3D simulations of yield-stress and shear-induced particle diffusion models

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Résumé :

On présente une méthode générale de simulation directe 3D par éléments finis d'écoulements de fluides présentant de fortes non-linéarités de comportement tels que fluides à seuil, ou suspensions à ségrégation induite par écoulement. Cette méthode utilise une technique d'adaptation de maillage a posteriori, qui permet d'obtenir une précision de calcul élevée pour un nombre limité de degrés de liberté du problème discrétisé. Différents exemples d'application seront proposés.

Abstract:

A general 3D finite elements method for fluid flows is presented. It focuses on the resolution of highly nonlinear flow models such as yield stress fluids and flow-induced segregation suspensions models. The method is based on an a posteriori mesh adaptation procedure that allows obtaining a high precision for controlled computational cost in terms of number of degrees of freedom of the discretized problem. Several application examples will be presented.

Mots clefs : finite elements method, yield stress fluids, flow induced segregation models, mesh adaptation

1 Introduction

The current work has been motivated by the study of paste extrusion. Very often, it is found that paste materials (which are basically made of a mixture of solid fillers dispersed at moderate to high volume fraction within a lubricant fluid) behave as yield-stress fluids when considering their apparent stationary flow curves. Recently, models of flow-induced segregation of solid fillers have been proposed [1, 2] to predict transient effects and non-homogeneous volume fraction effects observed in pastes and dense suspensions flows. The goal of this paper is to show the impact of such effects (apparent yield-stress and flow-induced segregation) in 3D paste extrusion flows. To reach this objective at reasonable computational cost, specific numerical techniques were used. In the following, flow model equations and numerical techniques are presented. Finally an application example is shown.

2 The physical model

2.1 Flow equations

The flow of concentrated suspensions takes place at low Reynolds number ($Re \ll 1$). The conservation equations for steady, incompressible flow are

$$\nabla \cdot \vec{u} = 0 \tag{1}$$

$$-\nabla p + \nabla \cdot \bar{\bar{\tau}} = 0 \tag{2}$$

Considering a generalised Newtonian fluid the stress tensor is expressed as follows

$$\bar{\bar{\tau}} = 2\eta \bar{\bar{\dot{\gamma}}} \tag{3}$$

with $\bar{\bar{\dot{\gamma}}}$ the strain rate tensor defined as

$$\bar{\bar{\dot{\gamma}}} = \frac{1}{2}\left(\nabla\vec{u} + (\nabla\vec{u})^T\right) \tag{4}$$

First the viscosity function $\overline{\eta}$ can be assigned as a function of strain rate in case of the Bingham [3] or Herschel-Bulkley [4] model. For example, using its Bercovier-Engleman [5] regularisation form, the Bingham viscosity is expressed as

$$\overline{\eta} = \eta + \frac{\tau_y}{\left(\dot{\gamma}^2 + \varepsilon^2\right)^{1/2}} \tag{5}$$

where η is the viscosity, τ_y the yield stress $\dot{\gamma}$ the second invariant of the strain rate tensor and ε a regularisation parameter.

An alternative is to consider a viscosity function obeying the Krieger-Dougherty [6] relationship

$$\overline{\eta} = \eta\left(1 - \frac{\phi}{\phi_{\max}}\right)^q \tag{6}$$

where ϕ is the filler volume fraction, η is the viscosity of the lubricant fluid, ϕ_{max} is the maximum packing fraction in the suspension and q a parameter usually equal to 2.

2.2 Diffusive-flux model

Phillips et al. [2] modelled the shear-induced particle migration due to the gradients in volume fraction and shear rate. The diffusion equation for the particle volume fraction ϕ defined in equation (6) can be written as

$$\frac{D\phi}{Dt} = \nabla\cdot\left[K_c a^2 \phi\nabla(\phi\dot{\gamma}) - K_\eta a^2 \dot{\gamma}\phi^2 \frac{1}{\eta}\frac{\partial\eta}{\partial\phi}\nabla\phi\right] \tag{7}$$

It is assumed that the density of the particles and the lubricant are equal and gravity and buoyant effects are neglected. The diffusion equation is solved with appropriate boundary conditions along the die surfaces, where it is assumed that the fluid does not slip ($\boldsymbol{u} = 0$). Obviously, no particles flow through the surfaces

$$\left\{K_c\phi\nabla(\phi\dot{\gamma}) + K_\eta\dot{\gamma}\phi^2\frac{1}{\eta}\frac{\partial\eta}{\partial\phi}\nabla\phi\right\}\cdot n = 0 \tag{8}$$

At flow entrance at initial time, particle concentration was assumed to be uniform, i.e. $\phi = \phi_0$.

3 Solution procedure

The Finite Element Method (FEM) was employed to solve numerically the governing equations with boundary and initial conditions. For both models (yield-stress models or shear-induced diffusion models) the velocity-pressure problem was solved using a P1+/P1 based mixed finite elements developed within a fully parallel SPMD (single program, multiple data) strategy [7-10]. The generalized diffusion equation (7) was solved using a modified version of the RFB (residual-free bubble) technique [11] applied to a P1 approximation.

A continuation method on the parameter ε was used to solve the non-linear Stokes problem (5) and a semi-implicit Euler scheme was used to solve the split time dependant problem (7). At each continuation or time step, an anisotropic mesh adaptation procedure was used [12, 13]. It consists in building a number of node-controlled target metric field based on the Hessian of the shear-rate field.

