A Numerical Method for the Transient Couette Flow of a Distributed-Order Viscoelastic Fluid*

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Abstract. This work presents a numerical method for the solution of two coupled distributed-order fractional differential equations, that appear in the pure tangential flow of fluids modelled by the Distributed-Order Viscoelastic Model. We prove the solvability of the method, and, perform numerical simulations of relaxation tests.

Keywords: Distributed-Order Fractional Derivatives · Numerical Methods · Finite Differences · Viscoelasticity.

1 Introduction

The word polymers comes from the Greek poly, meaning "many," and mere, meaning "parts," because the macromolecules of these compounds are formed by joining several units of small molecules called monomers.

Polymers were not invented by man, they already existed in nature. Some examples of macromolecules that have been used by man for thousands of years are in cotton, wool, silk, animal hooves, ivory and starch (which is found in

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vegetables and in the form of grains from seeds and roots of various plants, such as: Potato, wheat, rice, corn and cassava).

With the industrial revolution, the need to understand the behaviour of such complex materials increased, and several researchers began to develop experiments and theoretical models to understand this behaviour.

In the literature one can find several differential and integral models that can mimic the behaviour of complex material (such as polymers) under different deformations [1–10]. Each model has its own advantages and disadvantages when compared to others.

Recently, the research group devised a generalised viscoelastic model based on distributed-order derivatives of the Caputo type [11]. The model is able to fit well experimental rheological data obtained in the linear regime for food products (that behave as critical gels [12]).

To better understand the model behaviour, one can derive either analytical solutions or numerical methods. Since analytical solutions are difficult to obtain for such complex models (they are restricted to limited flows and geometries), numerical methods seem to be the only and best choice.

In this work we develop a numerical method for the solution of the 1D transient Couette flow of a Distributed-Order Viscoelastic Model (DOVM). The method is based on finite differences [8, 13].

The remaining of this work is organised as follows. In Section 2 the DOVM is introduced together with some basic definitions. The governing equations are presented in Section 3. Section 4 is devoted to the development of a numerical method and its validation. The numerical results are presented in Section 5. The work ends with the conclusions in Section 6.

2 The Distributed-Order Viscoelastic Model (DOVM)

In order to introduce the DOVM, some basic definitions are needed first.

Definition 1. *The* ***single order fractional derivative*** *in the* ***Caputo*** *sense* $(0 < \alpha < 1)$ *is given by [14]:*

$$ {}_0^C D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-t')^{-\alpha} \frac{df}{dt'} dt'. \tag{1} $$

Definition 2. *The* ***Caputo Distributed-Order Fractional Derivative*** $({}_0^C\mathbb{D}_t)$ *of a general function* f *is given by:*

$$ {}_0^C\mathbb{D}_t f(t) = \int_0^1 c(\alpha) {}_0^C D_t^\alpha f(t) \ d\alpha = \int_0^1 c(\alpha) \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-t')^{-\alpha} \frac{df}{dt'} dt' \ d\alpha \tag{2} $$

where the function $c(\alpha)$ (*acting as weight for the order of differentiation*) *is such that* $c(\alpha) \geq 0$ *and* $\int_0^1 c(\alpha)\ d\alpha = C > 0$ (*[15], [16]*).

The function $c(\alpha)$ is used to represent mathematically the presence of multiple memory formalisms. If $c(\alpha) = \delta(\alpha - \beta)$, where $\delta()$ is the delta Dirac function, then (2) reduces to the Caputo derivative ${}_0^C D_t^{\beta} f(t)$.

The Distributed-Order Fractional Viscoelastic Model (DOVM) is given by

$$\sigma(t) = {}_0^C \mathbb{D}_t \gamma(t). \tag{3}$$

were ${}_0^C\mathbb{D}_t$ is the distributed-order derivative of the Caputo type, $\sigma(t)$ is the stress and $\gamma(t)$ the strain or deformation.

The model can be seen as the classical Boltzmann model,

$$\sigma(t) = \int_0^t G(t - t') \frac{d\gamma(t')}{dt'} dt' \tag{4}$$

with the relaxation modulus $G(t)$ given in the form:

$$G(t) = \int_0^1 \frac{c(\alpha)}{\Gamma(1-\alpha)} t^{-\alpha}\, d\alpha. \tag{5}$$

Fore more details on the derivation of the DOVM model please consult the reference [11].

