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IDENTIFYING CONSTITUTIVE PARAMETERS OF VISCOELASTIC FLUIDS BY MEANS OF AN OPTIMAL CONTROL FORMULATION: SENSITIVITY ANALYSIS

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Abstract. *Computer predictions of physical events can be of great importance in improving the design of processes and systems. This is particularly true in the field of non-Newtonian fluids, in which very complex flows can take place associated to the modelling of real engineering applications. The reliability of the predictions, a chief issue on using computer modelling, can be improved by System Identification, which consists on the process of improving a mathematical model for a real system by combining physical principles with experimental or field data. The present article introduces an optimal control formulation to identify the rheological parameters of a class of non-Newtonian fluids. The effectiveness of the proposed formulation is assessed on a abrupt 4:1 contraction flow geometry.*

keywords: *Viscoelastic fluids, parameters identification*

Introduction

Nowadays, modelling plays a crucial role in controlling and optimizing industrial process by providing means of better understanding the involved phenomena and of improving the capacity of predicting future behavior, probably its key feature. The use of such models is mainly based on computational simulations, giving rise to two shortcomings concerning the reliability of the results: numerical pitfalls inherent to approximation methods, and uncertainties associated to non modelled dynamics and to parameters values. This last drawback can be alleviated by System Identification (Banks and Kunish, 1989), which consists on the process of improving a mathematical model for a real system by combining physical principles with experimental or field data. The main idea is to identify a set of parameters such that, over a desired range of operating conditions, the model outputs are close, in some well-defined sense, to the system outputs, when both are submitted to the same inputs. Due to the incompleteness of available information and unavoidable measurement errors, system identification only achieves an approximation of the actual system.

The present work is motivated by the need of improving the capability to predict the sophisticate dynamic mechanical response of non-Newtonian fluids. They often appear in very important industrial applications, ranging from oil exploitation to food manufacturing passing through biomedical processes.

Different approaches have been used to obtain rheological parameters. Bernardin and Nouar (1998) used experimental and numerical results of angular torque in a transient Couette flow of an Oldroyd fluid to identify rheological parameters. Sarkar and Gupta (2000) used finite element simulation to obtain results of entrance pressure drop in a contraction flow. These results are matched with experimental data to predict elongational viscosity parameters. The optimization scheme iteratively improves the value of elongational viscosity parameters by minimizing the difference between the entrance pressure drop predicted numerically and the ones obtained experimentally in a capillary rheometer. The results obtained showed that the method provides an attractive alternative for estimation of the elongational viscosity.

The modelling and simulation of non-Newtonian flows are based on mass and momentum conservation principles clustered with a constitutive equation that describes the material mechanical behavior. In Thompson et al. (1999), a nonlinear constitutive equation with remarkable performance in describing contraction flows of elastic fluids is introduced. In this work, an optimal control formulation is used to set the problem of identifying the rheological parameters associated to this constitutive equation. The optimal control formulation phrases the identification problem as the search for an optimal set of parameters that minimizes a performance index relating measured and modelled variables, as for instance comparing the pressure drop along the flow with the one predicted by the modelling. A crucial issue on estimation techniques applied to distributed parameter systems is to understand the role of the chosen performance index (cost function as known in optimization theory). Here, this is addressed by means of a sensitivity analysis (Gunzburger, 2003). Sensitivity analysis have its importance not only because it is frequently required to build up numerical algorithms for solving the parameter identification problem, but also because it provides a systematic tool to better understand complex phenomena involved in engineering systems.

In the present work, a sensitivity analysis for the identification problem mentioned above is presented. The effectiveness of the proposed formulation is assessed on a abrupt 4:1 contraction flow geometry.

The paper is organized as follows. First, the model to be used in the analysis of the non-Newtonian flows is introduced. Then, the identification problem is presented, and the sensitivity analysis is performed. Finally, the last section presents some remarks, comments and future perspectives.

Mathematical modelling

In the present section the nonlinear system of equations that governs the steady state flow of an viscoelastic fluid is summarized. The resulting mathematical problem is given by the mass and momentum equations and the constitutive relation. Bold is used to denote vectorial and tensorial fields .

For an incompressible fluid, the steady state mass conservation equation reduces to:

$$\operatorname{div} \mathbf{v} = 0 \tag{1}$$

where $\mathbf{v}$ is the velocity vector field. The momentum equation is given by:

$$\rho \operatorname{div}(\mathbf{v} \otimes \mathbf{v}) = -\nabla p + \operatorname{div}\mathbf{T} \tag{2}$$

where $\boldsymbol{\tau} = \mathbf{T} + p\,\mathbf{I}$ is the extra-stress, $\mathbf{T}$ is the stress tensor, I is the identity, p is the pressure and ρ is the mass density.

