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SIMULATION AND EXPERIMENTAL STUDIES OF THE PROCESS OF FILLING POROUS MATERIALS

BADANIE EKSPERYMENTALNE I SYMULACJA PROCESU WYPEŁNIANIA MATERIAŁÓW POROWATYCH

The article shows the results of simulation studies conducted on metal matrix composites applying the method of the dynamics of molecular particles. The described method has been illustrated with numerical examples of the simulation and verified by experiments. The numerical computations have been made on supercomputers available at the Academic Computer Centre in Kraków, while experimental studies were conducted by the Foundry Research Institute in Kraków.

Key words: simulation, casting, composite, solidification, porous media, particle dynamics

W pracy przedstawiono wyniki badań symulacyjnych kompozytów metalowych stosując metodę dynamiki cząstek molekularnych. Prezentowana metoda jest zilustrowana przykładami numerycznych symulacji oraz weryfikowana doświadczalnie. Obliczenia numeryczne prowadzono na superkomputerach w Akademickim Centrum Komputerowym w Krakowie, natomiast badania eksperymentalne zrealizowano w Instytucie Odlewnictwa w Krakowie.

1. Introduction

Simulation of fluid flow through porous media is a complicated modeling task, especially when analyzed in mesoscopic scale. Convenient approach to describe geometrically complex and irregular system is usage of interacting particles governed by the Newton law of motion. Applying particles instead of continuous model based on finite element or finite differences methods is much more flexible and enables geometry changes due to the flow.

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In this paper the possibilities of application of Dissipative Particle Dynamic (DPD) as a new tool in simulating the infiltration of porous medium by liquid metal are demonstrated. The DPD method is presented and the particle model of the system is described. Then the ways of generation of numerical models of the porous preform applied in and 3-D simulations are shown. Some results of simulation are shown in the paper.

The simulation studies were verified with experiments using to this end a specially designed preform see Górny [1, 10].

The ceramic preform (porous) contained zircon ($ZrSiO_4$), aluminium phosphate ($AlPO_4$), andalusite ($Al_{12}SiO_5$) and mullite. The preform had the density of 3.87 g/cm^3, apparent density of 0.75–0.80 g/cm^3, minimum compression strength of 1.5 MPa, open porosity 78–80%, common refractoriness above 175 sP, and refractoriness under loading of 1500°C. The preform was soaked with AK51 alloy characterised by pouring temperature of 650°C and placed in preheated mould (lower part 180°C, upper part 420°C) for the time of 30s. A real casting with component of composite part is also presented in the paper.

2. Particle approach to flow in porous medium and solidification

Simulation of fluid flow through porous media is a complicated modeling task, especially when analyzed in mesoscopic scale. Applying particles model governed by the Newton law of motion instead of continuous approach based on finite element or finite differences methods is much more flexible and enables easy geometry changes due to the flow.

Having possibility to choose from many particle models, such as Molecular Dynamics (MD), Granular Dynamics (GD), Lattice Gas Automata (LGA), we have decided to rely on Dissipative Particle Dynamics (DPD), an attractive mesoscopic simulation technique introduced by Hoogerbrugge and Koelman [2] and developed by Marsh et. al. [3], Español [4–5] and Avalos [6]. The method is based on MD principles, however contrary to MD atomic particles, the dissipative particles can be viewed as "clusters" of atoms or molecules. The DPD method consists essentially of a MD simulation, in which the force between particles consists of conservative, dissipative and Brownian components. It is intrinsically mesoscopic in nature, because it resolves only the center-of-mass motion of the droplets and avoids the description of its internal state.

We consider the 2-*D* and 3-*D* systems consisting of liquid metal placed initially above the porous material filled by the air and the slab on the top pushing the metal down The system is confined in the rectangular box with periodic boundary conditions. The entire system is built up of two types of interacting particles: the heavy, motionless particles, which represent the porous medium and the slab as well as the DPD "liquid particles", which can be treated as "droplets" of liquid metal and the air filling initially the pores.

