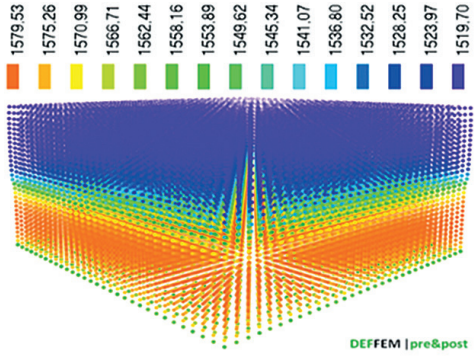

Fig. 2. Example temperature distribution of the computational domain

numerical simulation consisted in a free fall of a box (simulation domain) onto a substrate defined by dynamic particles. The simulation domain in the form of a box was divided in equal proportion into particles, to which temperatures of 1580°C and 1520°C were assigned respectively (Fig.1). The substrate temperature of 20°C was assumed in the computing process. Solutions domain consisting of 29 791 moving particles and 61 206 dynamic particles represents the boundary condition. The initial drop height for free fall case was set to 0.01 m. Other parameters were adopted as follows: initial smoothing length = 0.007 m, speed of sound 30 m/s and simulation time: 7.0 s. In the simulation no heat transfer to the environment was assumed. Figure 2 presents an example of temperature field distributions within the liquid steel volume for the simulation time equal to 1.0046051658706517E-002 second of the free fall. Analysing Fig. 2, one may observe temperature transfer within the liquid steel volume and first contact with heat transfer between the interface substrate–solution domain.

In Fig. 3, an example of temperature distribution of the boundary domain is presented. The maximum temperature reaches about 1292°C and is located in the centre of interface contact liquid steel-substrate, where an intensive area of solidification occurs. In the subsequent stages of the simulation (Fig. 5 and Fig. 6), as a result of contact with the ground, there is a free flow

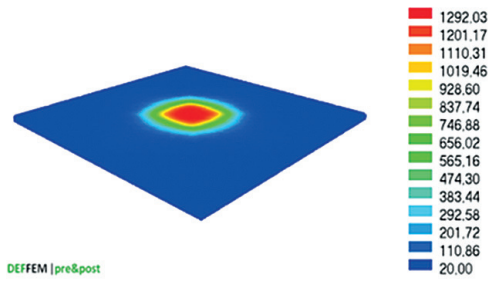

Fig. 3. Example temperature distribution of the boundary domain (time 0.23005412588462504 s.)

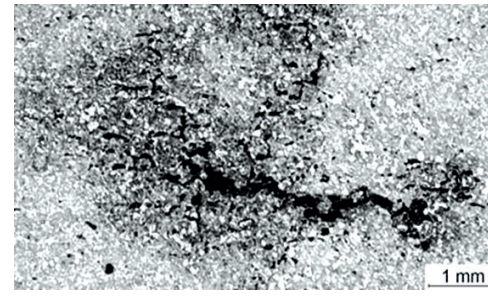

Fig. 4. Macrostructure of the sample centre with visible defects area after re-melting process at 1430°C

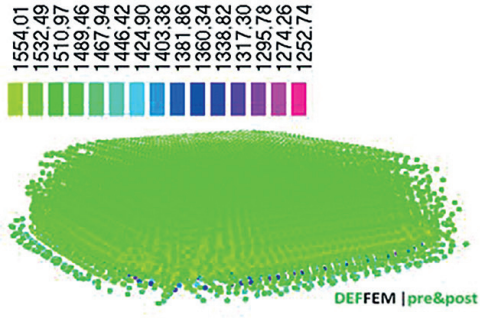

Fig. 5. Example temperature distribution of the computational domain (time 8.0122210271315705E-002 s.)