The stress tensor $\mathbf{T}$ is related to the flow kinematics by the nonlinear constitutive equation introduced in Thompson et al. (1999). The attractive aspect of this equation relies on the combination of its simplicity, which enables its use in numerical simulations, with its ability of describing the response of the material undergoing complex flows. A simplified version of the equation, which is capable of handling situations involving shear and extension, is introduced bellow

$$\mathbf{T} = \alpha_0 \mathbf{I} + \alpha_1 \mathbf{D} \tag{3}$$

where $\mathbf{D}$ is the rate of strain tensor, ($\mathbf{D} \equiv [\nabla\mathbf{v} + (\nabla\mathbf{v})^T]/2$), and the α_i's coefficients are assumed to be functions of the invariants of $\mathbf{D}$ and $\overline{\mathbf{W}}$, which is the relative-rate-of-rotation defined as

$$\overline{\mathbf{W}} = \mathbf{W} - \boldsymbol{\Omega} \tag{4}$$

In the equation above, $\mathbf{W} = [\nabla\mathbf{v} - (\nabla\mathbf{v})^T]/2$ is the vorticity tensor, and $\boldsymbol{\Omega}$ is a tensor related to the rate of rotation of $\mathbf{D}$ following the motion. If the set of unit vectors $\{\mathbf{e}_i^*\}$ is the basis consisting of the principal directions of $\mathbf{D}$ (i.e., the eigenvectors of $\mathbf{D}$), then the vector angular velocity of this basis is defined by

$$\frac{d\mathbf{e}_i^*}{dt} = \mathbf{w} \times \mathbf{e}_i^*, \qquad i = 1, 2, \text{ or } 3 \tag{5}$$

where d/dt denotes the material time derivative. The angular velocity $\mathbf{w}$ can be represented in the following tensorial form, $\boldsymbol{\Omega}$:

$$\boldsymbol{\Omega} \equiv \mathbf{w} \cdot \boldsymbol{\epsilon} \tag{6}$$

where $\boldsymbol{\epsilon}$ is the third-rank alternator tensor.

A straightforward manipulation leads to $\alpha_0 = -p$, while α_1 is related to the non-Newtonian viscosity function, η. In this work, the viscosity function is taken as a weighted average between extensional and shear viscosities, so that α_1 is given by:

$$\alpha_1 \equiv 2\eta = 2\eta_S(\dot\gamma)^{R^\theta}\eta_u(\dot\gamma)^{(1-R^\theta)} \tag{7}$$

where $\dot\gamma = (2tr(\mathbf{D}^2))^2$ and $R = -tr(\overline{\mathbf{W}})^2/tr(\mathbf{D}^2)$ is a a flow classifier, taking the values 0 in pure extension and 1 in shear flows. Besides, η_s and η_u stand for the shear and extensional viscosities. Moreover, θ is a new rheological parameter, which defines a different weighted average between shear and extensional viscosities, and it is proposed as an attempt to better describe the fluid behavior. All the parameters and constitutive functions must a priori be obtained to build a suitable model for numerical simulations. Indeed, the motivation of the present work relies on the determination of those parameters, and a methodology of determining θ is the focus here.

Appropriate boundary conditions must be selected in order to obtain an well-posed mathematical problem representing the actual flow to be simulated.

The shear and extensional viscosity functions $\eta_s(\dot{\gamma})$ and $\eta_u(\dot{\gamma})$, are given by the Carreau equation:

$$\eta_s = \eta_0 \left[1 + (\lambda_s \dot{\gamma})^2\right]^{\frac{n_s - 1}{2}} \tag{8}$$

$$\eta_u = \eta_0 \left[1 + (\lambda_u \dot{\gamma})^2\right]^{\frac{n_u - 1}{2}} \tag{9}$$

where η_0, λ_s, λ_u, n_s and n_u are rheological parameters.

Parameters Identification

The computational analysis of complex flows departs from a reliable modelling that often results in a nonlinear boundary value problem, normally referred to as the direct or forward problem in the context of parameter estimation. In this work, the direct problem consists on determining the steady state velocity and pressure fields for known geometry, constitutive parameters and boundary conditions. The numerical approximation of the direct problem requires sophisticate tools and, therefore, entails a significant challenge to the analyst.

This analysis can be meaningless, despite the quality of the applied numerical method, if the model itself is not capable of reproducing quantitatively the material response, what strongly depends upon the constitutive parameters. Obtaining those parameters leads to the so called inverse problem, in which available data related to the solution of the direct problem are used aiming at estimating either not or poorly known information required to solve the direct formulation.

The present section deals with the inverse problem concerning the parameter identification associated to the modelling introduced previously. This problem is cast in an optimal control framework in which $\boldsymbol{\Theta}$, the vector containing the sought parameters, plays the role of the control. Indeed, the proposed formulation can be extended to the case where the components of vector Θ are functions of the kinematic variables.

