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SPH simulations of three-dimensional non-Newtonian free surface flows

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ABSTRACT

In this paper, the smoothed particle hydrodynamics (SPH) method is extended to deal with three-dimensional (3D) non-Newtonian flows with complex free surfaces, in which the viscosity is modeled using the Cross model. In order to alleviate the so-called tensile instability which leads to particle clustering and unphysical fracture in fluid stretching, an artificial stress term is particularly incorporated into the momentum equation. For convenience in implementation of wall boundary condition in 3D, an enhanced treatment of solid boundaries is proposed to improve the computational performance. Parallelization is also developed to ensure affordable computational time of simulations involving millions of particles. The proposed SPH algorithm is validated by solving the Hagen–Poiseuille flow and comparing the SPH results with the available analytical solutions. To demonstrate the ability of the numerical method in simulating 3D non-Newtonian flows with free surfaces, three challenging engineering applications, including the impacting droplet, molding injection of a thin plate mold and a Z-shaped mold, and jet buckling, are investigated. It is found that the shear-thinning behavior can be well displayed in all cases, and the proposed SPH algorithm is stable and fairly accurate and agrees well with the available data.

1. Introduction

Simulation of free surface flows is an important and active research field in computational fluid dynamics, where the traditional grid-based numerical methods are extensively employed, including finite difference method (FDM), finite volume method (FVM) and finite element method (FEM). To cope with moving free surface and large deformation, complicated techniques of capturing and/or tracking the free surface as well as regenerating the computational grid are generally required, for instance, volume of fluid (VOF) [1], marker and cell (MAC) [2] and level set (LS) [3] methods. In the VOF approach, tracking of dynamical interface is accomplished by solving an additional partial differential equation for the filled fraction of each control volume. The MAC technique utilizes marker to track the free surface, while an additional implicit level set function is employed in the LS method.

On the other hand, many particle methods [4,5] have also been proposed in the Lagrangian framework to deal with the flows with moving free surface. Actually, particle methods have a variety of advantages over conventional grid-based methods. It is inherently suitable for simulating the flows with moving free surface and large deformation because the evolution of fluid particles can be readily obtained due to its purely Lagrangian mesh-free nature. Also, it is comparatively easier in numerical implementation, and is more straightforward to develop 3D model than grid-based methods. As a typical particle method, smoothed particle hydrodynamic (SPH) was first introduced by Lucy [4] and Gingold and Monaghan [5] in astrophysics to study the collision of galaxies. Recently, it has been extensively applied in a wide range of research areas, such as free surface flows [6–8], multi-phase flows [9–11], and non-Newtonian [12–14]. For more information on the SPH method, we refer the reader to the recent review of the method by Liu et al. [15].

As for the SPH simulation of non-Newtonian free surface flows, a two-dimensional (2D) dam-break problem of a Cross fluid was first investigated by Shao and Lo [16]. The impact of an Oldroyd-B droplet with a rigid plate was further simulated by Fang et al. [17], and it was found that an artificial stress term was required to remove the so-called tensile instability, which results in particle clustering and unphysical fracture in fluid stretching. With the employment of pressure Poisson equation to satisfy the incompressibility constraint, Rafiee et al. [18] solved the impacting droplet and jet buckling problems. More recently, Vázquez-Quesada and Ellero [19] simulated the flow of Oldroyd-B liquid around a linear array of cylinders confined in a channel and compared the dimensionless drag force acting on the cylinder with the available results. And Hashemi et al. [20] studied the movement of suspended solid bodies in Oldroyd-B fluid flows using an explicit weakly compressible SPH method.

The research works mentioned above are mainly considered in 2D space, and few 3D SPH simulations of non-Newtonian fluid

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flows have been carried out so far. This might be due to the massive memory requirement and the huge computational time, since the number of particles required in 3D is usually too large to be handled by a single processor. At present, some parallel techniques of the SPH method have been developed to reduce the computational cost. Specifically, Moulinec et al. [21] designed a parallel SPH code called *Spartacus-3D* to successfully simulate the 3D periodic hill flow and dam breaking flow. Ferrari et al. [22] proposed a new robust and accurate SPH scheme, and carried out the corresponding parallelization using the message passing interface (MPI) standard, together with a dynamic load balancing strategy. Recently, an open source SPH code called *JOSEPHINE* was developed by Cherfils et al. [23] to solve unsteady free surface flows.

This paper is directly motivated by the food and cosmetic product industries where the materials tend to be shear-thinning but not necessarily viscoelastic. The so-called shear-thinning effect is actually a common property of polymer solutions, in which the viscosity decreases with increasing local shear rate. In addition, 3D SPH simulations would be more significant to practical problems. Therefore, a parallel version of 3D SPH solver is developed in this study, and free surface flows of shear-thinning fluids, characterized by the Cross model, are further investigated. For convenience in implementation of wall boundary condition in 3D, an enhanced treatment of solid boundaries is proposed to improve the computational performance. The artificial stress term presented in [24,25] is also incorporated into the momentum equation to alleviate the so-called tensile instability. The proposed SPH algorithm is first validated by solving the Hagen–Poiseuille flow and comparing the SPH results with the analytical solutions. Then, three challenging test cases, *i.e.*, the spreading droplet, injection molding of a thin plate mold and a Z-shaped mold, and jet buckling, are investigated to demonstrate the ability of the numerical method in simulating 3D non-Newtonian free surface flows. Finally, the paper ends with some conclusions.

