A STRONG CRITERION FOR MICRO-STRUCTURED LIQUIDS IN WHICH THE MICRO-ELEMENT CAN BE REPRESENTED BY A VECTOR

Carlos R.A. dos Reis, carlos.ronaldo@gmail.com
Monica C. Matos, nicamatos@ig.com.br
Roney L. Thompson, rthompson@vm.uff.br
Grupo de Escoamento de Fluidos Complexos - LMTA – PGMEC, Department of Mechanical Engineering,
Universidade Federal Fluminense, Rua Passo da P\'atria 156,
Niteroi, RJ 24210-240, Brazil

Abstract. The purpose of these instructions is to serve as a guide for formatting papers to be published in the Proceedings *Based on the kinematic strong-weak criterion proposed by Tanner and Huilgol (1975), Tanner (1976) has developed a strong-weak criterion for a flowing system where hookean dumbbell micro-elements are present on a Newtonian solvent. Olbrich et. Al (1982) have extended this idea to more complex micro-structured liquids based not only on the kinematics of the main flow but also on micro-structure features of the micro-element and its interaction with the main flow. They could encompass, with the same theory, emulsions and polymeric liquids. The vector chosen to represent the main features of the micro-element can be a single one, as in the case of drops in a fluid, or can be an expectation value of a set of vectors, as in the case of polymer chains. The basic idea of these approaches is the identification of micro-structure-velocity-gradient, the velocity gradient experienced by the micro-element considered. After that, a Lyapunov exponent stability analysis is conducted. The problem identified with the application of this method is that the eigendirection correspondent to a positive real part of a Lyapunov exponent can be orthogonal to the orientation of the micro-element considered. Therefore, the eigendirections of the Lyapunov exponent analysis have to be filtered appropriately to exclude the plane defined by the orientation of the micro-element. Situations where the two methods do not coincide are explored to show that the filtered criterion over-performs the original one.*

Keywords: *Strong flows, micro-structured liquids, Lyapunov exponents*

1. INTRODUCTION

Solving a set of partial differential equations and appropriate boundary and initial conditions correspondent to a physical problem of interest in Mechanics is to find scalar, vector or tensor fields which obey that given set. These fields are generally filtered to interpret the results. In Fluid Mechanics, for example, it is common to calculate the streamlines (with a velocity field) and discover different flow patterns depending on specific parameters. It is also helping to plot tensor components or the deformation rate field. In general industrial processes, the analysis of a well-chosen diversity of fields increases the knowledge on the engineering problem and allows technical and economical decisions in order to optimize results: increase quality of the final product and decrease time and energy consumption. A change in a fluid mechanic part of an industrial process willing to increase its efficiency involve modifying combinations of four restrictions of the process: geometry, flow rate, materials which are involved and external forces. On manufacturing new devices to execute a certain process, generally, there is a stage of testing, that can be conducted numerically and/or experimentally, during which the efficiency of this device is measured. Not only experimentally, but numerically, is more expensive to change geometry and this is a challenge for the construction of new devices. Industrial processes such as: manufacturing anisotropic materials, oil recovery by polymer solutions in porous media, coating, separation of suspended and continuous phases, mixing, emulsification, preparation of medicines, food transportation, and many others, are connected to materials which are sensitive to flow type, i.e. respond differently when submitted to shear-like or extension-like flows (or any other-like flow). For these kind of non-Newtonian materials, an interesting quantity that can be calculated in order to give a better comprehension to what they are experiencing during a certain process, is a field of a persistence-of-straining parameter. This parameter is a flow classification dimensionless index which, in essence, gives a local instantaneous measure of how close a flow is from an extensional flow. In this approach, one can show that, for example, viscometric flows have a constant ``distance" from extensional ones or rigid body motions are in an opposite extreme. Hence, these results motivate the use of this parameter to classify motions. Astarita (1979) was probably the first one to propose a local objective criterion not restricted to Motions With Constant Relative Principal Stretch History (MWCRPSH) to capture the persistence-of-straining concept. The criterion proposed by Astarita (1979), however, was not valid for any 3-D kinematics. Thompson and Souza Mendes (2005a, 2007) developed a purely kinematic criterion based on the persistence-of-straining tensor and extended Astarita's previous work to general flows. As pointed by Thompson and Souza Mendes (2007), by purely kinematic it was meant that, for any given velocity field, that criterion yields local values for persistence of straining and, therefore, is not intended to analyze admissibility or classes of materials that can undergo a specific motion.

