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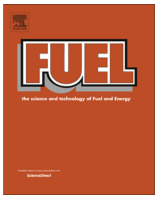

Modeling gelled fluid flow with thixotropy and rheological hysteresis effects

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HIGHLIGHTS

- We developed a constitutive model to consider thixotropy and rheological hysteresis in a gelled fluid flow.
- Using a proposed mode, the plain orifice flows have been simulated and rheological processes and hydrodynamic instabilities have been observed.
- We compared the thixotropic fluid flows with Newtonian and shear-thinning fluid flows.
- A parametric study has been conducted in terms of the rheological response rate in a proposed model.

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ABSTRACT

A new model has been developed for describing the rheology of thixotropic fluids. The model accounts for hysteresis effects when the fluid goes through multiple shearing events. To demonstrate the model capability, a series of unsteady, three-dimensional simulations are presented for flow through a plain orifice passage. The thixotropic liquid simulation showed the behavior generally bounded by Newtonian and shear-thinning liquids limits. For high Reynolds number injection conditions, quasi-periodic behavior is noted as in prior studies with Newtonian and shear-thinning fluids. The effect of fluid rheology and response rates is also parametrically considered to demonstrate the role of the model parameters.

1. Introduction

Flow of thixotropic fluids has attracted the attention of researchers given the natural occurrence of this flow in many processes related to the chemical, food and pharmaceutical areas. Studies of thixotropic fluids in well defined geometries of practical applications to industrial operations have been performed using both empirical and analytical approaches [1–3]. A simple example that demonstrates fluid response to shearing events is the flow through an orifice passage. Plain-orifice flows are widely found in metering applications due to ease of fabrication. Our group has studied the behavior of shear-thinning gelled fluids in orifice flows motivated by a rocket propellant application [4,5]. Gelling of the fuel (or oxidizer in a rocket application) has the potential to improve safety should leaks occur [6–8]. In addition, the use of energetic gelling agents could enhance performance in these applications.

Because of the high injection velocities required to atomize a gelled fuel, a very large range of shear rates are encountered in these injection processes [4,9,10]. At the high-speed injection conditions, the viscosity of the fluids approaches the so-called Newtonian plateau where viscosity becomes independent of shear rate.The limitations of simple shear-thinning modeling become apparent in this application and unreasonably high viscosity peaks periodically appeared in the low shear rate region downstream of the orifice inlet [4]. Due to the large shear and short flow times in this application, it became apparent that thixotripic and hysteresis effects could be quite important to describe the behavior of the fluid in this flowpath. It was this factor that motivated the present study. From a practical perspective, the high velocities encountered in the rocket application provides an excellent challenge as the shear rates for this application bound practically all other potential applications for a model of this type.

Major rheological phenomena pertinent to gelled fluid flow include shear-thinning, thixotropic and viscoelastic behavior. Shear-thinning behavior is common in many weak gels, and is characterized by a reduction in viscosity with increases of shear rate. This behavior is most commonly observed in inorganic gels [4,5,9,11]. Thixotropy accounts for the viscosity decrease with time under a given shear rate; presumably due to destruction (temporary or more permanent) of the network forming the gel under the action of the imposed shear. Silica-based organic gels are

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Nomenclature

E	flux vector	x	Cartesian coordinates
L	orifice length	α	response rate for shear-thinning
Q	solution vector or turbulence Q criterion	β	response rate for shear-thickening
V	mean flow velocity through the orifice	δ	Kronecker delta
Y	species	η	apparent viscosity
p	pressure	γ	strain rate tensor
e	equilibrium	λ	thermal conductivity or relaxation factor
i	index of the Cartesian coordinate or condition of the gel	ρ	density
n	shear-thinning power index	τ	stress tensor
u	velocity vector	0	stagnation quantity or zero shear quantity
v	viscous terms	∞	high shear Newtonian plateau quantity

reported to have thixotropy [12]. Lastly, viscoelasticity is a property which depends on the shear history and the properties of material and plays a key role in extrusion processes. Fluid relaxation from imposed shear can have either viscous or elastic character, or even a combination of both. Viscoelastic gels have a complex structure with rheological responses showing stresses that are a function of the applied strains and strain rates. The specific relationship of the resulting stress as a function of the applied strain rate indicates a time-dependent behavior of viscoelastic materials which is recognized as material that exhibit memory effects. The very complex rheology associated with thixotropic and viscoelastic fluids has presented a challenge in both characterization and in the modeling the flow of these gels.

