Second International Conference on CFD in the Minerals and Process Industries
CSIRO, Melbourne, Australia
6-8 December 1999

MODELLING OF FLOW IN POROUS MEDIA AND RESIN TRANSFER MOULDING USING SMOOTHED PARTICLE HYDRODYNAMICS

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ABSTRACT

A novel numerical method is presented for the simulation of flow in porous media, based on a mesoscopic-scale modelling using smoothed particle hydrodynamics. The method is demonstrated to provide encouraging results for both saturated and unsaturated porous media flow. The Darcy law is confirmed for low drift velocities in a saturated medium, while nonlinear behaviour is observed for higher values. The application of the method to mould filling demonstrates its ability to predict edge effects associated with resin transfer moulding. The time dependence of the computed resin surface for this unsaturated porous medium exhibits good qualitative agreement with experimental results.

INTRODUCTION

Flow in porous media occurs in many important industrial applications, including oil exploration, groundwater contamination by hazardous wastes, and packed bed chemical reactors. One specific area of increasing interest is resin transfer moulding (RTM), a process used to manufacture polymer composite components for, in particular, the aerospace and automotive industries (Potter, 1997). Liquid resin is forced under pressure into a mould containing a preform consisting generally of woven fibres. The properties of the resulting composite component are determined by a number of factors, including the design of the mould and preform as well as the dynamics of the resin flow.

A large range of numerical simulation methods have been employed over the years to study the flow in porous media. Many of these methods are based on macroscopic-scale models, using empirical simplifications of the governing equations such as the well-known Darcy law (see eg Kaviany, 1995). While traditional continuum methods have been extensively used, particle-based or Lagrangian methods exhibit a number of advantages. In particular, the treatment of the complex boundary conditions at either the microscopic or intermediate-level "mesoscopic" scale can be considerably simpler for particle methods.

Recently, a number of workers have analysed 2D and 3D mesoscopic-scale modelling of flow in porous media using lattice gas (Chen *et al.* 1991; Koponen *et al.* 1997) and lattice Boltzmann (Cancelliere *et al.* 1990; Spaid and Phelan 1997) methods. These studies have demonstrated that the Darcy law can be reproduced by such numerical methods. In addition, by varying the solid fraction in a system of randomly positioned spheres, good correlation of the calculated permeability with semi-empirical laws have generally been obtained. Koponen *et al.* (1998) have applied these methods to random fibre webs, which closely resemble fibrous sheets such as paper and non-woven fabrics.

Smoothed particle hydrodynamics (SPH) is a Lagrangian method for modelling mass flow and heat transfer. Material properties are approximated by their values at a discrete set of disordered points, or "SPH particles". As opposed to lattice gas and lattice Boltzmann methods, SPH is directly based on the resolution of the macroscopic governing equations, such as the Navier-Stokes equations. These equations are written as a set of ordinary differential equations for the mass and heat flux of the SPH particles. The SPH method has been developed over the past two decades, primarily for astrophysical applications (Monaghan, 1992). More recently, the method has been extended to incompressible enclosed flows (Monaghan, 1994; Cleary, 1998), and applied to industrial problems such as high velocity impact damage (Chen *et al.,* 1997) and high pressure die casting (Cleary *et al.,* 1999).

This paper presents the results of a study into the application of the SPH method to the simulation of flow in porous media. SPH has a number of properties that make it particularly well-suited for this type of problem:

- flow through the pore structure can be treated at a mesoscopic level, similar to that used in lattice gas and lattice Boltzmann simulations,
- complex physics, such as multi-phase flow, realistic equations of state, heat transfer and curing, can be included in a rigorous manner,
- complex geometries can be handled in a simple manner,
- extension from two- to three-dimensional flows is straightforward.

Two specific types of two-dimensional flow in porous media are considered in this paper. Firstly, the numerical simulation of flow in a saturated infinite porous media is presented. The results of these simulations allow a preliminary appraisal of the applicability of SPH for flow in porous media. Secondly, the flow in a channel almost completely filled with an unsaturated porous material is examined. This provides a relatively simple model of resin transfer moulding and, in particular, the analysis of "race-tracking" associated with edge effects in the mould filling process.