There are very representative industrial processes are related to complex microstructured fluids. In a mesoscopic approach, information about microstructure such as size and orientation, and its evolution counterparts stretch and rotation, are commonly brought into models by the introduction of a new local state variable: the conformation tensor. The conformation tensor can be represented by tensors of different, but the present framework is applied to second order tensors only. Depending on the physical context, the conformation tensor can be a representation of the expectation of local average value of microstructure features (being the case of polymeric liquids), or can be a single microstructure element (a drop suspended in a liquid, for example).

Hence, in this case, the constitutive model is broken into two parts. One part relates microstructure with kinematics of continuous phase. Generally this is done by an evolution equation for the conformation tensor. A general framework for an evolution equation for a symmetric second order conformation tensor can be found in Pasquali and Scriven (2004), for polymeric liquids and in Tucker and Moldenaers (2002) for a single ellipsoid droplet. The second part is dedicated to the relation between conformation tensor and stress. Since microstructured fluids are widely used in industry and conformation second order tensors are common entities to represent microstructure, a persistence-of-conformation-stretching parameter can be an interesting field in the analysis of certain processes.

When oil is being produced from a reservoir, it does not come alone. Generally it comes with water and gases. During the firs stage of separation, gas can be produced with high quality (very few parts of other components), but oil is still “contaminated” with water and water is still “contaminated” with oil. The problem of the first contamination is that above a certain level, the excess of water (more than 1 %volume fraction) inhibits some processes that are required for refinement and the production of derivatives such as gasoline or diesel. The second contamination problem concern environmental laws that do not allow a certain level of oil when water is rejected. A second stage of separation can be done by several methods, but one which is being more frequent is the use of hydro-cyclones. This method succeeds when there is the so-called *deoilering* hydro-cyclone, when the continuous phase is water. However, when the continuous phase is oil, for a reason which still being investigated, the process of separation by a hydro-cyclone does not give good results. One of the possible reasons for this failure can be associated to the breakage of the water drops inside the oil, due to action of the flow, making more difficult the process of migration inside the hydro-cyclone.

One of the aims of the present work is to study criteria that can be applied to micro-structured fluids that can be used to represent the break-up of these drops. These criteria are generally thought as measures of the kind of flow which is imposed to the drop, or a general micro-element.

2. MATERIAL RESPONSE AND FLOW CLASSIFICATION

Astarita (1979) proposed some conditions that a representative criterion should meet in order to classify flows. The criterion should be

A) Local. It should indicate the flow type at each position in a flow.

B) Objective. It should be invariant under changes of reference frame.

C) Generally applicable. It should not be restricted to certain classes of flows.

He also pointed out that a criterion could enjoy one of the following conditions

D) Purely kinematic.

E) Dependent on material properties and kinematics.

Thus, according to Astarita (1979) a criterion should be of type ABCD or ABCE. Thompson and Souza Mendes [1,2,3] developed an ABCD criterion and made a review on the subject.

Probably the first work on a flow classification scheme based on material response was done by Tanner (1976). He considered a collection of suspended elastic dumbbell particles (two beads connected by a linear, infinite extensible, spring) following the flow and discriminated flow conditions as strong or weak, depending on the ability of this given flow to distort microstructure. In the case considered, microstructure distortion was captured by examining the tendency of the couple material-flow on producing unbounded growth of the vector connecting the two beads of the dumbbell model.

