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Letter

Effect of fluid elasticity on the numerical stability of high-resolution schemes for high shearing contraction flows using OpenFOAM

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ABSTRACT

Viscoelastic fluids due to their non-linear nature play an important role in process and polymer industries. These non-linear characteristics of fluid, influence final outcome of the product. Such processes though look simple are numerically challenging to study, due to the loss of numerical stability. Over the years, various methodologies have been developed to overcome this numerical limitation. In spite of this, numerical solutions are considered distant from accuracy, as first-order upwind-differencing scheme (UDS) is often employed for improving the stability of algorithm. To elude this effect, some works been reported in the past, where high-resolution-schemes (HRS) were employed and Deborah number was varied. However, these works are limited to creeping flows and do not detail any information on the numerical stability of HRS. Hence, this article presents the numerical study of high shearing contraction flows, where stability of HRS are addressed in reference to fluid elasticity. Results suggest that all HRS show some order of undue oscillations in flow variable profiles, measured along vertical lines placed near contraction region in the upstream section of domain, at varied elasticity number $E \approx 5$. Furthermore, by E, a clear relationship between numerical stability of HRS and E was obtained, which states that the order of undue oscillations in flow variable profiles is directly proportional to E.

1. Introduction

Viscoelastic fluids are special category of non-Newtonian fluids which show viscous, elastic and non-linear responses to the flows. Such characteristics make these fluids very useful in daily routine works such as laundry liquids, glues, gels, oils, sauces, paints, etc. Also, these fluids are abundantly used in process and polymer industries. Typical industrial application includes extrusion and mould flow processes. In these processes, final outcome of the product depends significantly on the property and pattern of flow [1]. As these processes offer abrupt contraction to the flow of fluid, it gives rise to stress singularity near the re-entrant corner. At this point, the stress term rises exponentially to very high value. Hence, this problem is widely studied in past, both experimentally and numerically [2,3].

With the advancement in conventional rheometers, experimental works offer comparatively an easy prediction of flow properties [4]. However, this problem is numerically difficult to study due to the non-linear nature of constitutive equations [5]. Also, these works are subjected to loss of numerical stability at high Deborah numbers, commonly referred as high Deborah number problem (HDNP) [6]. To overcome this elevated issue of HDNP, numerous numerical methodologies have been put forward [7–14]. Amid this, some of the famous methodologies which can be applied to finite volume technique are both-side-diffusion (BSD) [11], log-conformation representation (LCR) [12], positive definiteness preserving scheme (PDPS) [13] and square-root conformation representation (SRCR) [14]. In the past, Jovani et. al [15] also presented split-stress approach in reference to OpenFOAM which resembles the BSD approach. This approach promotes numerical stability of the algorithm by adding additional diffusive terms on both sides of the momentum equation. While, other approaches promote numerical stability of the algorithm, by preserving positive definiteness of conformation tensor on discrete level [16].

As numerical stability of the algorithm is often considered important, accuracy of the results are usually overlooked for viscoelastic fluids. This problem was first addressed by Alves et al. [10], in which first-order upwind-differencing scheme (UDS) and second-order numerical schemes were compared. Broadly, accuracy of numerical solution depends heavily on the order of convective schemes [17]. These schemes are classified according to its polynomial relationship of control volume grid points. Numerical schemes relying only on the immediate neighbouring control volume grid point are referred as lower-order schemes. However,

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schemes relying on large number of control volume grid points are mentioned as higher-order (HO) schemes. These unbounded schemes though accurate, give rise to undue oscillations of numerical solutions for convection dominated flows. These unwanted oscillations can be suppressed by imposing any of these conditions: (1) total variation diminishing (TVD) [18], (2) convection boundedness criterion (CBC) [19]. To further improve the convergence and stability of numerical schemes, a special class of bounded schemes are used which are commonly known as high-resolution schemes (HRS) [19–23]. Over the last decade, some works were reported using HRS for viscoelastic fluids [6,15,16,24–26]. In broad terms, these works assessed the numerical stability of algorithm for different Deborah numbers. Also, these studies are limited to low shearing flows or creeping flows. Consequently, insufficient information is available on the numerical stability of high shearing flows. This article therefore presents a study of high shearing flows using the existing viscoelastic fluid flow solver [15] and HRS, wherein elasticity number is varied, in order to assess the numerical stability of HRS. In the present context of this paper, HRS are implemented using the blending factor (γ) method [21] in OpenFOAM.

The article is presented as follows: The governing equations for isothermal, incompressible and viscoelastic fluid are detailed in Sect. 2.1, followed by a brief description of BSD approach, numerical discretization and numerical algorithm in Sects. 2.2, 2.3 and 2.4, respectively. In Sect. 2.3, an overview of normalized variable approach and HRS are presented. Later in Sect. 3, flow geometry and mesh characteristics of planar contraction is outlined. Thereafter, under the results and discussion section, a comparative study of undue oscillations of flow variable profiles for HRS are detailed and assessment of numerical stability of HRS for varied elasticity number (E) are also presented, respectively. Finally, conclusions are reported based on these results which details the numerical stability of HRS in reference to E.

