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Simulation of Mould Filling and Phase Segregation in Powder Injection Molding with a Fully Explicit Vectorial Algorithm

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Abstract. A bi-phasic model is necessary for the simulation of phase segregation effects in PIM, which results in the solution of two coupled Navier-Stokes equations. Based on the previous explicit algorithms realized by the authors, a new explicit and vectorial algorithm for bi-phasic filling flow has been proposed and developed. By virtue of the new algorithm, all the global solutions are removed to provide the purely vectorial operations with a very efficient feature. The only matrix operations are strictly limited at the element level. Moreover, only the elements of equal-order interpolations are necessary with this new algorithm. In the filled domain, Incompressibility of the mixture is retained by a specially designed corrective feedback operation, with a systematic smoothing procedure to avoid the possibility of mesh lock. As all the global solutions are performed in vectorial forms, the computational cost is merely about proportional to the degree of freedom level. So the simulation of filling processes and phase segregation effects can be carried out with high efficiency, which provides the good suitability for simulation of the industrial problems in large scale. It is furthermore easy to be parallelized on a high performance multi-cluster system. The comparison of numerical results with the experiments proves the validity and efficiency of newly proposed algorithm.

Key words: PIM; Numerical Simulation; Bi-phasic; Phase Segregation

INTRODUCTION

The simulation of the injection stage in PIM is required to be capable for prediction of the powder segregation in the mould filling, which induces the use of bi-phasic model under the frame of mixture theory. The bi-phasic modeling of the mixture flow results in the solution of two coupled Navier-Stokes equations, which brings on the tremendous computation with the classical algorithms. For the sake of required efficiency in application to the industrial problems, the explicit algorithms proposed for simulation of the mould filling in single phase should be referred [1,2]. These algorithms exhibit the important advantage in efficiency by virtue of the application of dynamic models and the associated lumped mass matrices. For bi-phasic simulation of the MIM process, the authors proposed and realized the explicit algorithms for

prediction of the filling patterns and the important segregation effect [3], and an explicit algorithm with purely vectorial operation for filling flow of the single phase [4].

Based on the previous work, an explicit algorithm with purely vectorial operations for bi-phasic filling flows is developed. This new algorithm removes all the necessary global solution procedures to realize the high efficiency with purely vectorial operations. The manipulations of small matrices are restricted at the element level. The increase of computation is about proportional to the increase of DOF number. Moreover, the new algorithm is designed to use the elements of equal-order interpolations, instead of the MINI elements. So the developed solver can be easy integrated with the commercial pre- and post-processors. Incompressibility of the mixture is retained by a corrective feedback operation with the

systematic smoothing procedures to avoid the mesh locking. This numerical tool then provides adequate suitability for simulation of industrial problems in large scale. Furthermore, architecture of the new solver can be easily parallelized on a high performance multi-clusters. The comparison of numerical results with experiments proves well the validity and efficiency of the newly proposed algorithm.

BI-PHASIC MODELLING OF THE INJECTION STAGE IN MIM

The Eulerian description is classically used in the modeling of injection stage in MIM. Let t be the current instant in injection process: $t \in [0, T]$, where T stands for the total injection time. The total space in the mould is defined as a set Ω , where the vector X represents each spatial position. At each instant, the set Ω consists of two distinct subsets $\Omega^F(t)$ and $\Omega^V(t)$ to indicate the domain filled by feedstock and the remaining void portion practically filled by air. To identify these two parts at each instant, a field variable $F(X, t)$ is used to describe the filling state. It takes value 1.0 in the filled part and value 0 in the remaining void portion.

At each instant, evolution of the filling state variable is governed by an advection equation:

$$\frac{\partial F}{\partial t} + \nabla \cdot (\mathbf{V}^{ef} F) = 0 \quad (1)$$

In above equations, \mathbf{V}^{ef} is the effective velocity of mixture flow, which is defined as:

$$\forall X \in \Omega^F, \mathbf{V}^{ef} = \phi^s \mathbf{V}^s + \phi^f \mathbf{V}^f \quad (2)$$

where ϕ^s and ϕ^f are respectively the volume fractions of powder and binder phases in the mixture flow, \mathbf{V}^s and \mathbf{V}^f indicate the velocities of each distinct phases.