Since the dumbell model can capture elastic effects, the microstructure resists deformation through a restoring force. It can be shown that, for steady motions, the average end-to-end vector evolves like

$$\frac{d}{dt}\langle \boldsymbol{R}\rangle = \boldsymbol{L}\cdot\langle \boldsymbol{R}\rangle - 2\frac{H}{\zeta}\langle \boldsymbol{R}\rangle$$

where H is the constant spring stiffness and $zeta$ is the constant frictional factor between the beads and the solvent. The strong flow condition is determined by

$$\Rightarrow Max_{\mathrm{Re}}\left(\lambda_i^L\right) > 2\frac{H}{\zeta} \equiv \frac{1}{2\theta}$$

where Max_{Re} is a function that returns the maximum value of the real part of its arguments, lambda^L_i are the eigenvalues of the transpose of the velocity gradient L and \theta=\frac{\zeta}{4H} is the Rouse relaxation time. The idea developed by Tanner (1976), based on Tanner and Huilgol (1975), is to apply a classical linear stability method, finding the Lyapunov exponents of an equation of the form

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$$

If the eigenvalues of tensor **A** have a positive real part, this means that we have an unbounded growth of **x**. When applied to a micro-structure that can be represented by a vector, the resulting matrix can be interpreted as the velocity gradient that is experienced by the micro-element.

An interesting extension of this study was conducted by Doshi and Dealy (1987) by considering effects of Brownian forces in an exponential shear flow. One of the conclusions was that, in exponential shear flows, neglection of Brownian effects leads to strong flows only after a certain value of the product between exponential rate and relaxation time, an important dimensionless parameter of the problem. It is worth noting that these theoretical analysis were based on a specific model for the microstruture and its interaction with the main flow. The conclusions are, therefore, restricted to materials-processes that are well represented by them. For branched polymers undergoing the same flow, for example (Venerus, 2000), other results can be expected.

The work done by Olbricht et al. (1982) is remarkable in the sense that is probably the most complete criterion for flow classification that is related to material response available in literature. There was conducted a very elegant analysis extending Tanner (1976) results by the inclusion of other types of material responses then the ones predicted by the classical dumbbell. In their approach, they consider a more general evolution equation for conformation which was represented by a vector variable, ${\bf R}$, or its dyadic tensor, ${\bf R}{\bf R}$. The vector form is

$$\dot{\mathbf{R}} = (G\mathbf{D}+\mathbf{W})\cdot\mathbf{R} - G\frac{F}{1+F}(\mathbf{D}:\mathbf{rr})\mathbf{R} - \frac{\alpha}{1+F}\mathbf{R}$$

where ***D*** and ***W*** are , respectively, the symmetric and skew-symmetric parts of the velocity gradient and G, F and α are parameters that, when appropriately chosen represent the internal features of the micro-element and it interaction with the bulk flow. This equation encompasses a large variety of microstructured systems such as diluted emulsions and diluted polymeric solutions. The strong-flow criterion is to consider a similar to Tanner's approach and examine the eigenvalues of

$$L_{micro} = G\mathbf{D} + \mathbf{W} - \left(\frac{GF\mathbf{D}_{RR}}{F+1} + \frac{\alpha}{F+1}\right)\mathbf{I}$$

where L_{micro} can be interpreted as the velocity gradient that is experienced by the micro-element. Therefore, the same criterion is applied: if there is at least one eigenvalue of this tensor with a positive real part, the flow is considered strong.