3 Governing Equations for a 1D Transient Couette Flow

In fluid mechanics, Couette flow refers to the laminar flow of a viscous fluid in the space between two parallel planes (plates), one of which is moving relative to the other (Fig. 1).

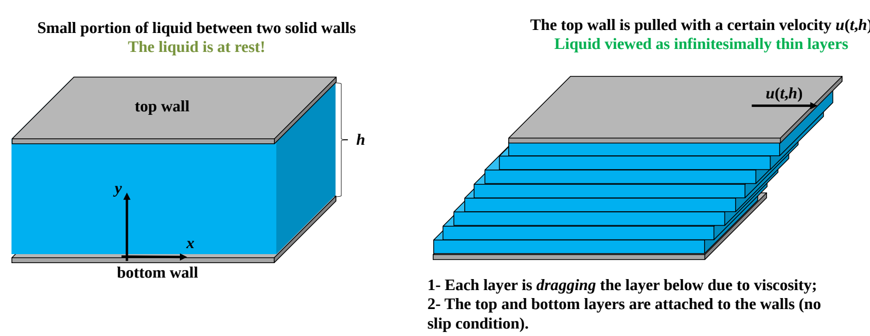

Fig. 1. Illustration of a Couette flow. A certain velocity $u(t, h)$ is imposed at the resting upper wall. As this wall moves along time, the displacement information travels along the different layers of fluid until it reaches the bottom wall. Note that these layers are merely illustrative.

The flow is driven by the drag force acting on it. This type of fluid is named after Maurice Marie Alfred Couette, a physics professor at the French University of Angers in the late 19th century.

The equations governing the 1D transient Couette flow are obtained from a simplification of the Navier-Stokes equations, together with an extra equation for the stress, given (in this case) by the DOVM. Note that we consider a small transient deformation, so that the DOVM (which is not invariant [9]) can be used (only invariant models can be used for large deformations).

We saw before that the stress was only a function of time, because, it was being measured at a specific point in space. In the 1D case, the stress $\sigma(t,y)$ and velocity $u(t,y)$ (that is obtained from the rate of deformation $d\gamma(t)/dt$ [9]) also vary in space (along y). In this particular flow, the stress has more than one component, being the one of interest denoted by σ_{xy} (shear stress). The governing equations are given by:

$$\rho\left(\frac{\partial u(t,y)}{\partial t}\right)=\frac{\partial \sigma_{xy}(t,y)}{\partial y} \tag{6}$$

$$\sigma_{xy}\left(t,y\right)=\int_0^t G(t-t')\frac{\partial u(t',y)}{\partial y}dt' \tag{7}$$

were ρ is the fluid density, and, it was assumed that only tangential movement exists. The velocity profile is given by $(u,v)=(u,0)$. This means that, for a fixed t, we can only see changes in velocity when moving in the transverse direction.

To solve this system of equations we do the following. First, we substitute (7) into (6), resulting in an integro-differential equation for the velocity:

$$\rho\left(\frac{\partial u(t,y)}{\partial t}\right)=\frac{\partial}{\partial y}\left(\int_0^t\int_0^1\frac{c(\alpha)}{\Gamma(1-\alpha)}(t-t')^{-\alpha}d\alpha\frac{\partial u(t',y)}{\partial y}dt'\right). \tag{8}$$

Second, with the velocity profile obtained from solving (8) we can easily calculate the stress from (7). (8) can be rewritten by changing the integration and differentiation order. This results in the following system of integro-differential equations that will be solved numerically:

$$\rho\left(\frac{\partial u(t,y)}{\partial t}\right)=\int_0^1\frac{c(\alpha)}{\Gamma(1-\alpha)}\int_0^t(t-t')^{-\alpha}\frac{\partial^2 u(t',y)}{\partial y^2}dt'd\alpha \tag{9}$$

$$\sigma_{xy}\left(t,y\right)=\int_0^1\frac{c(\alpha)}{\Gamma(1-\alpha)}\int_0^t(t-t')^{-\alpha}\frac{\partial u(t',y)}{\partial y}dt'd\alpha \tag{10}$$

4 Numerical Method

This Section is dedicated to the discretisation and numerical solution of equations (9) and (10). To test the convergence of the method we analyse the precision of the numerical scheme by comparing the numerical results with generalised analytical solutions.