The volume fractions of each phase should satisfy the saturation conditions at each spatial position. In the filled domain, this relationship is expressed as

$$\phi^s + \phi^f = 1 \text{ and } \frac{\partial \phi^s}{\partial t} + \frac{\partial \phi^f}{\partial t} = 0 \quad (3)$$

By mass conservation, both powder and binder phases are regarded as intrinsically incompressible, with their proper densities ρ^{s_0} and ρ^{f_0} . Their apparent densities in the mixture, expressed by ρ^s and ρ^f , are related to their volume fraction by the following relationship:

$$\rho^s = \phi^s \rho^{s_0} \text{ and } \rho^f = \phi^f \rho^{f_0} \quad (4)$$

Then the mass conservation for the flows of each

phase in the filled domain $\forall X \in \Omega^F$ is described as

$$p \in \{s, f\}, \frac{\partial \rho^p}{\partial t} + \nabla \cdot (\rho^p \mathbf{V}^p) = 0 \quad (5)$$

As the proper densities of each distinct phase remain constants, their mass conservation can be written as:

$$p \in \{s, f\}, \frac{\partial \phi^p}{\partial t} + \nabla \cdot (\phi^p \mathbf{V}^p) = 0 \quad (6)$$

The saturation of volume fractions in the mixture and the mass conservation for each phase result in the incompressibility of the mixture flow:

$$\forall X \in \Omega^F, \nabla \cdot \mathbf{V}^{ef} = 0 \quad (7)$$

The same operations are performed for both the filled and void domain to keep the consistency of the algorithm, but incompressibility of the mixture is attentively maintained only in the filled domain with exactly determined parameters. As the Reynolds number is sufficiently small in case of the PIM injection, the equations of momentum conservation for two distinct phases can be reduced to two coupled Stokes equations. In the filled domain $\forall X \in \Omega^F$ and for each phase $p \in \{s, f\}$, these equations are expressed as

$$\rho^p \frac{\partial \mathbf{V}^p}{\partial t} = -\nabla (\phi^p P) + \nabla \cdot (\mu_p \dot{\epsilon}_p) + \rho^p \mathbf{g} + \mathbf{m}^p \quad (8)$$

where P represents the pressure field in the mold, μ_s and μ_f are the viscosities for the flows of powder and binder phase in the filled domain, ρ^s and ρ^f are their apparent densities, \mathbf{g} is the gravitational acceleration. At each position, the coupling terms \mathbf{m}^s and \mathbf{m}^f for momentum exchange are proportional to the difference of velocities between these two phases:

$$\mathbf{m}^s = k (\mathbf{V}^f - \mathbf{V}^s), \mathbf{m}^f = k (\mathbf{V}^s - \mathbf{V}^f) \quad (9)$$

where k is an interaction coefficient.

THE FULLY VECTORIZED PROCEDURE FOR EXPLICIT SOLUTION

The MINI elements are generally used to avoid the mesh locking for the simulation of incompressible flows. But the new algorithm is based on the elements of equal order interpolations and a special smoothing procedure. So that the interpolations of different field variables are written as:

$$\{V^s, V^f, V^{ef}\} = \sum_{i=1}^n N_i \{V_i^s, V_i^f, V_i^{ef}\} \quad (10)$$

$$\{P, F, \phi^s, \phi^f\} = \sum_{i=1}^n N_i \{P_i, F_i, \phi_i^s, \phi_i^f\} \quad (11)$$

in which N_i stands for the interpolation functions, n is the number of nodes in the element.

The determination of filling state and the fields of volume fractions by Taylor-Galerkin and Galerkin methods remain the same as in the previous work [3], so they are not specifically introduced.

By virtue of the explicit procedures, the solution of momentum equation (8) is realized by three fractional steps: 1) solution for the effect of phase interaction 2) solution for the effects of viscous diffusion and 3) solution to maintain the incompressibility conditions. In the filled domain $\forall X \in \Omega^F$ and for each phase $p \in \{s, f\}$, the equations of the three fractional steps are described in the next parts:

Phase Interaction

The solution of interaction effects between the flows of two distinct phases is expressed as:

$$\rho^p \frac{\partial(V_{n+}^p - V_n^p)}{\partial t} = \mathbf{m}^p \quad (12)$$