SMOOTHED PARTICLE HYDRODYNAMICS

In the SPH method, the interpolated value of any field A at position $\mathbf{r}$ is approximated by

$$A(\mathbf{r}) = \sum_b m_b \frac{A_b}{\rho_b} W(\mathbf{r} - \mathbf{r}_b, h) \quad , \tag{1}$$

where the value of A associated with particle b at $\mathbf{r}_b$ is denoted by A_b. The mass and density of particle b are denoted by m_b and ρ_b, respectively. $W(\mathbf{r},h)$ is a spline-based interpolation kernel of radius twice the interpolation length h. The kernel is a C^2 function that approximates the shape of a truncated Gaussian function; the sum in Eq. (1) is thus restricted to all particles b within a radius $2h$ of $\mathbf{r}_b$.

The use of an interpolation kernel allows smoothed approximations to the physical properties of the material to be calculated from the particle information. The smoothing formalism also provides a means to determine gradients of material properties. The gradient of the function A is then given by

$$\nabla A(\mathbf{r}) = \sum_b m_b \frac{A_b}{\rho_b} \nabla W(\mathbf{r} - \mathbf{r}_b, h) \quad , \tag{2}$$

In this way, the SPH representation of the hydrodynamic governing equations can be built from the Navier-Stokes equations.

The most appropriate choice of SPH continuity equation is

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = \sum_b m_b (\mathbf{v}_a - \mathbf{v}_b) \nabla W_{ab} \quad , \tag{3}$$

since it is Galilean invariant, has good numerical conservation properties and is not affected by free surfaces. The following form of the SPH momentum equation is used

$$\frac{\mathrm{d}\mathbf{v_a}}{\mathrm{dt}} = \mathbf{f} - \sum_b m_b \left[\left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) - \frac{\xi}{\rho_a \rho_b} \frac{4\mu_a \mu_b}{(\mu_a + \mu_b)} \frac{\mathbf{v}_{ab} . \mathbf{r}_{ab}}{\mathbf{r}_{ab}^2 + \eta^2} \right] \nabla W_{ab} \quad , \tag{4}$$

where $\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b$, $\mathbf{f}$ is a body force (per unit mass), μ the dynamic viscosity, and ξ and η are constants. The above formulation is more sophisticated than the original SPH momentum equation of Monaghan (1994); it automatically ensures continuity of stress across material interfaces, and allows multiple materials with viscosities varying by up to five orders of magnitude to be accurately simulated.

SPH is actually a quasi-compressible method and the pressure is given by the equation of state

$$P = P_0 \left[\left(\frac{\rho}{\rho_0} \right)^\gamma - 1 \right] \quad , \tag{5}$$

where P_0 is the magnitude of the pressure and ρ_0 is the reference density. For the present study, the ratio of specific heats $\gamma = 7$ is used. The speed of sound c_s in the material is given by

$$c_s^2 = \frac{\gamma P_0}{\rho_0} = \alpha V^2 \quad , \tag{6}$$

where V is the characteristic or maximum fluid velocity. Typically, α is chosen to be around 100 which ensures that the density variation is less than 1% and the flow can be regarded as incompressible.

Two types of boundary conditions have been used in the present study. Periodic boundaries are applied by simply replacing SPH particles that move outward across the boundary by inward moving particles at the corresponding opposite boundary. External solid walls are modelled by placing "boundary particles" along the boundary. These particles exert Leonard-Jones forces on the SPH particles in the normal direction; appropriate interpolation of these forces produces arbitrary, smoothly-defined boundaries. In the tangential direction, the particles are included in the summation for the shear force to give non-slip boundary conditions at the walls (see Cleary and Monaghan (1993) for more details). Note that the solid walls need not necessarily be stationary; a moving wall is used, for example, to model flow ahead of a piston injecting resin into a preform.

The above set of ordinary differential equations is integrated in time using an explicit predictor-corrector scheme, which has a time step limited by the Courant condition.

In summary, the SPH method does not require a computational mesh. The SPH particles contain all the computational information and are free to move throughout the computational domain. The Lagrangian nature of SPH means that the particles will automatically follow complex flows. This makes the method particularly suited for fluid flows involving complex boundaries and free surfaces.