The DPD particles defined by mass M_i, position $\boldsymbol{r}_i$, and momentum $\boldsymbol{p}_i$ interact with each other and with the "heavy particles" via two-body, short ranged force, which is a sum of conservative $\boldsymbol{F}_C$, dissipative $\boldsymbol{F}_D$ and Brownian $\boldsymbol{F}_B$ components where:

$$\mathbf{F}_C = \pi \cdot \omega(r_{ij}) \cdot \mathbf{e}_{ij},\ \mathbf{F}_D = \gamma \cdot M \cdot \omega(r_{ij}) \cdot (\mathbf{e}_{ij} \circ \mathbf{v}_{ij}) \cdot \mathbf{e}_{ij},\ \mathbf{F}_B = \frac{\sigma \cdot \theta_{ij}}{\sqrt{\delta t}} \cdot \omega(r_{ij}) \cdot \mathbf{e}_{ij} \qquad (1)$$

and $\omega(\boldsymbol{r}_{ij})$ is a weight function dependent on the distance between particles i and j, $\boldsymbol{e}_{ij}$ is a unit vector pointing from particle i to particle j, θ_{ij} is a random variable with zero mean and unit variance, while π, γ and σ are the scaling factors for each type of interactions. The temporal evolution of the particle ensemble obeys the Newtonian equations of motion.

In our model we use the modified DPD collision operator presented in [2–5]. We employ improved 2nd order ($o(\Delta t^2)$) numerical scheme to integrate the equations of motion for the particle system. The "leap-frog" algorithm is used for the particle positions $\boldsymbol{r}_i^n$, but the Adams-Bashforth scheme for the particle velocities $\boldsymbol{v}_i^n$ and momenta $\boldsymbol{p}_i^n$. The scheme is a reasonable compromise between the low-order schemes used previously [2–6] and the less efficient but implicitly stable and self-consistent, higher-order schemes. For multi-component fluid, where $k = g(i)$ and $l = g(j)$ mean the types of particle i and j, respectively, the equations of motion can be represented in the following discretized form.

$$\mathbf{p}_i^{n+\frac{1}{2}} = \mathbf{p}_i^{n-\frac{1}{2}} + \sum_{j \neq i} \left[\pi_{kl} \cdot \omega_1(\boldsymbol{r}_{ij}^n) - \gamma_{kl} \boldsymbol{M}_{kl} \cdot \omega_2(\boldsymbol{r}_{ij}^n) \cdot (\mathbf{e}_{ij}^n \circ \tilde{\mathbf{v}}_{ij}^n) + \frac{\sigma_{kl} \cdot \theta_{ij}}{\sqrt{\Delta t}} \cdot \omega_1(\boldsymbol{r}_{ij}^n) \right] \mathbf{e}_{ij}^n \cdot \Delta t \qquad (2)$$

$$\mathbf{r}_i^{n+1} = \mathbf{r}_i^n + \frac{\mathbf{p}_i^{n+\frac{1}{2}}}{M_i} \cdot \Delta t, \quad \mathbf{p}_i^n = \frac{\mathbf{p}_i^{n+\frac{1}{2}} + \mathbf{p}_i^{n-\frac{1}{2}}}{2} \qquad (3)$$

$$\tilde{\mathbf{v}}_i^n = \frac{1}{2 \cdot M_i} \left(3 \cdot \mathbf{p}_i^{n-\frac{1}{2}} - \mathbf{p}_i^{n-\frac{3}{2}} \right),\ \tilde{\mathbf{v}}_{ij}^n = \tilde{\mathbf{v}}_i^n - \tilde{\mathbf{v}}_j^n,\ \mathbf{r}_{ij}^n = \sqrt{(\mathbf{r}_i^n - \mathbf{r}_j^n)^2},\ \mathbf{e}_{ij}^n = \frac{\mathbf{r}_i^n - \mathbf{r}_j^n}{\mathbf{r}_{ij}^n} \qquad (4)$$

$$\omega_1(\boldsymbol{r}_{ij}^n) = \frac{3}{\pi r_c^2 n} \cdot \left(1 - \frac{r_{ij}^n}{r_c} \right),\ \omega_2(\boldsymbol{r}_{ij}^n) = \frac{6}{\pi r_c^2 n} \cdot \left(1 - \frac{r_{ij}^n}{r_c} \right)^2,$$

$$M_{ij} = \begin{cases} M_i & \text{if } g(i) = g(j) \\ \dfrac{2M_i \cdot M_j}{M_i + M_j} & = \text{if } g(i) \neq g(j), \end{cases} \qquad (5)$$

where:

M_{kl} – the mass of DPD particle; for interactions between particles of different kind ($k \neq l$) the geometric mean is computed,