Equation (12) is discretized by a Galerkin method resulting in solution procedure:

$$\begin{aligned} \mathbf{M}^s \frac{(V_{n+}^s - V_n^s)}{\Delta t} &= \mathbf{K}^I \bullet (V_n^f - V_n^s) \\ \mathbf{M}^f \frac{(V_{n+}^f - V_n^f)}{\Delta t} &= \mathbf{K}^I \bullet (V_n^s - V_n^f) \end{aligned} \quad (13)$$

where V_{n+}^s and V_{n+}^f are the intermediate velocity fields, the mass matrices \mathbf{M}^s and \mathbf{M}^f for solid and fluid phase are defined as:

$$\mathbf{M}^p = \mathbf{A} \int_{\Omega} N^T \rho^p N d\Omega$$

in which \mathbf{A} stands for the FEM assembling operation. These two matrices should be lumped into diagonal form to get the explicit solution. \mathbf{K}^I is a stiffness matrix for the interaction effect that can be written as:

$$\mathbf{K}^I = \mathbf{A} \int_{\Omega} N^T k N d\Omega$$

Viscous Diffusion

The fractional step for the effect of viscous diffusion in the flow of each phase p is expressed as:

$$\rho^p \frac{\partial(V_{n+}^p - V_n^p)}{\partial t} = \nabla \bullet (\mu_p \dot{\epsilon}_p) + \rho^p \mathbf{g} \quad (14)$$

Equations (14) is discretized by Galerkin method and it results the following operations:

$$\mathbf{M}^p \frac{(V_{n+}^p - V_n^p)}{\Delta t} = \mathbf{F}^\sigma(V_{n+}^p) + \mathbf{F}_{ext}^p \quad (15)$$

where V_{n+}^p are the intermediate velocity fields, \mathbf{F}^σ represents the viscous diffusion effects, \mathbf{F}_{ext}^p are the external load vectors associated to gravitational effects and boundary conditions.

Incompressibility

The global solution of pressure fields is considered to be indispensable for keeping the incompressibility of the mixture. In the former explicit algorithms, these solutions prevent the simulation from high efficiency, especially for the large scales industrial models. The new algorithm is designed based on the nature of filling process to keep incompressibility of the mixture without the solution of pressure field. The intermediate velocity fields obtained by the previous fractional step are corrected by a dilatancy coefficient to keep the incompressibility. This coefficient is determined by a feedback from the actual state compared to the incompressibility condition. As the incompressible domain increases gradually in the filling process, the flows in filled domain can be updated at each time step to satisfy the incompressibility condition. In the filled domain $\forall X \in \Omega^F$ and for each phase $p \in \{s, f\}$, the procedure for correction on intermediate velocity fields to keep the incompressibility is expressed as

$$\rho^p \frac{\partial(V_{n+1}^p - V_{n+}^p)}{\partial t} = -\phi^p \nabla \bullet [\lambda_{n+1} (\nabla \bullet V_{n+}^{ef}) \mathbf{I}] \quad (16)$$

in which λ_{n+1} is the factor determined by the state of intermediate velocity fields and the condition of incompressibility in the filled domain. Equations (16) are discretized by the Galerkin method to form the solution procedure as:

$$\mathbf{M}^p \frac{(V_{n+1}^p - V_{n+}^p)}{\Delta t} = \phi^p \mathbf{F}^d(\lambda_{n+1}, V_{n+}^{ef}) \quad (17)$$

where \mathbf{F}^d is the term for incompressibility correction. Numerically the term $\mathbf{F}^d(\lambda_{n+1}, V_{n+}^{ef})$ is built as:

$$\mathbf{F}^d(\lambda_{n+1}, V_{n+}^{ef}) = -\mathbf{A} \int_{\Omega} \mathbf{B}^T \mathbf{I}^e \lambda_{n+1} \bar{\mathbf{d}}_{sm}(V_{n+}^{ef}) d\Omega^e \quad (18)$$

where $\bar{\mathbf{d}}_{sm}(V_{n+}^{ef})$ are the values evaluated at Gauss points to account the compressive ratio of the effective velocity V_{n+}^{ef} in each element, which consists of the intermediate velocity fields obtained from previous fractional step by equation (2). To avoid the numerical

trouble caused by the locking of elements, these values are smoothed locally in the patch with their neighbour elements by a systematic procedure. \mathbf{B} is the interpolation function matrix \mathbf{N} , \mathbf{I}^e is a constant vector. λ_{n+1} is the corrective coefficient determined by a special feedback procedure, which will be introduced later.