FLOW IN A SATURATED POROUS MEDIUM

The creeping flow of an incompressible, isothermal, single-phase fluid through a porous medium is governed by the well-known Darcy law. A body force $\mathbf{f}$ applied to a Newtonian fluid completely filling a porous medium with permeability $\mathbf{K}$ gives rise to drift velocity $\mathbf{u}_\mathrm{D}$ given by

$$\frac{\mu}{\mathbf{K}} \mathbf{u}_\mathrm{D} = \mathbf{f} \quad . \tag{7}$$

Here $\mathbf{K}$ is a second-order symmetric tensor, which may have non-zero off-diagonal elements if the porous medium is anisotropic (Kaviany 1995). Equation (7) is a formulation of the Darcy law, and is valid provided that viscous forces dominate over the inertia forces, i.e.

$$Re_p = \frac{\rho u_p d_p}{\mu} < 1 \quad , \tag{8}$$

where u_p is the average pore velocity and d_p is a characteristic length scale of the pores.

For flows in which inertia forces can not be neglected, a linear relationship between the applied force and drift velocity, as expressed by the Darcy law, is not observed. A number of semi-empirical relationships, which include a further term nonlinear in $\mathbf{u}_D$ on the left-hand side of Eq. (7), have been proposed to model such flows. The Ergun equation (Kaviany 1995) is an example of a relationship that is commonly employed when inertial effects play a significant role in the flow through a porous medium.

Within the framework of the SPH methodology, a porous medium can be modelled by the inclusion of a number of "fixed particles" within the flow domain. These particles provide a similar contribution to both the continuity and momentum equations as the mobile SPH particles. However, fixed particles are not influenced by the resulting forces, remaining stationary (it being implicitly assumed that the porous medium structure provides the necessary counteracting force).

Since there is considerable freedom in the choice of the number, location and clustering of the fixed particles, such a model allows a large degree of flexibility to tailor the properties of the porous medium. In addition, the interpolation kernel W used in the SPH formalism can be modified to alter the specific nature of the inter-particle interactions. Such flexibility is of particular importance for the modelling of a wide range of porous media flow conditions.

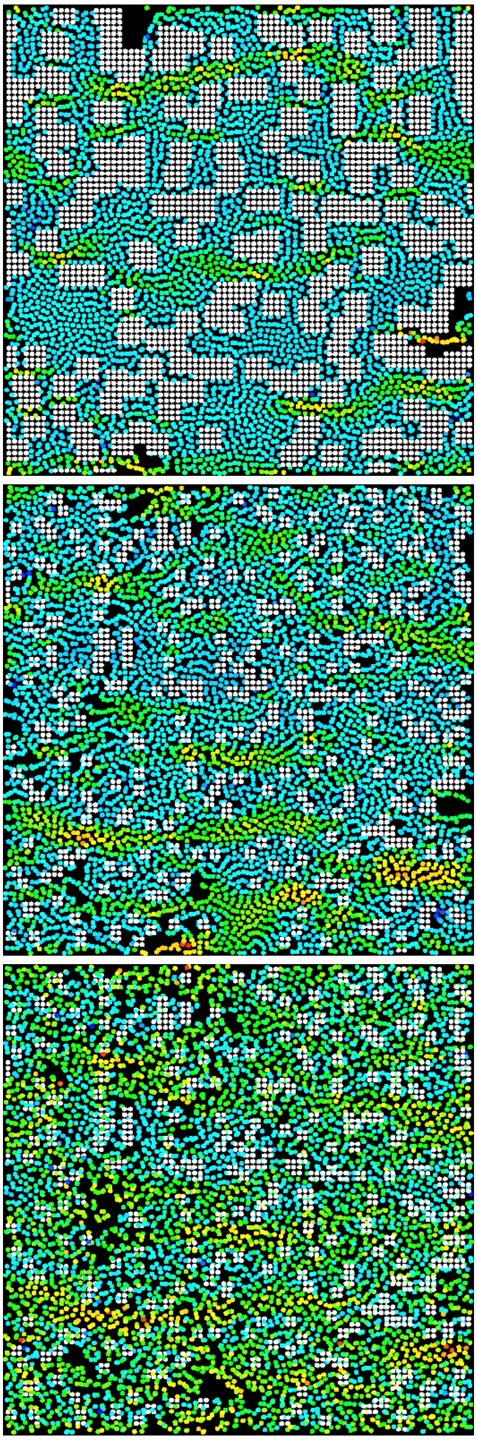
The present study is concerned exclusively with isotropic porous media, for which $\mathbf{K} = K\mathbf{I}$. Nevertheless, it should be noted that by using an appropriate spatial distribution of fixed particles, anisotropic media can also be modelled. In addition, the present study is limited to two-dimensional simulations. Such a mathematical construction can be considered as a model for a medium in which the pore structure is aligned in layers. These properties are exhibited by planar fibrous materials, such a polymer films, paper and non-woven fabrics.