4 Example of computation

The simulation of a 3-D Bingham flow with a yield stress of τ_y = 3 10^5 Pa and viscosity η = 3 10^4 Pa.s flowing at maximum speed of 1.4 mm/s within half a slit die of 30 mm gap is shown figure 1. The regularisation parameter was 10^{-4} times the apparent strain rate, obtained using 16 continuation steps. Number of nodes is approximatively 28 800, which can be considered as low with respect to the obtained precision. Indeed, one can observe that mesh adaptation allows obtaining a rather good description of

unyielded zones (defined as the zones for which the stress field magnitude is lower than τ_y). This result was obtained in ~2 h using a 16 Amd Opteron 6134 processors cluster equipped with an Infiniband DDR 20 Gb/s network.

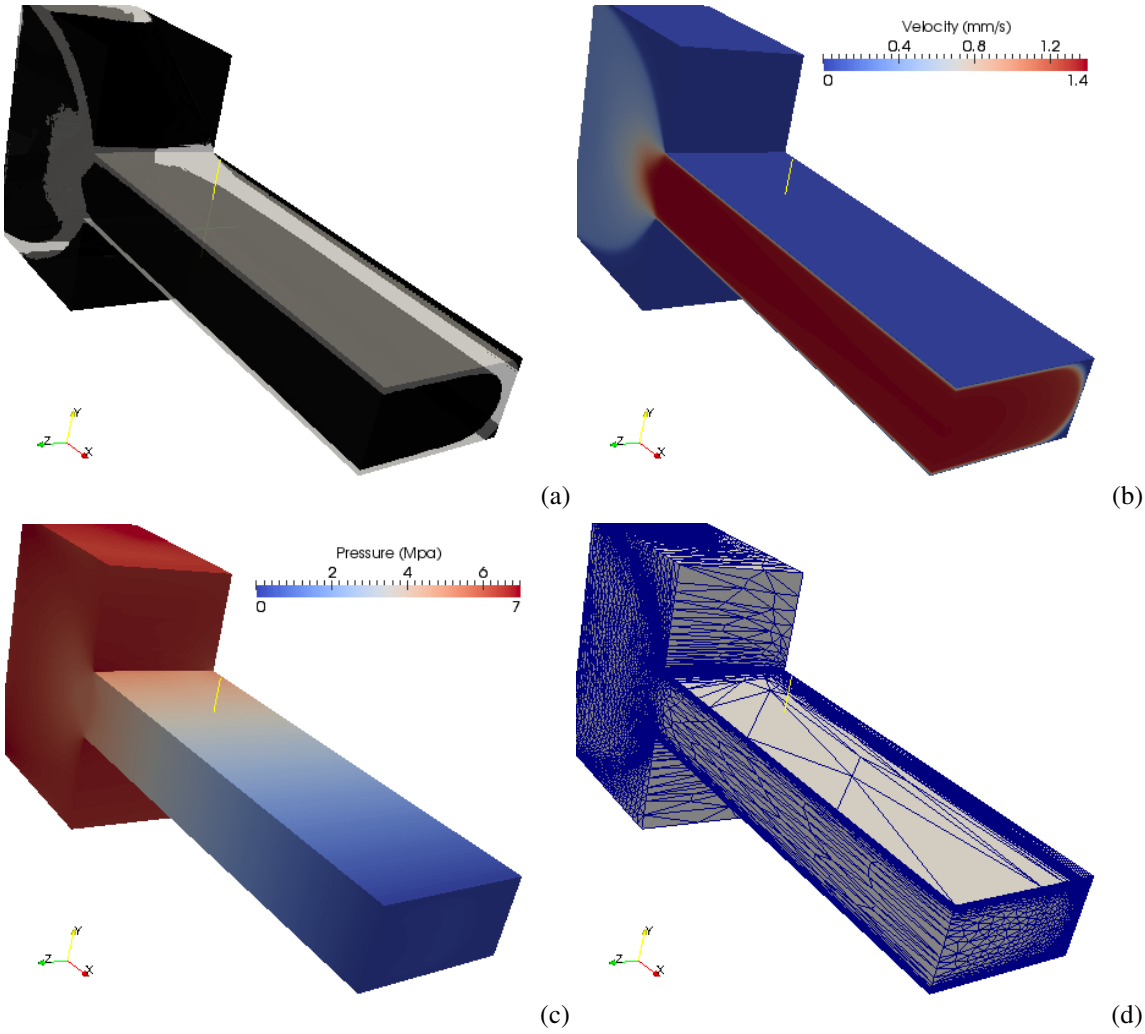

FIG. 1 – 3-D simulation results (symmetry plane is on the left face). (a) Unyielded zones (in black) produced by a Bingham fluid inside a rectangular die. (b) Norm of the velocity field. (c) Pressure field. (d) Adapted mesh. It can be noticed that the undeformed zones in the die occupy most of the region and the flow is mostly a plug.

5 Conclusion

The FEM has been employed to solve non-linear and/or time-dependent flows of yield-stress and shear-induced particle diffusion models, allowing a high precision for controlled computational cost in terms of number of degrees of freedom of the discretized problem. Several application examples will be presented during the conference. In particular, a comparison of flow fields between yield-stress fluids and flow-induced segregation fluids exhibiting similar stationary flow curves will be presented.

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