π_{kl} – the scaling factor for conservative part of collision operator,

γ_{kl} – dissipative force coefficient,
σ_{kl} – the scaling factor for Brownian motion,
r_c – cut-off radius, and for $r_{ij} < r_c$, $\omega_1(r_{ij}) = \omega_2(r_{ij}) = 0$,
n_D – average particle density in D-dimensional system ($D = 2, 3$),
$\omega_1()$ and $\omega_2()$ – are the weight functions defined so that

$$n_D \cdot \int_0^r \omega_m(r)\, d\boldsymbol{r} = 1 \text{ for } m = 1, 2.$$

We assume that n – particle density – is a constant and the density ρ_k of the kth particle system is equal to:

$$\rho_k = S_k \cdot m_k \cdot n, \tag{6}$$

where m_k is the mass of atom (or molecule) of fluid k, S_k – scaling factor, $M_k = S_k \cdot m_k$ is a mass of DPD particle. The gravitational force is acting only on the slab, while the particles representing the porous material are motionless.

The 2D simplified model has been treated as a vehicle to analyze the overall velocity of liquid flow depending on the density and porosity of the porous material. The artificially generated porous structure have been generated as a regular mesh of circles, where their radii and distances hare been treated as parameters. Two analyses have been completed: the first one for the varying radii and distances, while keeping the density constant, and the second one for changing density of the material. The velocity profiles have been calculated and the liquid front shape has been analyzed.
Sample snapshots of 2D simulation are presented in Fig. 1.

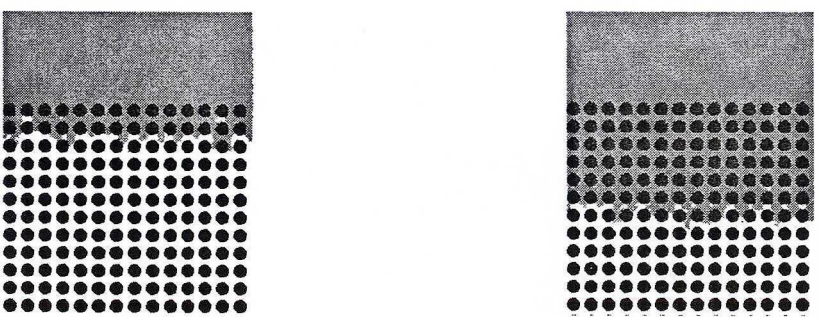

Fig. 1. Two snapshots from 2-D DPD simulation, showing the process of flooding of the higher layers of the porous material

Instead of generating an artificial regular structure, in 3-D simulations we have employed the results coming from the simulation of droplets coalescence in binary fluid [8–9], which enable generating the porous irregular structures of a given porosity and average size of pores. By removing one fluid, the remaining structure resembles the porous preform used in the experiment (see Fig. 2).

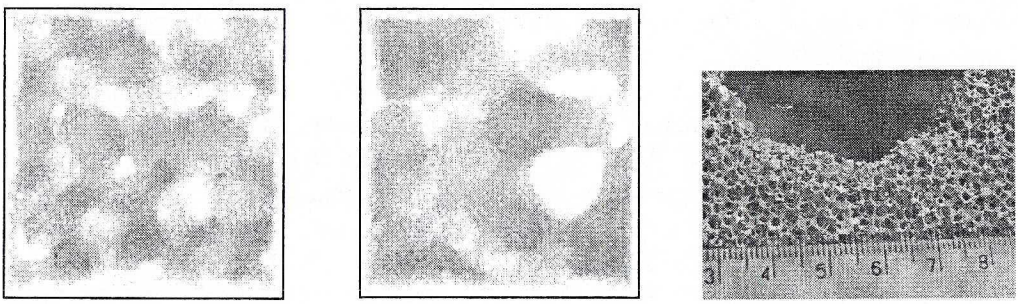

Fig. 2. Two different models representing the structures of the same porosity but different average pore size, of the 3-D preform (here X–Y projections) generated by using droplets coalescence simulation. The structures are compared to the ceramic preform used in the experiment

The model generated this way is more realistic than the others. Moreover, formation of the porous medium is similar to the real technological processes used in the preform production. However, as is shown in the following section, the faults in the model, e.g., too narrow channels resulting in lower permeability, may cause some side effects.

The sample simulation was performed for liquid Sn ($T = 573$ K) under pressure $P = 3$At. The pressure is larger than in the experiment (0.7–1 At) in order to accelerate the process of pores flooding thus shorteing the simulation time. Because the model is isothermal, the average temperature of the system (preform + slab + metal + air) is the same during the simulation. The parameters of DPD forces were computed by using continuum limit and kinetic theory equations [3–6].