In a saturated porous medium, the entire (non-isolated) pore volume is filled with fluid. A convenient means to construct initial conditions for the SPH modelling of such a medium is to establish an array of particles, of which an appropriate number are randomly assigned as fixed particles. The porosity ε of the medium can be defined by

$$\varepsilon = 1 - \frac{number\ of\ \ fixed\ \ particles}{total\ number\ of\ \ particles} \quad . \qquad (9)$$

The present model is, however, not intended to give an accurate representation of the microscopic pore-scale behaviour of the flow. Except for certain academic examples, such a microscopic representation would involve a very complex fluid-solid interface to represent the detailed pore structure. Rather, the present SPH model is intended as an intermediate level, mesoscopic-scale representation. The model aims to provide the correct global behaviour of the flow, while also enabling the possibility to include more fine-scale details than are not available from a macroscopic model.

Three different examples of such a model of an isotropic saturated porous medium are shown in Fig. 1. For each of these examples, the medium has been constructed from a 80x80 array of particles. A constant body force $\mathbf{f} = f_0\mathbf{x}$ (from left to right) is applied to the medium. Periodic boundary conditions are imposed at each of the four edges of the array.


$\varepsilon = 0.6$, $f_0 = 10$

$\varepsilon = 0.8$, $f_0 = 1$

$\varepsilon = 0.8$, $f_0 = 500$

Figure 1: Examples of flow in 2D porous media having different porosity and applied force. Fixed particles are coloured white, while mobile particles are coloured according to their velocity magnitude. (Note that the colour scale is not the same for each plot.)

The plots in Fig. 1 show that the body force produces a movement of the mobile SPH particles through the void regions surrounding the fixed particles. The preferred path of the mobile particles across the medium has a tortuosity determined by the placement of the fixed particles. While the local velocity of the individual particles contains time-varying **x** and **y** components, the **y** component of the time-averaged drift velocity is found to be negligible.

A series of simulations has been undertaken to provide a more quantitative analysis of the induced drift velocity. An isotropic porous medium of dimension 80 mm square was constructed from an 80x80 array of particles, in the above-described manner. The porosity of the medium was fixed at ε = 0.8, the fluid density and dynamic viscosity were chosen to be ρ = 1000 kg m^{-3} and μ = 0.1 Pa s, respectively. Different values of the applied force f_0 (applied in the **x** direction) were considered.

Figure 2 presents the calculated time-averaged drift velocity as a function of the amplitude of the applied force. These results show that for low applied force (for which the relation (8) is satisfied), the induced drift velocity is proportional to the force. Since the porosity (and hence the permeability) of the medium and the fluid viscosity were constant for the simulations, these results are thus in agreement with the Darcy law, Eq. (7). For higher applied force, corresponding to a Re_p greater than unity, a nonlinear relationship is observed between the force and the resulting drift velocity.