4.1 Discretisation of the Velocity and Shear stress Equations

We will now derive a numerical method for the solution of the system (9)-(10), with boundary and initial conditions of Dirichlet type:

$$u(t,0)=0,\ u(t,h)=\phi_h(t), \quad 0<t<T, \tag{11}$$

$$u(0,y)=\frac{\partial u(0,y)}{\partial t}=0,\ \sigma_{x,y}(0,y)=0, \quad y\in[0,h],\ h>0 \tag{12}$$

Note that the viscoelastic fluid is at rest and fully relaxed at $t=0^-$.

Numerically, we need to obtain an approximation for all the operators (time and spatial derivatives). For that, we consider a uniform space mesh on the interval $[0,h]$, defined by the gridpoints $y_i=i\Delta y$, $i=0,\dots,N$, where $\Delta y=\frac{h}{N}$. For the discretisation of the fractional time derivative we also assume a uniform mesh, with a time step $\Delta t=T/S$ and time gridpoints $t_s=s\Delta t$, $s=0,1,...,S$.

At $t=t_s$ the integral on the right-hand side of the momentum equation can be written as,

$$\begin{aligned}&\int_0^1\frac{c(\alpha)}{\Gamma(1-\alpha)}\int_0^{t_s}(t_s-t')^{-\alpha}\frac{\partial^2u(t',y)}{\partial y^2}dt'd\alpha\\ =&\int_0^1\frac{c(\alpha)}{\Gamma(1-\alpha)}\sum_{j=0}^{s-1}\int_{t_j}^{t_{j+1}}(t_s-t')^{-\alpha}\,\frac{\partial^2u(t',y)}{\partial y^2}dt'd\alpha\end{aligned} \tag{13}$$

for $s=1,...,S$. We define u_i^s as the approximation of $u(t_s,y_i)$, $i=1,...,N-1$, $\ s=1,...,S$. The following approximation is considered for the integration in time:

$$\begin{aligned}\int_{t_j}^{t_{j+1}}(t_s-t')^{-\alpha}\,\frac{\partial^2u(t',y)}{\partial y^2}dt'&\approx\frac{u_{i+1}^{j+1}-2u_i^{j+1}+u_{i-1}^{j+1}}{(\Delta y)^2}\int_{t_j}^{t_{j+1}}(t_s-t')^{-\alpha}\,dt'\\&=\frac{u_{i+1}^{j+1}-2u_i^{j+1}+u_{i-1}^{j+1}}{(\Delta y)^2}\,\frac{\Delta t^{1-\alpha}d_{sj}(\alpha)}{1-\alpha}\end{aligned} \tag{14}$$

with $d_{sj}(\alpha)=(s-j)^{1-\alpha}-(s-(j+1))^{1-\alpha}$.

This results in the following discretized equation:

$$\rho\frac{\partial u(t,y)}{\partial t}=\int_0^1F(\alpha)d\alpha \tag{15}$$

with

$$F(\alpha)=\frac{c(\alpha)\Delta t^{1-\alpha}}{\Gamma(2-\alpha)(\Delta y)^2}\sum_{j=0}^{s-1}(u_{i+1}^{j+1}-2u_i^{j+1}+u_{i-1}^{j+1})d_{sj}(\alpha). \tag{16}$$

A simple first order approximation for the time derivative, and the use of the midpoint rule to approximate the integral in the interval $[0,\ 1]$ considering the gridpoints $\alpha_l = (l - 1/2)\Delta\alpha$, $l = 1, ..., P$, $\Delta\alpha = 1/P$, leads to the following discretized velocity equation:

$$\begin{aligned} \rho \frac{u_i^s - u_i^{s-1}}{\Delta t} &= \Delta\alpha \sum_{l=1}^{P} M(\alpha_l) \\ &= \Delta\alpha \sum_{l=1}^{P} \frac{c(\alpha_l)\Delta t^{1-\alpha_l}}{\Gamma(2-\alpha_l)(\Delta y)^2} \sum_{j=0}^{s-1} (u_{i+1}^{j+1} - 2u_i^{j+1} + u_{i-1}^{j+1}) d_{sj}(\alpha_l) \end{aligned} \tag{17}$$

for $i = 1, ..., N-1$ and $s = 1, ..., S$ (for each time step we need to solve a system of equations).