2. Numerical methodology

2.1. Governing equations

The governing mass and momentum conservation equations for isothermal, incompressible and viscoelastic fluid in vector form are written as:

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \tag{2}$$

where $\boldsymbol{u}$ refers to the velocity vector, ρ refers to the density, p refers to the pressure and $\boldsymbol{\tau}$ refers to the total stress. This total stress can be decomposed into viscous and elastic parts:

$$\boldsymbol{\tau} = \boldsymbol{\tau}_\mathrm{S} + \boldsymbol{\tau}_\mathrm{P}, \tag{3}$$

where $\boldsymbol{\tau}_\mathrm{S}$ denotes the solvent (viscous) contribution and $\boldsymbol{\tau}_\mathrm{P}$ denotes the polymeric (elastic) contribution. The viscous term $\boldsymbol{\tau}_\mathrm{S}$ is further detailed as under:

$$\boldsymbol{\tau_S} = \eta_\mathrm{S} \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\mathrm{T}\right]. \tag{4}$$

In this equation, η_S refers to the solvent viscosity. And, the polymeric term $\boldsymbol{\tau}_\mathrm{P}$ referred in Eq. (3), depends upon the viscoelastic fluid model. As the simplest viscoelastic models (UCM and Oldroyd-B) does not predict the shear-thinning characteristics of the fluid, so the single-mode Giesekus model [27] is being considered for formulation of constitutive equation. Moreover, this model enables decent prediction of first and second stress differences for the mobility factor α in the range of $0 < \alpha < 0.5$.

$$\boldsymbol{\tau}_\mathrm{P} + \lambda \overset{\nabla}{\boldsymbol{\tau}}_\mathrm{P} + \alpha \frac{\lambda}{\eta_\mathrm{P}} (\boldsymbol{\tau}_\mathrm{P} \cdot \boldsymbol{\tau}_\mathrm{P}) = \eta_\mathrm{P} \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\mathrm{T}\right], \tag{5}$$

where η_P represents the polymeric contribution of shear viscosity, λ represents the relaxation time, α represents the mobility factor and $(\boldsymbol{\tau}_\mathrm{P} \cdot \boldsymbol{\tau}_\mathrm{P})$ represents the non-linear term, which corresponds to qualitative description of viscoelastic properties [27–29]. And, $\overset{\nabla}{\boldsymbol{\tau}}_\mathrm{P}$ refers to the upper convected derivative which is defined as under [30]:

$$\overset{\nabla}{\boldsymbol{\tau}}_\mathrm{P} = \frac{\mathrm{D}\boldsymbol{\tau}_\mathrm{P}}{\mathrm{D}t} - (\nabla \boldsymbol{u})^\mathrm{T} \cdot \boldsymbol{\tau}_\mathrm{P} - \boldsymbol{\tau}_\mathrm{P} \cdot \nabla \boldsymbol{u}. \tag{6}$$

By substituting Eq. (6) in Eq. (5), following constitutive equation is obtained:

$$\begin{aligned} &\frac{\boldsymbol{\tau}_\mathrm{P}}{\lambda} + \frac{\delta \boldsymbol{\tau}_\mathrm{P}}{\delta t} + \nabla \cdot (\boldsymbol{u}\boldsymbol{\tau}_\mathrm{P}) + \frac{\alpha}{\eta_\mathrm{P}} (\boldsymbol{\tau}_\mathrm{P} \cdot \boldsymbol{\tau}_\mathrm{P}) \\ &\quad = \frac{\eta_\mathrm{P}}{\lambda} \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\mathrm{T}\right] + (\nabla \boldsymbol{u})^\mathrm{T} \cdot \boldsymbol{\tau}_\mathrm{P} + \boldsymbol{\tau}_\mathrm{P} \cdot \nabla \boldsymbol{u}. \end{aligned} \tag{7}$$

Thus, by substituting Eqs. (3), (4) and (7) into Eq. (2), give rise to the complete governing momentum equation for viscoelastic fluids.

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) - \nabla \cdot \eta_\mathrm{S} \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\mathrm{T}\right] = -\nabla p + \nabla \cdot \boldsymbol{\tau}_\mathrm{P}. \tag{8}$$

These equations though complete in all aspects, are subjected to the loss of numerical stability when solvent viscosity ($\eta_\mathrm{S} \approx 0$) reduces to negligibly small value. To overcome this shortcoming, both-side-diffusion (BSD) approach is considered in the present study [11].

2.2. Both-side-diffusion approach

In momentum equation, non-linear hyperbolic stress term ($\boldsymbol{\tau}_\mathrm{P}$) is calculated based on the constitutive equation. When $\eta_\mathrm{S} \rightarrow 0$, elliptic diffusive term on the left-hand-side (LHS) of Eq. (8), reduces to zero. This absence of an explicit diffusive term makes these equations difficult to converge for high shearing flows. In order to overcome this limitation, an additional diffusion term is added on both sides of momentum equation. Thus, Eq. (8) changes to:

$$\begin{aligned} &\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}\boldsymbol{u}) - \nabla \cdot (\eta_\mathrm{S} + \eta_\mathrm{P}) \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\mathrm{T}\right] \\ &\quad = -\nabla p - \nabla \cdot \eta_\mathrm{P} \left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\mathrm{T}\right] + \nabla \cdot \boldsymbol{\tau}_\mathrm{P}. \end{aligned} \tag{9}$$

This approach of adding diffusive terms is commonly referred as BSD approach. In above equation, all terms on the LHS are implicitly treated and remaining right-hand-side (RHS) terms are explicitly added as a source. In case of numerical convergence, these added terms cancel each other.

2.3. Numerical discretization

In this section, the governing flow equation (referred in Eq. (9)) are integrated over a control volume and gauss divergence theorem is applied over it, to give a set of discretized equations [17]. In this equation, unsteady, time-dependent terms are discretized using the Crank Nicolson scheme and convective terms of momentum and constitutive equations are discretized using the high resolution scheme (HRS). While, remaining terms are discretized using the central difference scheme. All flow variables are stored using the non-staggered, collocated grid arrangement of OpenFOAM. And localize normalized variable approach [21] is being considered for formulation of HRS.

2.3.1. Normalized variable approach

Figure 1 shows the actual plot of convected variables and distances of the control volume, along positive flow direction. These variables and distances are normalized using the localize normalized variable approach for any arbitrary control volume mesh.