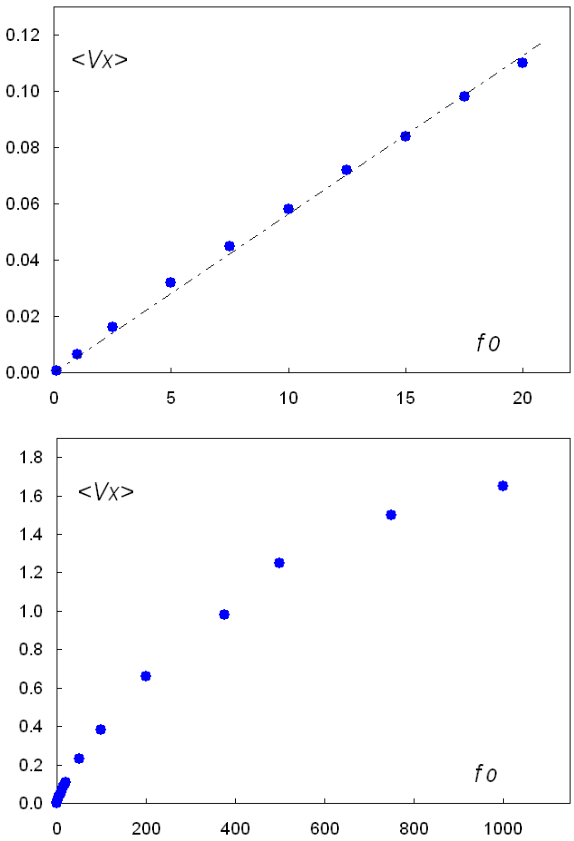


Figure 2: Dependence of the drift velocity <*Vx*> on the applied force f_0 for (top) low values and (bottom) wide range of values of applied force. (The straight line in the top figure represents a linear dependence.)

RESIN TRANSFER MOULDING

In the previous section, flow in an infinite saturated porous medium was considered. While this may be a valid approximation for some problems, in a number of applications the time-dependent filling of the porous medium is of critical importance. For such applications it is necessary to model the finite extent of the porous medium and the propagation of the fluid free surface.

A particular example of flow in a finite unsaturated porous medium occurs in resin transfer moulding (RTM). The RTM process is used to manufacture polymer composite components. Liquid resin is forced under pressure into a mould containing a preform. The preform is chosen according to the desired properties of the resulting composite component, and generally consists of woven fibres. A number of other factors are also important, including the dynamics of the resin flow. Small clearances may exist between the fibre preform and the mould edges due to the unravelling of fibre bundles during the cutting of the preform, imperfect fitting or deformation of the preform. Such defects influence the resin flow, with high permeability regions leading to "race-tracking"; these edge effects can result in the production of unsatisfactory composite components.

The present study provides a very simplified modelling of mould filling in the RTM process. Important effects such as fibre wetting, the removal of entrapped air, and resin curing are not considered. However, it should be noted that many of these more complex phenomena can be incorporated in a straightforward manner into the SPH methodology.

A preliminary study of mould filling, including edge effects, has been undertaken. The geometry considered is similar to that described by Young and Lai (1997), and consists of a rectangular channel of length 220 mm and width 80mm (as shown in Fig. 3). The preform, comprised of an isotropic porous material, occupies all of the channel except for a 5 mm gap at one side. Numerical simulations have been undertaken for a number of preform porosities, ranging from ε = 0.3 to 0.9. The fluid (liquid resin) is injected into one end of the channel, ahead of a piston moving at 0.1 m/s. The resin has a density ρ = 1200 kg m^{-3} and a dynamic viscosity μ = 0.2 Pa s.

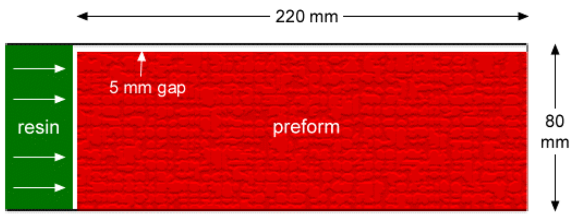


Figure 3: Schematic diagram of geometry used for the resin transfer moulding study. (The left side section of the resin has been truncated for clarity.)

The filling with resin of this rectangular mould containing a gap between the preform and side wall gives rise to two-dimensional flow. For the SPH simulation of the mould filling process, the porous preform was constructed by randomly removing particles from an array of N_f = 16,200 particles, the resulting number of fixed particles being given by (1-ε)N_f. In the initial state, the preform was considered to be empty, containing only fixed particles (with no enclosed mobile SPH particles). The resin was modelled by 11,770 SPH particles, corresponding to a resolution of 1 particle/mm. A moving wall condition was applied at the left boundary, which forced the mobile SPH particles into the inter-particle spaces of the porous preform. Fixed wall conditions are applied at the horizontal upper and lower boundaries.