After solving each system of equations, an approximation of velocity at time and space mesh points is known, and, the evolution shear stress equation, equation (10), can be easily obtained for the same time and space mesh points using:

$$\sigma_{xy}{}_i^s = \Delta\alpha \sum_{l=1}^{P} \frac{c(\alpha_l)\Delta t^{1-\alpha_l}}{2\Gamma(2-\alpha_l)\Delta y} \sum_{j=0}^{s-1} (u_{i+1}^{j+1} - u_{i-1}^{j+1}) d_{sj}(\alpha_l) \tag{18}$$

where $\sigma_{xy}{}_i^s$ is the approximation of $\sigma_{xy}(t_s, y_i)$, $i = 1, ..., N-1$, $\quad s = 1, ..., S$.

4.2 Solvability

In the matrix form, (9) writes:

$$AU^s = \rho U^{s-1} + \sum_{j=0}^{s-2} B_j U^{j+1} + \sum_{j=0}^{s-2} C_j, \quad s = 1, 2, ..., S \tag{19}$$

where

$$U^j = [u_1^j,\, u_2^j,\, ..., u_N^j]^T, \tag{20}$$

$$B_j = \begin{pmatrix} 2Q & -Q & & & & \\ -Q & 2Q & Q & & & \\ & -Q & 2Q & Q & & \\ & \ddots & \ddots & \ddots & & \\ & & & & & \\ & & & -Q & 2Q & Q \\ & & & & -Q & 2Q \end{pmatrix}, \tag{21}$$

with

$$Q = \Delta\alpha\Delta t \sum_{l=1}^{P} \frac{c(\alpha_l)\Delta t^{1-\alpha_l}}{\Gamma(2-\alpha_l)\Delta y^2} d_{sj}(\alpha_l). \tag{22}$$

C_j is given by,

$$C_j = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \\ Q\phi_h(t_{j+1}) \end{pmatrix}. \tag{23}$$

A is a tridiagonal matrix

$$A = \begin{pmatrix} \rho+2M & -M & & & & \\ -M & \rho+2M & -M & & & \\ & -M & \rho+2M & -M & & \\ & \ddots & \ddots & \ddots & & \\ & & & & & \\ & & & -M & \rho+2M & -M \\ & & & & -M & \rho+2M \end{pmatrix}$$

with

$$M \equiv M(\Delta\alpha, \Delta t, \Delta y) = \Delta\alpha \Delta t \sum_{l=1}^{P} \frac{c(\alpha_l)\Delta t^{1-\alpha_l}}{\Gamma(2-\alpha_l)(\Delta y)^2}. \tag{24}$$

A is a strictly diagonal dominant matrix and therefore the system is uniquely solved.

4.3 Validation

To assess the robustness of the numerical method, we developed a non-smooth analytical solution (for the velocity equation), by imposing a certain velocity profile, through the inclusion of correcting source terms, $f(t, y)$.

We consider the following problem:

$$\begin{cases} \rho \dfrac{\partial u(x,t)}{\partial t} -_0^1 \dfrac{\Gamma(5/2-\alpha)}{\Gamma(1-\alpha)} \displaystyle\int_0^t (t-s)^{-\alpha} \dfrac{\partial^2 u(x,t)}{\partial y^2} ds = \dfrac{x^3 \log(t) - 6\sqrt{\pi}(t-1)tx}{2\sqrt{t}\log(t)} \\ u(0,y) = 0, \ 0 < y < h \\ u(t,0) = 0, \ u(t,L) = t^{1/2}h^3 \ 0 < t \leq 1 \end{cases} \tag{25}$$

with analytical solution $u(t, y) = t^{1/2}y^3$.

To evaluate the accuracy of the numerical predictions, we define:

$$\varepsilon_{\Delta t,\Delta y} = \max_{k=1,\ldots,N-1} \left| u\left(t_i, y_k\right) - u^{num}\left(t_i, y_k\right) \right|, \ i = 1, 2, ..., S \tag{26}$$

Fig. 2 shows the 3D plot of the analytical solution and the results obtained numerically for $h = 0.1$, $t = 0.5$, $\Delta\alpha = 0.1$, $\Delta t = 0.01$ and $\Delta y = 0.002$. This resulted in $\varepsilon_{\Delta t,\Delta y} = 1.40337 \times 10^{-6}$. For a courser mesh with $\Delta\alpha = 0.2$, $\Delta t = 0.1$ and $\Delta x = 0.02$ we still obtained a small error $\varepsilon_{\Delta t,\Delta y} = 1.41838 \times 10^{-5}$.