Roughly speaking, the optimal control problem relates some measured data (like, for instance, the pressure drop along the flow) to its model counterpart value. Therefore, $\boldsymbol{\Theta}$ is intended to drive the model adaptation such that the difference between measured and model response achieves a minimum. In formal terms, the problem is defined by

Problem (P) : Find a minimum of the cost function $\mathcal{J}(p, \mathbf{v}; \Theta)$
subject to the state equations (1), (2) and (3)
and boundary conditions.

The choice of the cost function $\mathcal{J}$ plays a crucial role in obtaining the sought parameters, and it is very difficult to have any a priori idea of its best form. Typically, the square of the difference is taken (e.g : $\mathcal{J}(\Delta p; \Theta) = [(\Delta p - \Delta p_{mes}]^2)$, leading to a least square constrained problem, which might be solved by means of a numerical technique. Indeed, least square formulations are the most often used approach in this sort of problem.

Numerical Solution

The optimization problem **(P)** introduced in the last section can be solved through a gradient method which is summarized in the following expression, representing a typical iteration of a gradient minimization method

$$\Theta_{l+1} = \Theta_l - \gamma_t\, \mathcal{L}^{'}(\Theta_l) \quad (l = 1, ..., n) \tag{10}$$

where γ_t is the step length of the algorithm and $\mathcal{L}^{'}$ stands for the gradient of the Lagragian $\mathcal{L}$ defined as

$$\begin{aligned} \mathcal{L}(\mathbf{v}, p, \boldsymbol{\tau}, \lambda, \pi, \xi; \Theta) = \mathcal{J}(\mathbf{v}, p, \boldsymbol{\tau}) + \int_\Omega \lambda.\mathrm{div}\ \mathbf{v}\ d\Omega \\ + \int_\Omega \pi.(\rho\ \mathrm{div}(\mathbf{v}\otimes\mathbf{v}) - \nabla\ p + \mathrm{div}\ \boldsymbol{\tau})\ d\Omega + \int_\Omega \xi.(\boldsymbol{\tau} - G(\mathbf{v}, \Theta))\ d\Omega \end{aligned} \tag{11}$$

where λ, π, ξ are the Lagrange multipliers responsible for enforcing the state equations restrictions in the optimization formulation and G is a compact notation for the constitutive equation.

The most delicate aspect of the proposed algorithm is the computation of the gradient. A direct computation would lead to very troublesome numerical problem involving the sensitivities of the state fields with respect to the sought parameters. This computational burden can be circumvented by the use of an adjoint problem (Gunzburger, 2003).

The proposed numerical algorithm is summarized bellow.

Step 0 - Set $l = 0$ and choose the initial guess Θ_0
Step 1 - Solve the direct problem and obtain $(\Delta p)_l$
Step 2 - Compute $\mathcal{L}^{'}(\Theta)_l$
Step 3 - Choose a decent step γ_l
Step 4 - Update the sought parameters by using $\Theta_{l+1} = \Theta_l - \alpha_t \mathcal{L}^{'}(\Theta_l)$
Step 5 - Check convergence. If yes (i.e., if $|\mathcal{J}| \leq 10^{-4}$), end. If no, go to step 1

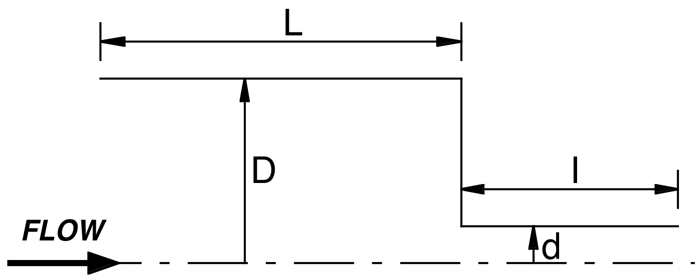

Figure 1: The geometry.

Sensitivity Analysis

The effectiveness of the proposed formulation is assessed on an axisymmetric abrupt 4:1 contraction flow, shown in Fig. 1. The motivation for using this geometry is twofold: the reproduction of experimental likely scenarios and the generation of extensional and shear contributions to flow kinematics. The boundary conditions are: uniform inlet velocity, impermeable and no-slip walls and developed flow at outlet. The dimensionless lengths (L/d, were d is the upstream tube diameter) of the upstream and downstream tubes were equal to 2. The mass and momentum conservation equations (eqs. 1 and 2), together with the constitutive equation described above (eq. 3), were discretized by the finite volume method (Patankar, 1980). Staggered velocity components were employed to avoid unrealistic pressure fields. The pressure-velocity coupling was handled by an algorithm based on SIMPLEC (Van Doormaal and Raithby, 1984). The resulting algebraic system was solved by the TDMA line-by-line algorithm, coupled with the block correction algorithm (Settari and Aziz, 1973) to increase the convergence rate. The solution was considered converged when the normalized residue of the conservation equations was less than 10^{-3}.