Khakhar and Ottino (1986) have given an interpretation of G, F and α for the case of slender drops. In this case, these coefficients are non-linear. They found the following expressions for these parameters

$$G = \frac{\left(1 + \frac{25}{2}\left(\frac{a}{R}\right)^2\right)}{\left(1 - \frac{5}{2}\left(\frac{a}{R}\right)^3\right)} \approx \left(1 + 15\left(\frac{a}{R}\right)^3\right)$$

$$\alpha = \frac{\sigma}{2\sqrt{5}\mu_e a} \frac{(1+F)(R/a)^{1/2}}{1+0{,}8p(R/a)^3}$$

$$F = G - 1$$

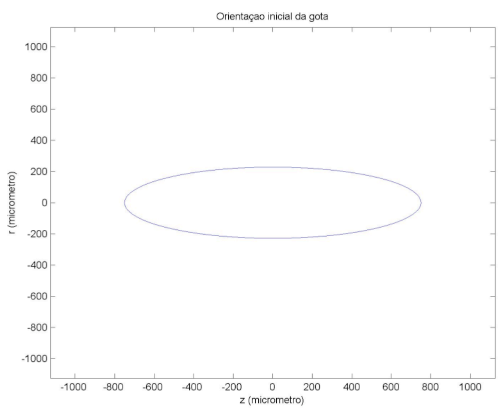
where $R = |\mathbf{R}|$ is the length of the drop, μ_e is the viscosity of the fluid the drop is immersed, μ_i is the viscosity of the drop and $p = \mu_i / \mu_e$ is the viscosity ratio. The model above is valid in the case of slender drops $(a / R << 1)$ for a low viscosity ratio ($p << 1$).

3. THE PRESENT APPROACH

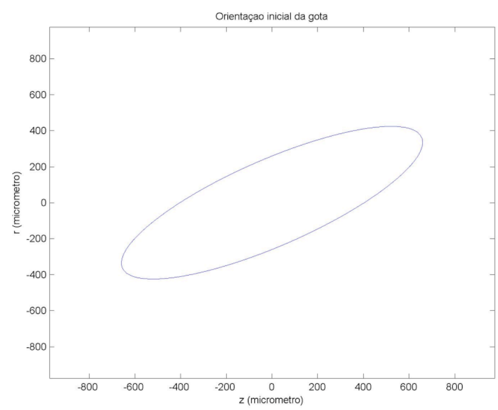
The first part of this work is related to the investigation of the evolution of a drop of water when immersed on a continuous phase of oil with typical features of the field of Jubarte in Campos bay. For this purpose we will use the evolution equation proposed by Olbritch et al. (1982), with the coefficients as suggested by Khakhar and Ottino (1986). The parameters used were given in a work report of PETROBRAS. They are

- Oil Viscosity (μ_e) = 50,6 cP = 0,0506 Pa.s
- Oil density (ρ_e) = 950,6 kg/m³
- Water Viscosity (μ_i) = 1,0 cP = 0,001 Pa.s
- Water density (ρ_i) = 1050,0 kg/m³
- Interfacial tension (σ) = 25 dina/cm = 0,025 N/m
- Mean diameter of a spherical drop = 50μm

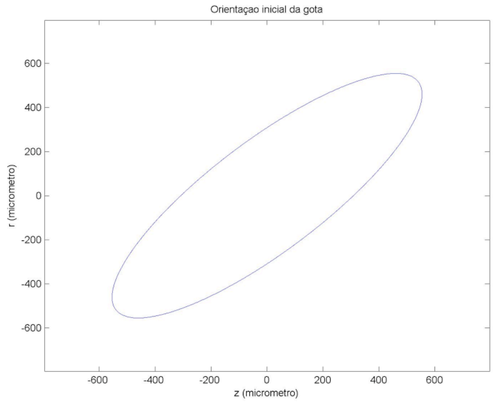
In fact we have computed this evolution with 5 different initial orientations: 0, π/6, π /4, π /3, and π /2 as shown by the figures below



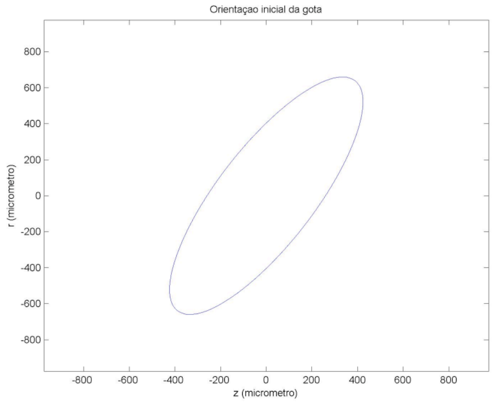
(a)