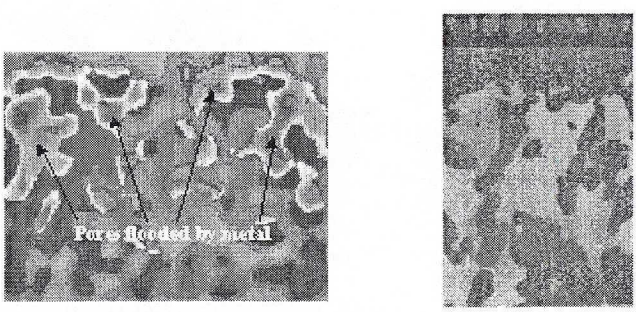

Fig. 3. The X–Y cut plane from 3-D DPD simulation (left) and experiment (right) showing the clusters of pores flooded by metal on the front of liquid Sn

The rest of preform is permeable. In Fig. 2 we show the process of filling the pores in time. As is shown, the air is removed down and the pores are being filled by the metal completely. In Fig. 3 (left) we present the cut-plane from the snapshot of 3-D DPD simulation in larger scale than in Fig. 2. It represents the liquid Sn front layer. Unlike in

Fig. 2 (on the left and centre), the shaded spots represent not the single pores but the clusters of pores filled by the liquid metal. The similar picture was obtained in the experiment (see Fig. 2 on the right).

The dissipative particle dynamics method, despite its limitations can be used as an important supplementary method together with experiment and classical simulation techniques in investigation of fluid flows in porous media. In comparison with classical finite elements and finite difference methods it opens the perspectives of semi-mesoscopic simulations of the flows, giving direct insight into the processes occurring in a single pore or small clusters of pore channels. By using the DPD simulations of phase separation in binary fluid one can mimic the technological processes thus enabling modeling the realistic porous structures, which can be employed in further experiments. Assuming more realistic potentials between particles in the porous material and DPD particles from liquid one can simulate also the interactions between liquid metal and ceramic material, e.g., in order to model damage of the material caused by the temperature and high pressure.

3. Conclusions

The adopted mathematical model of the flow and soaking of DPD preform as well as a, based on this model, simulation of the liquid metal flow and shaping of temperature field in time is an approximation comparable with true measurements and enabling closer evaluation of a non-isothermal flow – evaluation qualitative rather than quantitative, and if quantitative – very rough only.

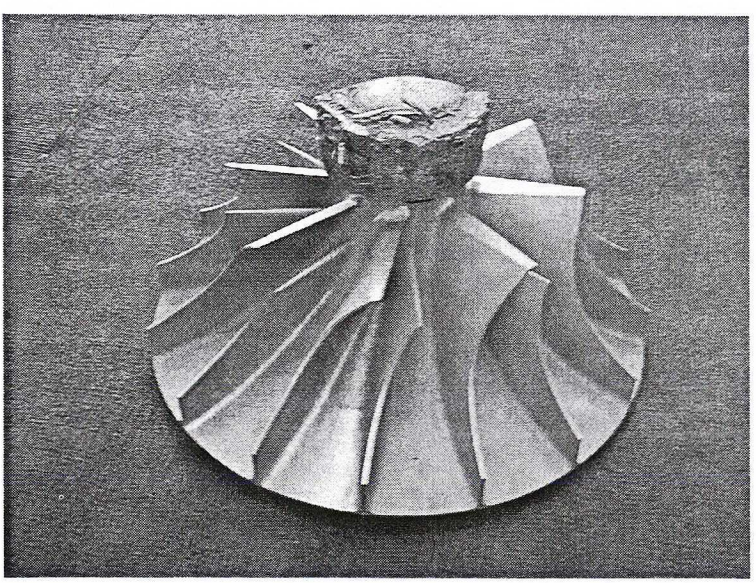

Fig. 4. Real casting with component of composite part

To make experimental verification, an industrial installation for casting with counter-pressure, operating at WSK – Rzeszów, was used. This was the Bulgarian equipment of the following operating parameters: capacity 300 kg, locking force 1200 kN, ejecting force 600 kN, ejecting stroke 150 mm, and plate travel 1000 mm; the plate dimensions were $1100 \times 1600 \times 800$ mm see Górny [1, 10] The difference in pressures during manufacture of casting was 0.07–0.12 MPa as well as 0.5 MPa (Fig. 4).

The presented method and the results obtained are expected to enable production of materials characterised by the required properties and a more precise quantitative description of the examined phenomena.

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