A 82×56 uniform mesh per zones was employed in the numerical solution, with more concentration in the neighborhood of the contraction plane. Some mesh tests were performed with a Newtonian fluid, and the result obtained for the corner vortex detachment length (approximately equal to $0.17D$) was in good agreement with experimental and numerical results available in the literature.

First of all, some results of streamlines, flow classifier R and viscosity function are presented. Although the complete momentum equation was integrated numerically, for the results presented in this paper inertia was kept negligible ($Re \equiv \rho\overline{u}D/\eta_0 = 1 \times 10^{-2}$). All results were obtained for the following parameters: $\eta_0 = 2.65\,\text{Pa.s}$, $\lambda_u = 5.2 \times 10^{-2}$s, and $\lambda_s = 7 \times 10^{-2}$s. Figures 2 and 3 show the streamlines for different set of rheological parameters: $n_u = 1.5, n_s = 0.8, \theta = 1$ and $n_u = 2.25, n_s = 0.9, \theta = 1$, respectively. It can be observed the presence of the corner vortex. For the cases analyzed, the detachment length is almost equal to the Newtonian value, due to the fact that these fluids don't present a strong extensional behavior. More significant differences between Newtonian and non-Newtonian fluids could be observed by increasing n_u and θ. Unfortunately this is not an easy task from the computational standpoint due to convergence problems. It is worth mentioning that the convergence of the iterative algorithm applied to solve the problem is very difficult to be achieved. Indeed, this numerical burden has been under discussion in the literature for several years. Flow classifier and viscosity fields for the same rheological parameters are depicted in Figs. 4 to 7. It can be observed that shear flow ($R \simeq 1$) occurs in the neighborhood of the walls, and also everywhere away from the contraction plane. Extensional flow ($R \simeq 0$) occurs in a large region located just upstream the contraction plane, and a nearly rigid body motion ($R > 1$) occurs in the corner vortex. Analyzing Figs. 6 and 7, it can be noted that there is a smooth viscosity variation near the contraction region.

From now on some preliminary results associated to the parameter identification problem will be presented. The proposed formulation is expected to handle the identification of several different parameters simultaneously. Despite of that, here only the new rheological parameter θ is assumed as unknown. This allows to a deeper understanding of the role played by θ, as a sensitivity analysis (Guzbunger, 2003) is performed. Further, it leads to a simpler numerical problem which is suitable for assessing and testing the proposed formulation.

In the tests presented here, the experimental data is replaced by the numerical response of the direct problem, solved for a prescribed value of θ. Therefore, the used data is noisy free. Moreover, the cost function is chosen as the square of the difference of the pressure drop through the contraction (entrance pressure drop), which is determined by extrapolating the average pressure drop obtained at the developed flow region of the upstream tube, and the one obtained at the downstream tube, as it is shown in Fig. 8.

As mentioned before, a critical step on the numerical algorithm is computing the gradient $\mathcal{J}'$. Here, it is accomplished by using an approximated finite differences scheme, e.g.

$$\mathcal{J}' = \lim_{\Delta\theta \to 0} \frac{\mathcal{J}(\theta + \Delta\theta) - \mathcal{J}(\theta)}{\Delta\theta} \tag{12}$$

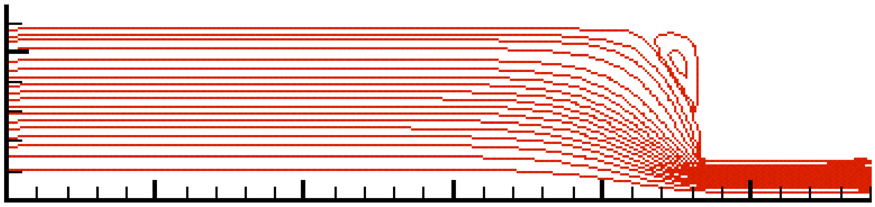

Figure 2: Streamlines for $n_u = 1.5, n_s = 0.8, \theta = 1$.

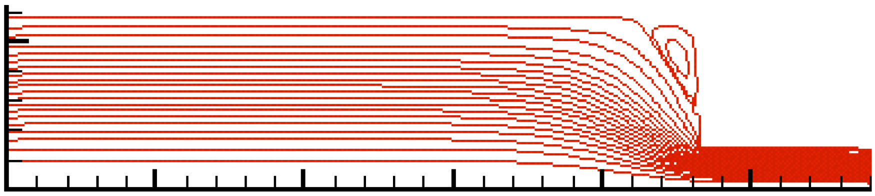

Figure 3: Streamlines for $n_u = 2.25, n_s = 0.9, \theta = 1$.