2. Governing equations

In a Lagrangian frame, the governing equations for the flow of an isothermal, transient, weakly compressible fluid can be written as

$$\frac{d\rho}{dt} = -\rho\frac{\partial v^\beta}{\partial x^\beta}, \tag{1}$$

$$\frac{dv^\alpha}{dt} = \frac{1}{\rho}\frac{\partial\sigma^{\alpha\beta}}{\partial x^\beta} + F^\alpha, \tag{2}$$

where ρ is the fluid density, x^β is the spatial coordinate, v^β is the βth component of the fluid velocity, and $\sigma^{\alpha\beta}$ is the (α,β)th component of the Cauchy stress tensor. The term F^α denotes the αth component of the acceleration due to external forces. d/dt is the material time derivative operator, *i.e.*, $d/dt = \partial/\partial t + v^\beta\partial/\partial x^\beta$.

The Cauchy stress tensor in Eq. (2) is decomposed into the ordinary isotropic pressure p and the extra-stress tensor $\tau^{\alpha\beta}$

$$\sigma^{\alpha\beta} = -p\delta^{\alpha\beta} + \tau^{\alpha\beta}, \tag{3}$$

where $\delta^{\alpha\beta} = 1$ if $\alpha = \beta$ and $\delta^{\alpha\beta} = 0$ if $\alpha \neq \beta$.

2.1. Rheological models

Both Newtonian and non-Newtonian fluid flows are considered in this paper, and the popular Cross model is introduced as the rheological model. The constitutive equation for $\tau^{\alpha\beta}$ is given by

$$\tau^{\alpha\beta} = 2\mu(\dot\gamma)d^{\alpha\beta}, \tag{4}$$

where $\mu(\dot\gamma) = \rho\upsilon(\dot\gamma)$ is the dynamic viscosity, $\upsilon(\dot\gamma)$ is the kinematic viscosity, $\dot\gamma$ is the local shear rate defined by

$$\dot\gamma = [2\mathrm{tr}(d^{\alpha\gamma}\cdot d^{\gamma\beta})]^{1/2} \tag{5}$$

and $d^{\alpha\beta}$ is the rate-of-deformation tensor given by

$$d^{\alpha\beta} = \frac{1}{2}\left(\frac{\partial v^\alpha}{\partial x^\beta} + \frac{\partial v^\beta}{\partial x^\alpha}\right). \tag{6}$$

The symbol "tr" denotes the trace of matrix.

The kinematic viscosity $\upsilon(\dot\gamma)$ representing the shear-thinning nature of the fluid is chosen as [26]

$$\upsilon(\dot\gamma) = \upsilon_\infty + \frac{\upsilon_0 - \upsilon_\infty}{(1 + (K\dot\gamma)^m)}, \tag{7}$$

where m, υ_0, υ_∞ and K are given positive constants. As for the Newtonian fluid flow, the kinematic viscosity is equivalent to υ_0, *i.e.*, $K = 0$.

2.2. Equation of state

Generally, there are two typical approaches for solving the governing equations, namely the incompressible SPH [27] and the weakly compressible SPH [28,29] methods. In the incompressible SPH method, a pressure Poisson equation is particularly employed to enforce a divergence-free velocity field, and the fluid pressure is further evaluated accordingly. However, the pressure in the weakly compressible SPH algorithm is explicitly calculated from a simple thermodynamic equation of state. The time-consuming solution of linear system of equations is avoided in weakly compressible SPH algorithm, and thus is quite suitable for 3D large-scale SPH simulations. In this study, we follow the latter approach by using the following two equations of state [13,30]:

$$p(\rho) = c^2\rho^2/2\rho_0 \tag{8}$$

and

$$p(\rho) = c^2(\rho - \rho_0), \tag{9}$$

where c is the speed of sound and ρ_0 is the initial fluid density. To ensure that the artificial compressible flow is sufficiently close to the behavior of truly incompressible fluid, the Mach number should be less than 0.1 in practice [13]. Note that Eq. (8) is only applied to the Hagen–Poiseuille flow in Section 4.1, while for flows with free surface studied in Sections 4.2-4.4, Eq. (9) is used to obtain almost zero pressure level on the free surface.

3. Smoothed particles hydrodynamics

3.1. Basic SPH methodology

In the SPH method, the fluid domain Ω is discretized into a finite number of particles with associated physical quantities, such as density, pressure, mass and velocity. The fields of the particle of interest are determined by relevant information of neighboring particles within the support domain. An arbitrary function $A(\mathbf{r})$ defined at the position $\mathbf{r} = (x, y, z)$ can be expressed by the following integral:

$$\langle A(\mathbf{r})\rangle = \int_\Omega A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}', h)d\mathbf{r}', \tag{10}$$

where W is the so-called kernel function and h is the smoothing length. The chosen kernel function should satisfy several conditions, such as normalization, compact condition, and delta function property. In this paper, the popular quintic spline kernel [18] is used for all simulations.