The values for compressive ratio of the effective velocity field at each Gauss point is defined as:

$$\bar{\mathbf{d}}(\mathbf{V}_{n++}^{ef}) = \frac{1}{3} \text{Tr}(\dot{\mathbf{e}}_{n++}^{ef}). \quad (19)$$

A smoothing operation is chosen in the new proposed algorithm to avoid the numerical difficulties. It is a systematic operation without any piecemeal operations [5]. The smoothed nodal values \mathbf{d}_{sm} for the compressive ratios are obtained by

$$\mathbf{M}_0 \mathbf{d}_{sm}(\mathbf{V}_{n++}^{ef}) = \mathbf{A} \int_{\Omega} \mathbf{N}^T \bar{\mathbf{d}}(\mathbf{V}_{n++}^{ef}) d\Omega^e \quad (20)$$

in which \mathbf{M}_0 is a pseudo mass matrix lumped in diagonal form. It is built as

$$\mathbf{M}_0 = \mathbf{A} \int_{\Omega} \mathbf{N}^T \mathbf{N} d\Omega^e$$

So that equation (18) gets the following form:

$$\mathbf{F}^d(\lambda_{n+1}, \mathbf{V}_{n++}^{ef}) = - \mathbf{A} \int_{\Omega} \mathbf{B}^T \mathbf{I}^e \lambda_{n+1} \mathbf{N} d\Omega^e \mathbf{d}_{sm}(\mathbf{V}_{n++}^{ef}) \quad (21)$$

By the interpolation in each element, there exists the relationship $\bar{\mathbf{d}}_{sm} = \mathbf{N} \mathbf{d}_{sm}^e$ for the values at Gauss points.

Determination of the Scale Dilatancy Parameter λ

The determination of the scale dilatancy coefficient λ_{n+1} is a key issue of the new proposed method. The average compressed values of the intermediate velocity field in the filled domain Ω^F are used to determine λ_{n+1} for the feedback correction at each time step. The way to obtain λ_{n+1} is expressed as:

$$\lambda_{n+1} = \frac{\langle \mathbf{D}(\phi^s \mathbf{V}_{n++}^s + \phi^f \mathbf{V}_{n++}^f) \rangle_{sum}}{\Delta t \langle \mathbf{D}(\frac{(\phi^s)^2}{\mathbf{M}^s} + \frac{(\phi^f)^2}{\mathbf{M}^f}) \mathbf{I}_{cm}^F(\mathbf{V}_{n++}^{ef}) \rangle_{sum}} \quad (22)$$

where the notation $\langle \rangle_{sum}$ stands for the sum of all nodal values in the filled portion, \mathbf{D} is a divergence operator, while \mathbf{I}_{cm}^F substitutes the expression:

$$\mathbf{I}_{cm}^F(\mathbf{V}_{n++}^{ef}) = \mathbf{A} \int_{\Omega^F} \mathbf{B}^T \mathbf{I}^e (\nabla \cdot \mathbf{V}_{n++}^{ef}) d\Omega^e \quad (23)$$

When the λ_{n+1} is obtained, it can be introduced into equation (18) for the correction to satisfy the incompressibility condition in the filled domain. The same operations are performed in the void portion but no means to maintain a strict incompressibility. The choice for λ_{n+1} coefficient for this domain needs only to keep stability of the calculation.

NUMERICAL VALIDATIONS AND COMPARISONS WITH EXPERIMENTS

In order to verify the results of simulation by the new algorithm, a mould cavity with the form of tensile specimen is chosen. For 2D case, the triangular elements with linear interpolations are used. The mesh of the mould cavity is shown in Figure 1. For the simulation model, the pressure 16 MPa is imposed on two opposite inlets of the mould cavity. The cavity walls are assigned to be sliding without friction. 316L based feedstock is chosen for the injection. The viscosity values for metal powder and polymer binder are 35 Pa.s and 28 Pa.s respectively[6,7]. Initial volume fractions of the two distinct phases are 0.55 and 0.45 respectively. The values of their pure densities are 8 g.cm⁻³ and 1.5 g.cm⁻³ respectively. The interaction coefficient is chosen to be 2×10¹⁰ Pa.s.m⁻².

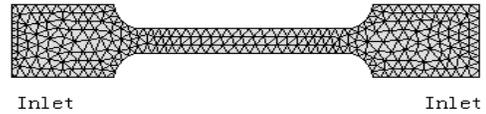


FIGURE 1. Mesh with triangle element

Mould Filling Simulation

By the new vectorial algorithm, the filling state at instant of 75% and 95% filled ratio is shown in Figure 2 and Figure 3, the white bands in post-processing indicate the position of filling fronts.