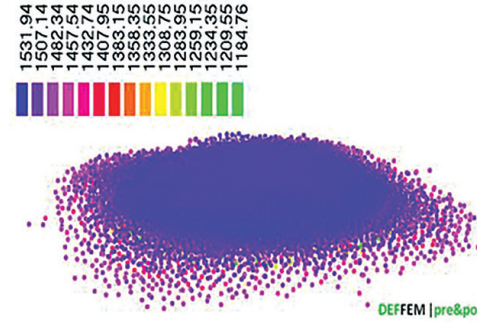

Fig. 6. Example temperature distribution of the computational domain (time 0.18009102709323876 s.)

of liquid steel on the substrate surface together with simultaneous solidification. The second simulation variant was oriented for a test hybrid solver and possibility to predict defects (porous zone formation) within the volume of a sample (see Fig. 4) as well as robustness of the hybrid solver. Cylindrical specimens with a diameter of 10 mm and a length of 125 mm were tested with a Gleeble 3800 thermo-mechanical simulator [5]. A specimen was heated by resistance heating, with an automatically controlled alternating current being introduced into the specimen through cooper grips.

At the first stage of a physical simulation, the specimen was rapidly heated up to 1350°C at the heating rate of 20°C/s. At the second stage, the specimen was slowly heated up to 1430°C at the heating rate of 1°C/s and held at this temperature for 30 seconds. Finally, the specimen was cooled down to nominal temperature and after holding for 10–60 seconds (this time depends on simulation variant) cooled down to ambient temperature. To prevent oxidation, the specimen was located in a vacuum chamber. A transparent quartz sleeve was used to protect against potential leakage of metal during re-melting. In order to find out the temperature distribution along the heating zone within the specimen, temperatures are continuously measured at several locations of the sample. A special thermocouple was mounted in the core of the specimen and gave access to the radial temperature gradient. More details about experimental methodology can be found in [5]. The hybrid methodology of numerical modelling consists of three main steps:

1) In the first stage (resistance heating process), a classic DEFFEM thermal solver based on FEM is applied in order to estimate temperature distribution within the volume of a sample [5].
2) In the second stage, a hybrid DEFFEM solver is used. The mesh is re-built and particles are generated within the volume of a sample together with their temperature initialization based on interpolation temperature from FEM mesh nodal results (Fig. 7).

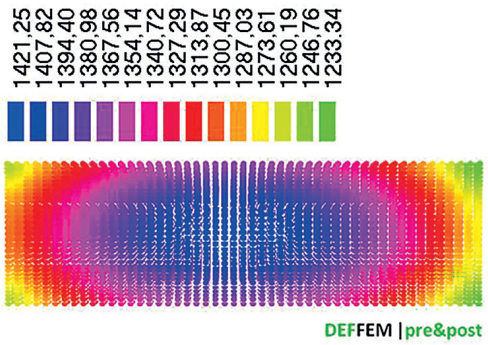

Fig. 7. Particles temperature distribution in the longitudinal-section of a sample after interpolation based on FEM mesh nodal results, just before cooling down to ambient temperature

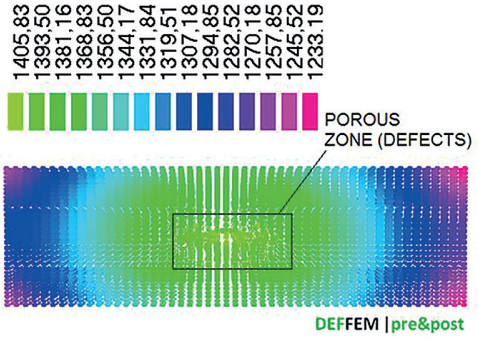

Fig. 8. Particles temperature distribution in the longitudinal-section of a sample after finishing solidification process with visible defects within the sample volume