We can therefore conclude that the numerical method converges easily to the singular analytical solution, illustrating the robustness of the numerical scheme.

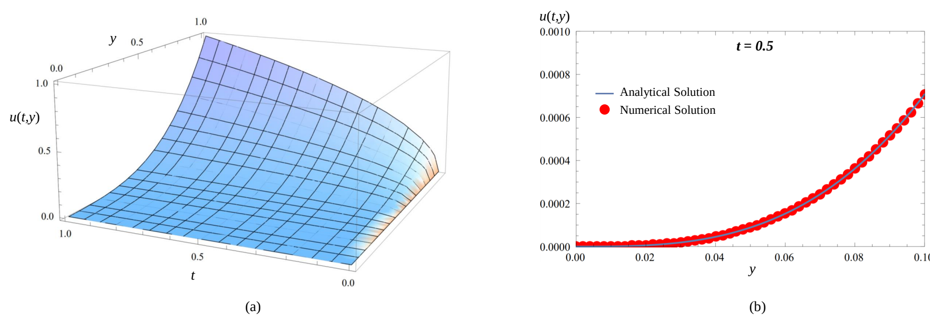

Fig. 2. (a) 3D plot of the analytical solution given by $u(t, y) = t^{1/2}y^3$. (b) Comparison between the analytical and numerical solutions for $h = 0.1$, $t = 0.5$, $\Delta\alpha = 0.1$, $\Delta t = 0.01$ and $\Delta y = 0.002$ ($\varepsilon_{\Delta t,\Delta y} = 1.40337 \times 10^{-6}$).

5 Numerical Results

One way to experimentally characterise viscoelastic fluids is to perform a relaxation test, i.e., we impose a step displacement given by $\gamma = \gamma_0 H(t - a)$ (with $H(t)$ the Heaviside function) and measure the stress response to this deformation. At time $t = a$ we impose a constant deformation, and we observe that the stress relaxes until it becomes zero (Fig. 3).

To mimic the step-strain test illustrated in Fig. 3, the upper wall suddenly starts moving at $t = 0^+$ with a tangential velocity given by,

$$u\left(t, h\right) = \frac{\Delta_{wall}}{\psi\sqrt{\pi}} e^{-\frac{(t-t_d)^2}{\psi^2}}. \tag{27}$$

and then stops (after a period of $\Delta t_{exp} \approx 50\ ms$). Then we observe how the tangential stress in the fluid relaxes.

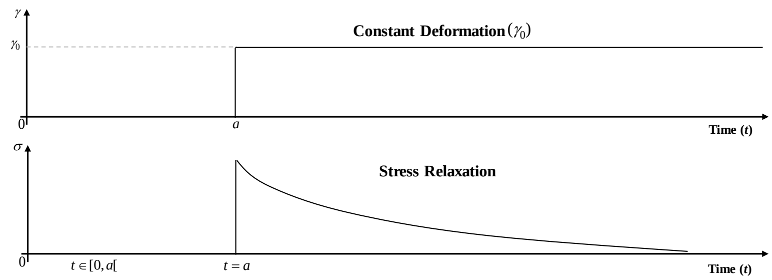

Fig. 3. Stress relaxation of a viscoelastic material after a step displacement.

As $\psi \to 0$, the velocity converges to the Dirac delta function multiplied by the displacement of the upper wall, $\Delta_{wall}\delta(t)$ (assuming $t_d = 0$). The need for the delay time, t_d, comes from the initial condition $\frac{du(0,h)}{dt} = 0$. This step-strain is illustrated in Fig. 4.

Fig. 4 (a) shows the initial and final state of the deformation. After 50 ms the upper wall stops moving (the displacement is Δ_{wall}). Fig. 4 (b) shows the variation of the upper wall velocity along the 50 ms. For this case we considered a deformation ($\gamma_0 = \Delta_{wall}/h$) of 100%.