Figure 4 shows, for a preform porosity of $\varepsilon = 0.5$, the location of the fluid particles at selected times during the mould filling. The free surface of the resin is seen to be initially convex, due to the Poiseuille-like flow that is established in the channel before the resin reaches the preform. As the resin enters the region partially-filled by the preform, the free surface rapidly becomes concave in shape, due to the lower permeability in the preform than in the gap. As the resin is forced further into the channel, its free surface appears to reach a steady-state shape.

As seen from Fig. 5, this shape depends on the porosity (and, therefore, the permeability) of the preform. For high preform porosity, the flow in the perform is only slightly retarded with respect to that in the gap region. This leads to a free surface that is only slightly curved, as observed at the top of Fig. 5. As the preform porosity is decreased, the relative permeability in the preform decreases, and the resin free surface becomes more highly curved. For the lowest values of porosity considered in this study (shown at the bottom of Fig. 5) the influence of this race-tracking behaviour is observed over the majority of the preform cross-section.

Since the parameters chosen for the present study do not coincide with those used in the experimental work of Young and Lai (1997), direct comparison of the results obtained can not be made. Nevertheless, the qualitative features of the race-tracking behaviour described above are observed in their reported experimental data. In particular, the time dependence of the curved shape of the free surface, and its dependence on the preform permeability, as predicted by the SPH model appears to correspond well with the experimental results.

CONCLUSION

A novel approach to modelling of flow in porous media has been presented. The study of mesoscopic-level modelling using smoothed particle hydrodynamics has demonstrated the ease of implementation of such a Lagrangian approach. The application of a constant body force to a saturated isotropic porous medium has been shown to produce a drift velocity in the direction of the force that satisfies the required linear relationship of the well-known Darcy law. For sufficiently large amplitude of the applied force, the SPH simulations predict a nonlinear relationship between the force and the resulting drift velocity, in qualitative agreement with experimentally observed behaviour. In addition, the SPH modelling has been applied to mould filling in the resin transfer moulding process. The predicted behaviour of the resin flow in the unsaturated porous preform material appears to be in qualitatively good agreement with available experimental data.

The present study should be regarding as a preliminary investigation of the application of SPH modelling to flow in porous media. A number of simplifications have been made regarding the nature of the porous medium, in particular, isotropic, isothermal and two-dimensional. It should be straightforward to overcome these simplifications within the framework of the SPH modelling. This will be a subject of future investigations. In addition, while the present study has concentrated on a qualitative analysis of the numerical results, a detailed quantitative study will also be forthcoming.

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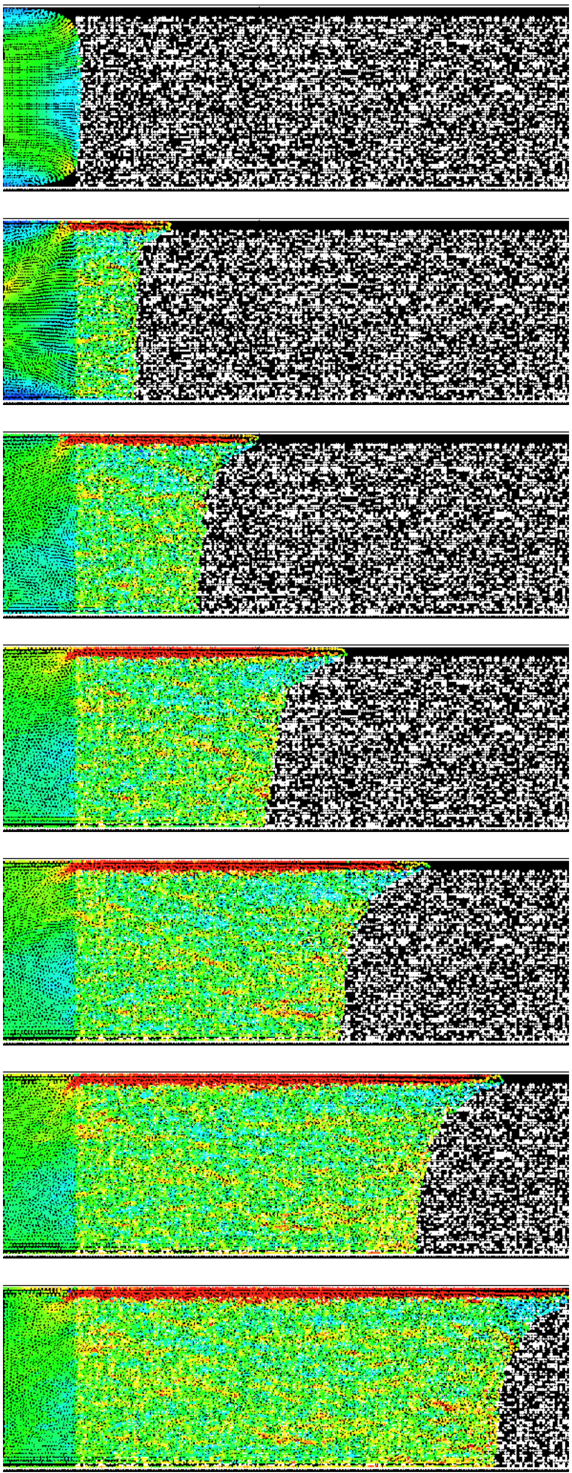