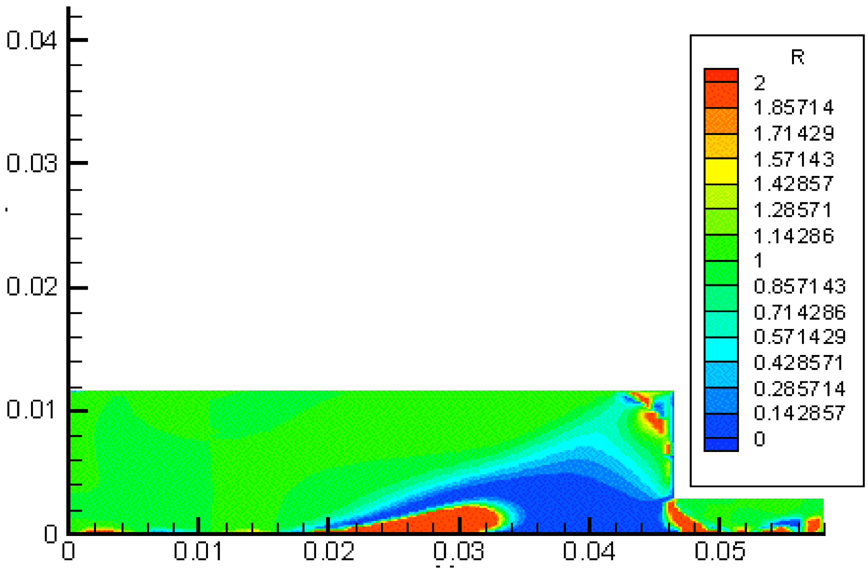

Figure 4: Flow classifier R for $n_u = 1.5, n_s = 0.8, \theta = 1$.

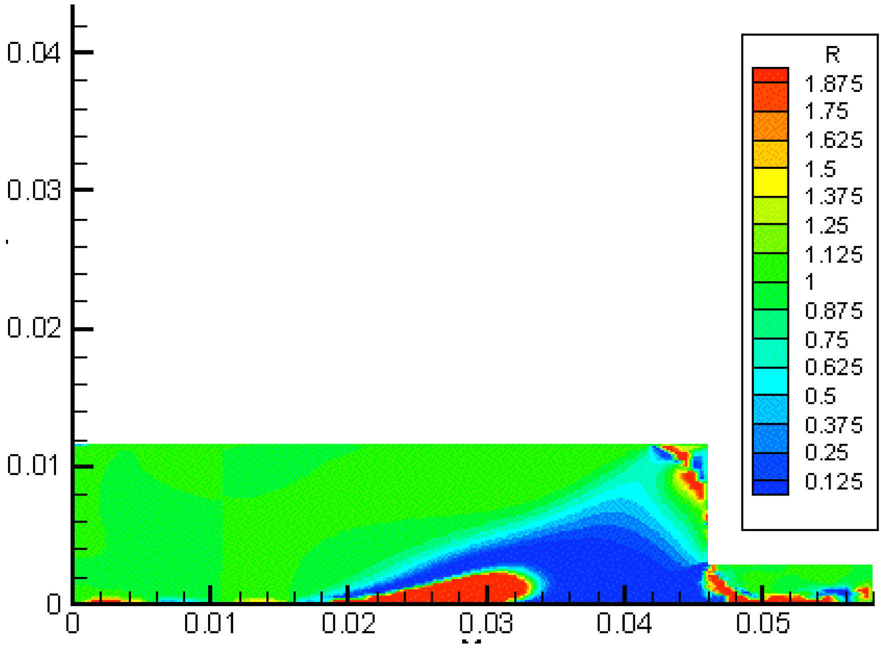

Figure 5: Flow classifier R for $n_u = 2.25, n_s = 0.9, \theta = 1$.