Physically, the breakdown of a gel structure under imposed shear can be attributed to internal collisions and Brownian motion. These behaviors give rise to a bulk rheological behavior often refered to as fluid thixotropy. Factors governing thixotropic response include imposed shear forces and molecular motion arising from the characteristics of the molecules forming the fluid, as well as micro and macro structural characteristics of the fluid. For most thixotropic gels, the rate of structure breakdown is generally more rapid than that of its reconstruction. The structure may never be fully recovered to the original unstrained condition (jello is classic example). The recovery time, or overall degree of recovery is of obvious interest in many application as a gelled fluid is delivered to a container for long term storage and eventual usage.

The objective of this study is to develop a general numerical treatment for thixotropic effects that is suitable for inclusion in a multidimensional computational fluid dynamic (CFD) tool. All fluids which have some sort of a macrostructure as exhibited by colloidal systems or gels may exhibit thixotropy because the forces keeping that macrostructure in place may not be enough to stand high shear forces during testing or in a flow. The relationship between the applied shear and the ability of the material to recover its gel structure is one of the main causes of thixotropy especially when the material cannot recover the original structure within a time that is associated with the residence in the flowpath. For example, flocculated colloidal particles, mean alignment of fibre-like particles, high entanglement density of polymeric structures, or even molecular associations can contribute to gel network breakdown under applied shear events. Metal particle addition into the gel may also play a role as a flocculated particle system. The model must accurately reflect this time-dependent behavior in order to capture thixotropic effects.

As an example, Green and Weltzman [13] indicated basic principles of the hystersis loop in the pigment/vehicle system and characterize the thixotropic system by means of hystersis loop. In addition, Santos et al. [14] characterized this behavior for particulate gels by considering a ramp-up and ramp-down of shear imposed in a rotational rheometer. Fig. 1 indicates the viscosity hysteresis observed during ramp-up and ramp-down of the imposed shear rate. This rheological response would be common for many industrial processes that route fluid through a plumbing network to a storage vessel. To effectively simulate this type of behavior, memory of the initial shearing events must be included within the rheological model.

2. Model description

2.1. Computational framework

Computations reported here used the in-house, unstructured finite volume solver, GEMS (General Equation and Mesh Solver). [15,16] GEMS is a coupled, density-based equation solver using a preconditioning method for incompressible fluid flows. It solves the momentum equations in conjunction with the continuity, energy and species equation described below.

$$\frac{\partial Q}{\partial t}+\frac{\partial (E_i-E_{vi})}{\partial x_i}=0 \tag{1}$$

where the vectors, Q, E_i, and E_{vi}, are given by:

$$E_i=\begin{pmatrix}\rho u_i\\ \rho Y u_i\\ \rho u_i u_j+\delta_{ij}p\\ \rho u_i h^0-p\end{pmatrix}\quad Q=\begin{pmatrix}\rho\\ \rho Y\\ \rho u_j\\ \rho h^0-p\end{pmatrix}\quad E_{vi}=\begin{pmatrix}0\\ \rho D\frac{\partial Y}{\partial x_i}\\ \tau_{ij}\\ \tau_{ij}u_j+\lambda\frac{\partial T}{\partial x_i}\end{pmatrix} \tag{2}$$

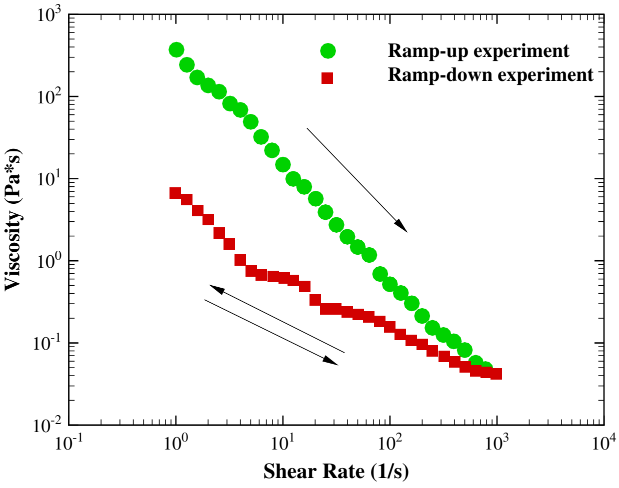

Fig. 1. Rheological hysteresis from the 4% silica/JP-8 experiment using a rotational rheometer [14].