Figure 4: SPH particle locations, coloured by velocity, at selected times (top to bottom: 0.32, 0.68, 1.03, 1.39, 1.74, 2.10, 2.45 s) during the mould filling for a preform porosity of $\varepsilon = 0.5$. (Flow is from left to right.)

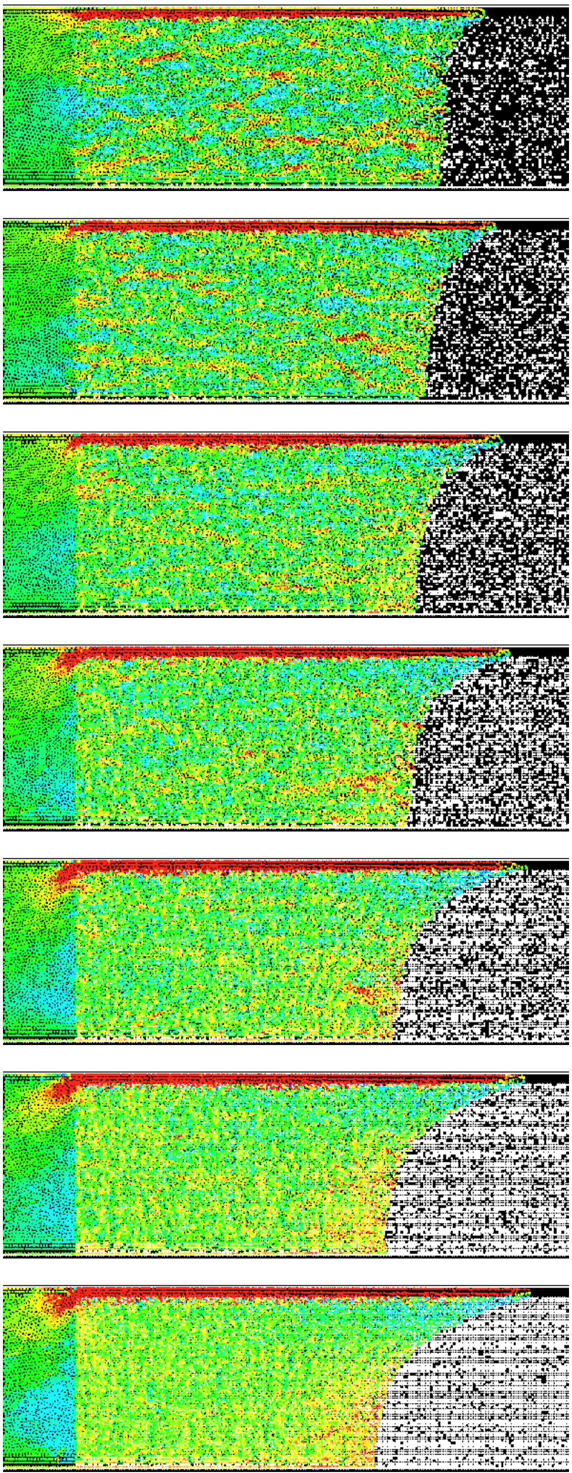

Figure 5: SPH particle locations, coloured by velocity, at $t = 2.10$ s during the mould filling for different preform porosity (top to bottom: $\varepsilon = 0.7$ to 0.1 by intervals of 0.1). (Flow is from left to right.)