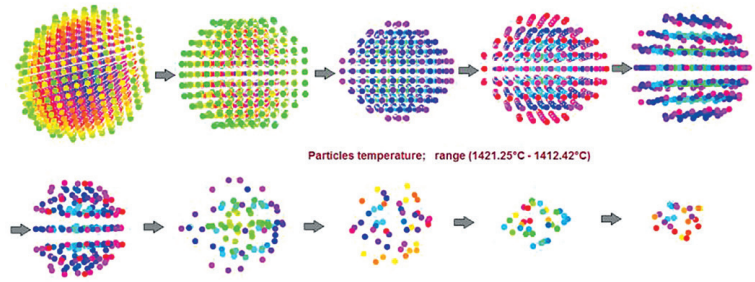

Fig. 9. Mushy zone evaluation over the simulation time of solidification process

3) In the third stage, the solidification process is performed (hybrid solver). The particles temperature distribution after finishing solidification is presented in Fig. 8. While analysing Fig. 8, one may observe that particles temperature drops below the solidus temperature and in the centre of the sample a porous zone (defects area) was formed. The obtained results are similar to the results received from physical simulations. The computer simulation results are promising, however the DEFFEM hybrid solver required further validation tests based on physical simulations.

The maximum temperature of 1421.5°C occurs in the sample centre and is higher than the solidus temperature of about 9°C (Fig. 7). The surface temperature on the FEM mesh equals 1380°C [5]. The total gradient temperature in the cross-section of the sample is 41.25°C. Based on such temperatures as references temperatures, a mushy zone can be estimated within the volume of the sample (Fig. 9). The volume of the mushy zone decreases over the simulation time to reach the minimum volume after 0.3 seconds from the start of solidification process.

Such result is nearly half faster than the results obtained from the physical simulation. In Fig. 10, the temperatures changes versus time for the experiment and a hybrid model is presented. According to physical results, the solidification process lasts 0.6 seconds. At the beginning of solidification process within about 0.2 seconds, temperature changes between the

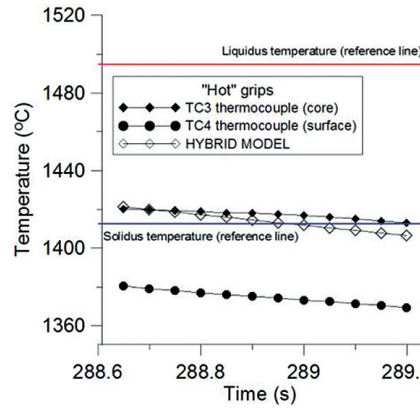

Fig. 10. Temperatures changes versus time (experiment and hybrid model)

computer and physical simulations were very convergent. The whole process of solidification was finished 0.35 seconds faster for the computer simulation than during the physical simulation. The main reason of such differences is the admission of linear approximation of enthalpy changes versus temperatures in the numerical model and adoption of a constant heat exchange coefficient in the FEM model [5]. The impact of these simplifications will be examined in the next research project.

4. Conclusions

The article presents test simulations allowing the quality and capabilities of a hybrid solver as regards fluid flow simulation, taking into account thermal effects or simulation of the solidification processes in terms of their further development by subsequent sub-models to be evaluated. The solidification process was calculated by applying the enthalpy method in the SPH formulation to solve a heat transfer problem. The phase transition model from liquid to solid was treated by considering the effect of latent heat and non-isothermal phase change on the model of heat transfer. The conducted simulations indicate that the assumed and implemented model solutions (shrinkage cavity and heat transfer during liquid mixing) are correct. Further work related to the developed solution will focus on making the liquid-solid phase interaction model more specific by adding a particular force between the mushy and solid phases, or the procedure of particle grouping and taking into account its movement within the mixed zone (liquid and solid phases).

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References

[1] Monaghan J.J., *Smoothed particle hydrodynamics*, Annual Review of astronomy and Astrophysics, Vol. 30, 1992, 543–574.
[2] Monaghan J.J., *Simulating free surface flows with SPH*, Journal of Computational Physics, Vol. 110, 1994, 399–406.
[3] Crespo A.A.J.C., et al., *Boundary conditions generated by dynamic particles in sph methods*, Cmc -Tech Science Press, Vol. 5, 2007, 173–184.
[4] Cleary P.W., Monaghan J.J., *Conduction modelling using smoothed particle hydrodynamics*, J Comput Phys, vol. 148, 1999, 227–264.
[5] Hojny M., *Modeling of Steel Deformation in the Semi-Solid State*, Advanced Structured Materials, vol. 78, Springer 2017.