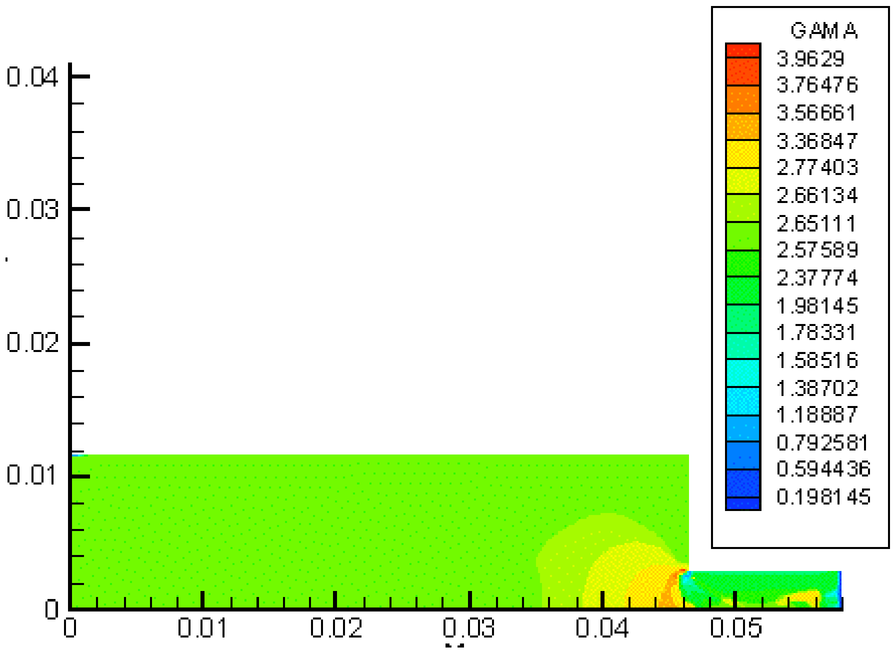

Figure 6: Viscosity field for $n_u = 1.5, n_s = 0.8, \theta = 1$.

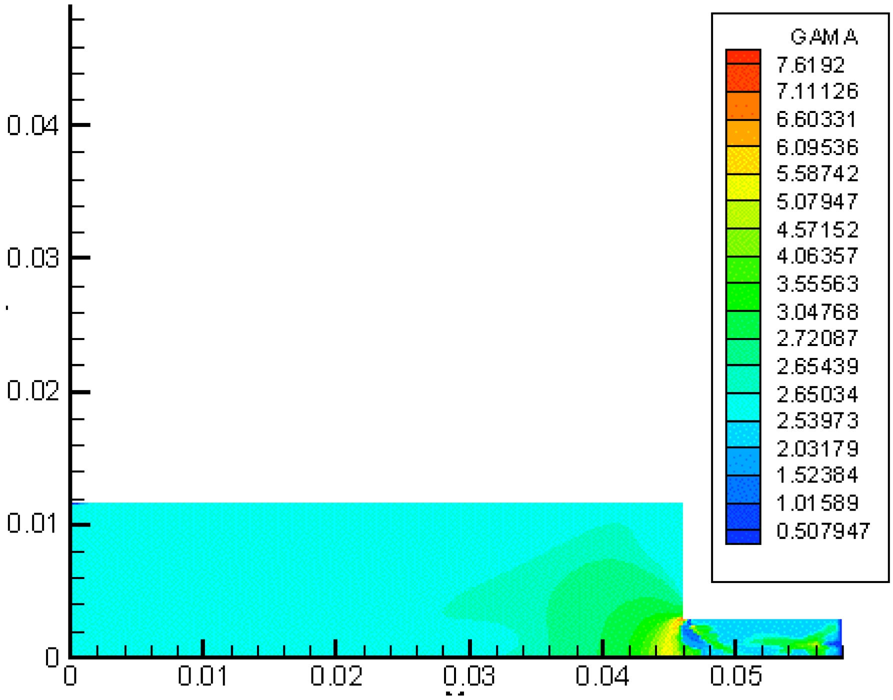

Figure 7: Viscosity field for $n_u = 2.25, n_s = 0.9, \theta = 1$.

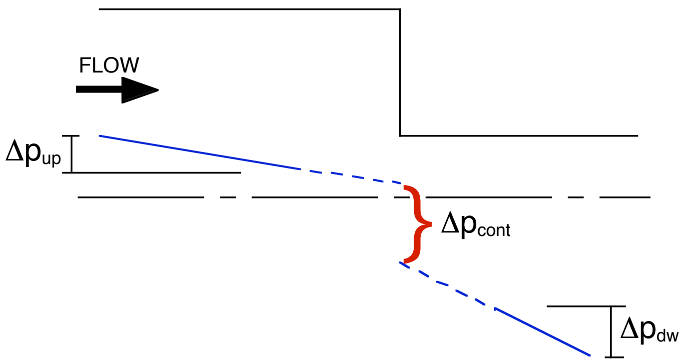

Figure 8: Pressure drop through the contraction.

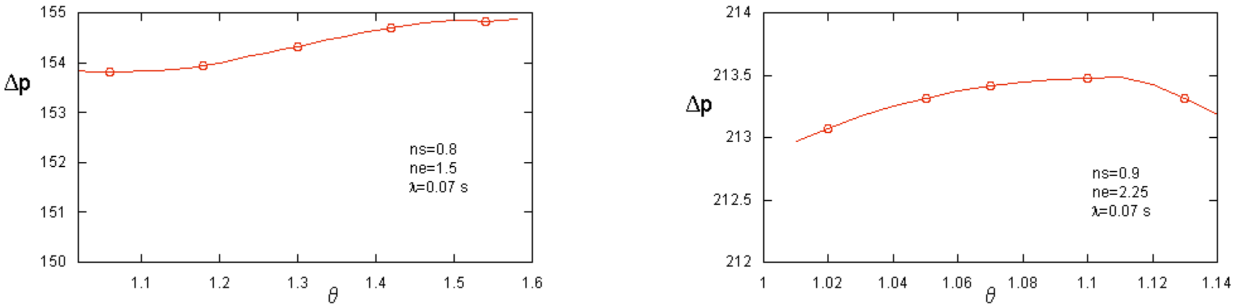

Figure 9: Pressure drop through the contraction versus θ for $n_u = 1.5, n_s = 0.8$ and $n_u = 2.25, n_s = 0.9$.