(b)



(c)



(d)

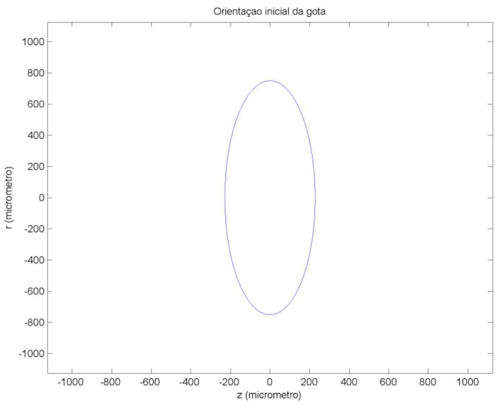


Figure 1 – Initial orientations of the drop of water immersed in oil considered: a) 0, b) π/6, c) π /4, δ) π /3, and e) π /2.

One of the main ideas developed here is to based on the fact that there is an infinity of possibilities, when examining the evolution equation proposed by Olbritch et al. (1982), to transform it to a the form $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$, therefore leading to different sets of Lyapunov exponent solutions. We advocate that the best choice is to consider

$$\mathbf{L}_{\text{mod}} = G\mathbf{D} + \mathbf{W} - \left(\frac{GF\mathbf{D}_{RR}}{F+1} + \frac{\alpha}{F+1} \right) \hat{\mathbf{e}}_{\mathbf{R}} \hat{\mathbf{e}}_{\mathbf{R}}$$

4. RESULTS

4.1 Simple shear flow

The results show, as expected, that there is an attractor direction at $\theta = 0$. The evolution of the orientation of the five drops considered are shown in Fig. 2. Here we can see a monotonic behavior between the different drops.

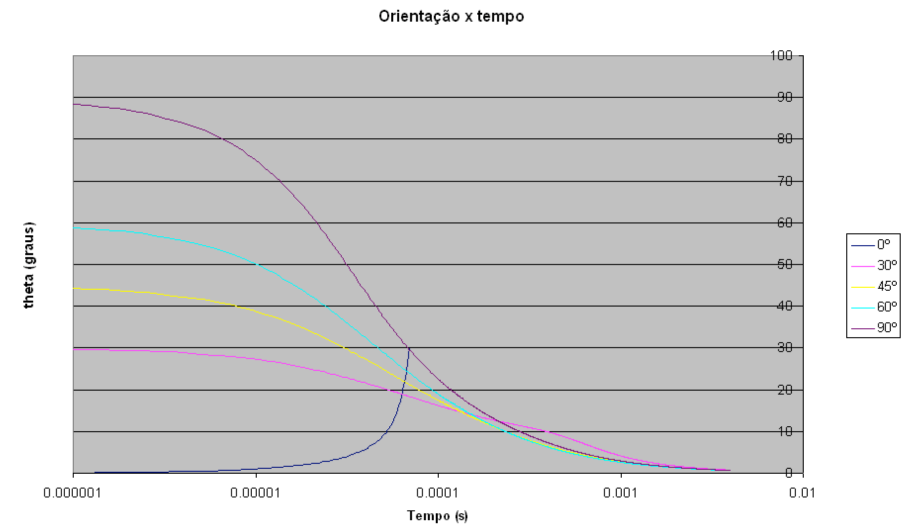
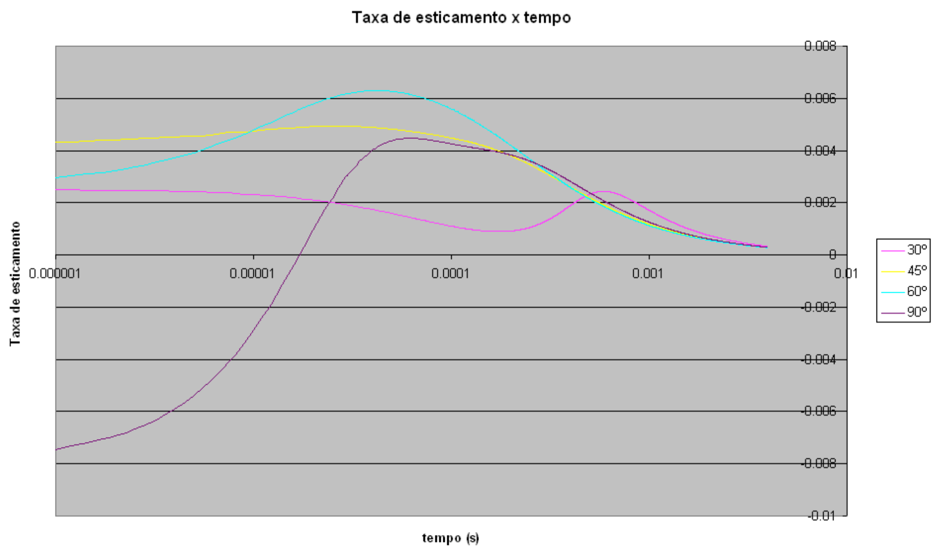