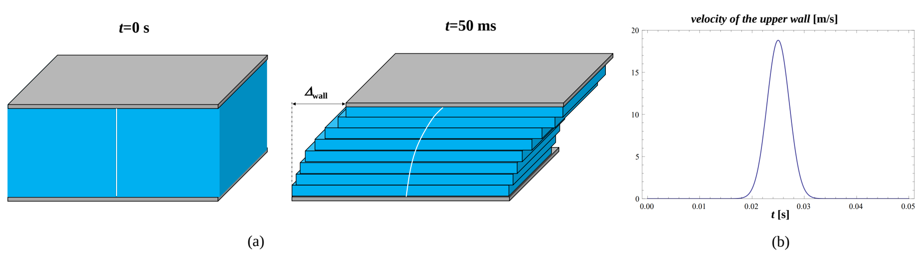

Fig. 4. Step displacement. (a) Initial and final state of the deformation. After 50 ms the upper wall stops moving (the displacement is Δ_{wall}). (b) Variation of the upper wall velocity along the 50 ms. The deformation ($\gamma_0 = \Delta_{wall}/h$) is 100%, $\psi = 0.003$ and the delay (t_d) is 0.025 seconds.

5.1 Case Study

After some preliminary experiments with the step-strain problem, the trade-off between simulation time and accuracy resulted in a mesh size of $\Delta t = 2 \times 10^{-3}$, $\Delta y = 2.5 \times 10^{-3}$ and $\Delta\alpha = 0.1$. Note that these parameters are dimensional and not scaled with the relaxation of the fluid. This happens because the DOVM represents an infinite set of relaxations weighted by the function $c(\alpha)$.

Fig. 5 shows the stress relaxation test in a narrow gap Couette cell following a sudden straining deformation (the upper wall moves) for $\gamma_0 = 100\%$, $\psi = 0.003$ and $t_d = 0.025$ seconds.

We have considered different $c(\alpha)$ functions in order to understand the influence of this weighting function on the relaxation of the DOVM.

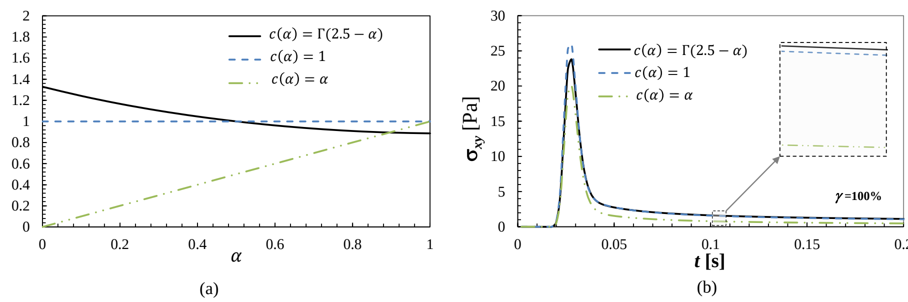

Fig. 5. (a) Three different functions $c(\alpha)$. (b) Stress relaxation test in a narrow gap Couette cell following a sudden straining deformation (the upper wall moves) for $\gamma_0 = 100\%$) and different functions $c(\alpha)$.

As expected, for the case $c(\alpha) = \alpha$ we obtained a higher rate of relaxation when compared to $c(\alpha) = 1$ or $c(\alpha) = \Gamma(2.5 - \alpha)$ (Fig. 5 (a) and (b)). This happens because for $c(\alpha) = \alpha$ we attribute smaller weights to low values of α (elastic behaviour) and bigger weights to high values of α (Newtonian behaviour - instantaneous relaxation) (Fig. 5 (a)). The model with $c(\alpha) = 1$ also presents a higher rate of relaxation when compared to the model with $c(\alpha) = \Gamma(2.5 - \alpha)$ (see the inset in Fig. 5 (b)).

These results allow one to conclude that the implementation of the numerical method is physically correct, and that the new DOVM allows for a broader spectrum of relaxations, when compared to the classical viscoelastic models.

6 Conclusions

A new numerical method for solving the 1D Couette flow of a Distributed-Order Viscoelastic Model has been developed. We proved the solvability of the numerical scheme and analysed its convergence considering a non-smooth solution. The numerical method was used to study the relaxation of fluids (governed by the DOVM) under a step-strain.

This prototype numerical scheme can be improved by considering high order approximations in its derivation. This is an ongoing work, where we also analyse the convergence and stability of the fully discretized family of numerical schemes for this kind of problems.

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