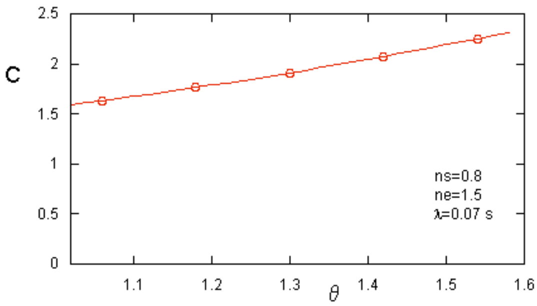

Figure 10: Couette correction factor versus θ for $n_u = 2.25, n_s = 0.9$.

First of all, a sensitivity analysis was performed to evaluate the influence of parameter θ on entrance pressure drop. The results are shown in Fig. 9, for $n_u = 1.5, n_s = 0.8$ and $n_u = 2.25, n_s = 0.9$. The other rheological parameters were held fixed ($\eta_0 = 2.65$ Pa.s, $\lambda_u = 5.2 \times 10^{-2}$s, and $\lambda_s = 7 \times 10^{-2}$s). The first case ($n_u = 2.25, n_s = 0.9$) shows the existence of two possible solutions for some values of entrance pressure drop. It can also be observed that the variation of entrance pressure drop is very small in the range of θ analyzed. In the second case the results are better, since the pressure drop increases monotonically with θ. However, again only a mild variation of the pressure drop is observed. Based on this results, a dimensionless entrance pressure drop, the Couette Correction factor, was investigated as a new comparison parameter. The Couette Correction factor is defined as the ratio between pressure drop through the contraction and wall shear stress in the developed region of the downstream tube. As it can be observed in Fig. 10, for the same case ($n_u = 2.25, n_s = 0.9$), the Couette Correction factor seems to be much more sensitive to θ than the pressure drop, and it should be used in future analysis.

Figures 11 to 13 show the influence of parameter θ on cost functional $\mathcal{J}$ and its derivative $\mathcal{J}'$. Figure 11 show $\mathcal{J}$ and $\mathcal{J}'$ for $n_u = 1.5$ and $n_s = 0.8$. It can be noted that $\mathcal{J}$ is very sensitive to θ, and its derivative presents a reasonable variation for the range of θ investigated. These results show that the adopted cost functional can be used to the identification of the sought parameter. Simmilar results are obtained for the other cases: $n_u = 2, n_s = 1$, Fig. 12, and $n_u = 2.25, n_s = 0.9$, Fig. 13. However, for $n_u = 1.5, n_s = 0.8$, it can be observed that two minimum values of J are obtained in a very small range of θ.

Finally, Fig. 14 shows the number of iterations needed to obtain the parameter θ for $n_u = 1.5, n_s = 0.8$ and $n_u = 2.25, n_s = 0.9$. It can be observed that convergence is obtained with a relatively small number of iterations in both cases.

Final Remarks

The present work presents a sensitivity analysis in the context of identifying rheological parameters of non-Newtonian fluids. The obtained results confirm the adequacy of the proposed cost function involving the pressure drop along the flow, which is a key aspect on the identification formulation.

The next steps of the present work rely on carrying out the identification of the θ parameter by using the contraction flow analyzed here, which, in turn, can be reproduced in a laboratory.

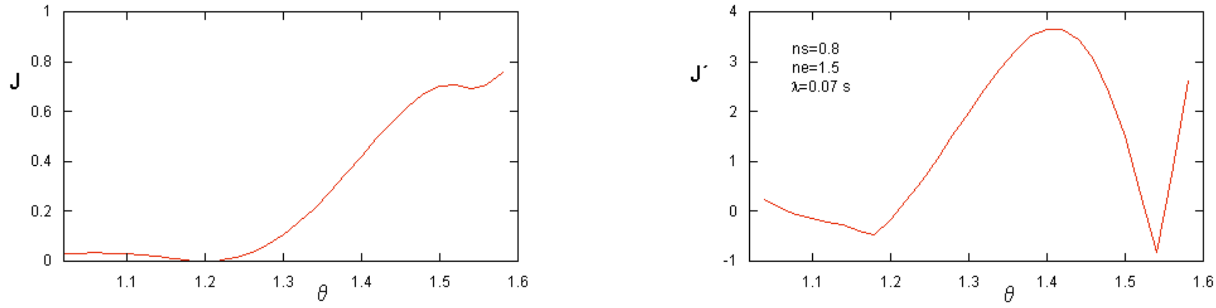

Figure 11: Cost functional $\mathcal{J}$ and $\mathcal{J}'$ versus θ for $n_u = 1.5, n_s = 0.8$.