FIGURE 2. Filling fronts of the mixture flow corresponding to 75% of filling state



FIGURE 3. Filling fronts of the mixture flow corresponding to 95% of filling state

Powder Volume Fraction

At the fully filled state, the contours of solid volume fraction are shown in Figure 4. It is almost symmetrical to the centre of tensile specimen. The values decrease from the maximum near two inlets to the minimum at the centre of the specimen. The average values of volume fraction along the length of tensile specimen are shown in Figure 5. The location in abscissa axis represents its distance from the left end of specimen, as shown in Figure 4.

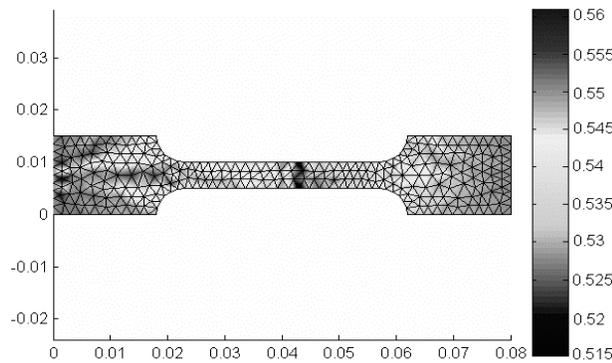


FIGURE 4. Solid volume fraction field at fully filled state

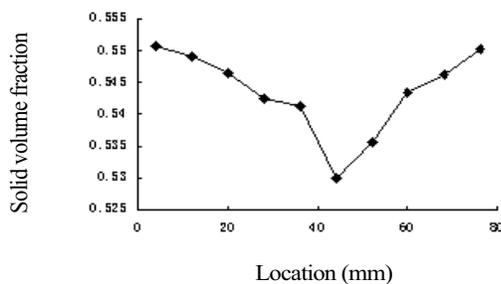


FIGURE 5. Solid volume fraction along the length of tensile specimen

Based on the values of solid volume fraction along the length of tensile specimen, the density values can be calculated and compared with the results of experiments [8], shown in Figure 6 and Figure 7. The density values obtained by simulation along the length of tensile specimen have the same tendencies with the ones obtained by experiments. The maximum density difference between

two sets of the values is less than 4.5%, it is relatively good.

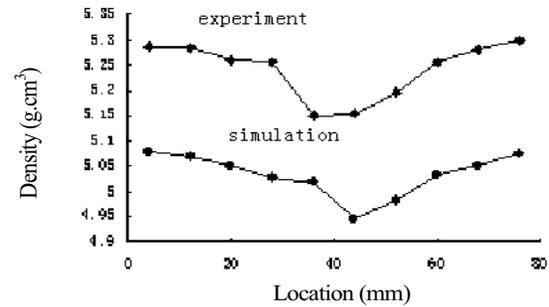


FIGURE 6. Comparison between the density values obtained from experiment and simulation

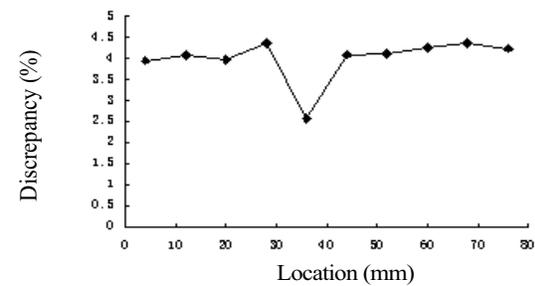


FIGURE 7. Discrepancy of the density values obtained by experiment and simulation

CONCLUSION

The prediction of the powder segregation effects in the injection stage of the PIM technology requires the application of bi-phasic model under the frame of mixture theory. For such a purpose, an explicit algorithm with fully vectorial operations is proposed and validated. This new algorithm is especially powerful for efficient simulation of the mould filling processes and phase segregation effects in PIM, that reinforces significantly the industrial applications of numerical simulations. By virtue of the new algorithm, there is neither the global solution, nor the creation of global matrix in the simulation. The computation can be carried out in fully vectorial operations with high efficiency. The comparison of numerical results with experiments proves the validity and efficiency of newly proposed algorithm.

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