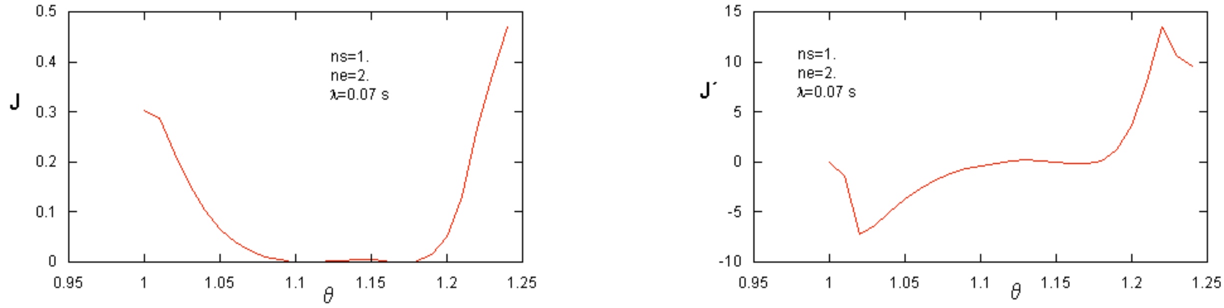

Figure 12: Cost functional $\mathcal{J}$ and $\mathcal{J}'$ versus θ for $n_u = 2, n_s = 1$.

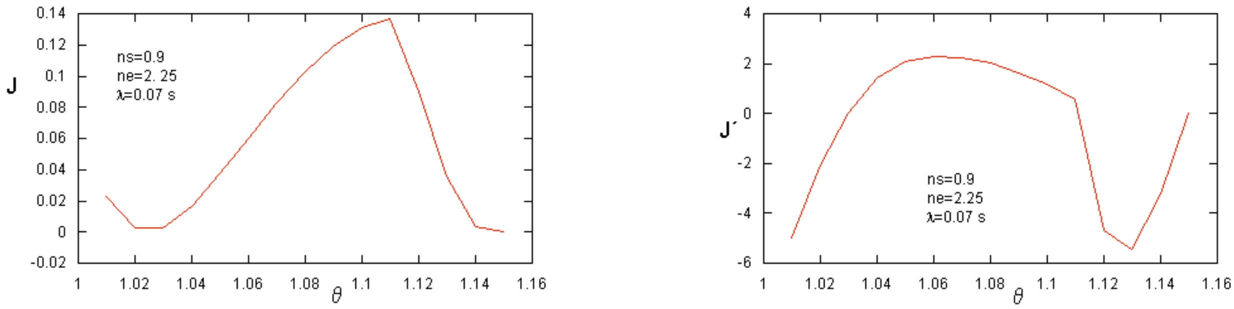

Figure 13: Cost functional $\mathcal{J}$ and $\mathcal{J}'$ versus θ for $n_u = 2.25, n_s = 0.9$.

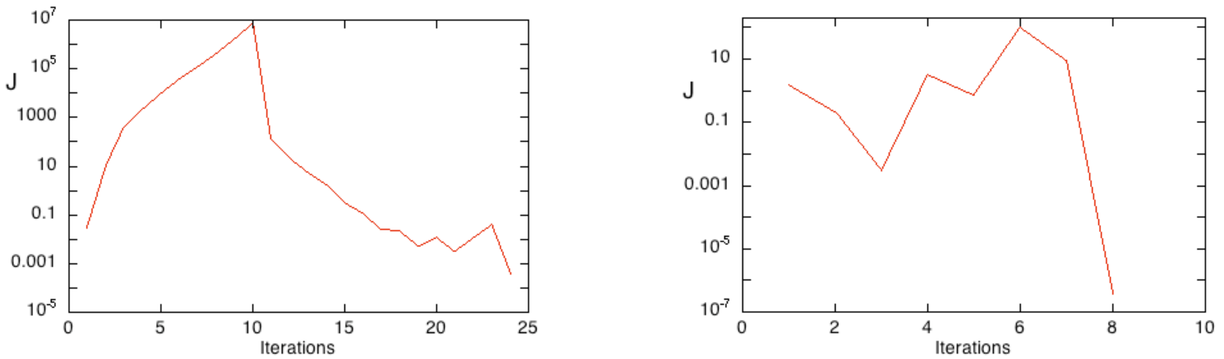

Figure 14: Cost functional $\mathcal{J}$ for $n_u = 1.5, n_s = 0.8$ and $n_u = 2.25, n_s = 0.9$.

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