Figure 2. Evolution in time of the orientation of five differently oriented drops in a shear flow.

In the case of the stretching rate computed for the different drops as depicted in Fig. 3, we can see that there is a



more

Figure 3. Evolution in time of the stretching rate of five differently oriented drops in a shear flow.

complex competition between rate of rotation and rate of deformation. Therefore, we can see the cross-over evolution between the drops. This happens because the orientation of maximum stretching rate, which is $\pi /2$ in the case of shear flows, is different from the orientation of maximum deformation rate, which is $\pi /4$ in the case of shear flows.

4.2 Extensional flows

For extensional flows, we can see, from Fig. 4, that, again, we have a monotonic behavior. It is worth noticing that in the case of a drop initially aligned to a main axis of the flow, there is no change in its orientation. It is also interesting to note that $\pi /2$ consists of an unstable orientation attractor, while 0, is a stable orientation attractor, since every orientation in between these values are attracted to the second one. This fact shows that uniaxial extension is a strongly aligning flow.

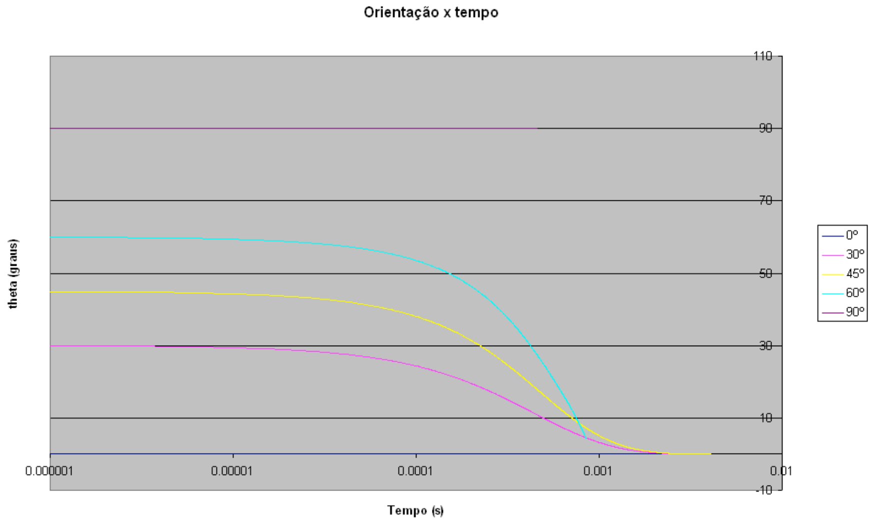


Figure 4. Evolution in time of the orientation of five differently oriented drops in an extensional flow.

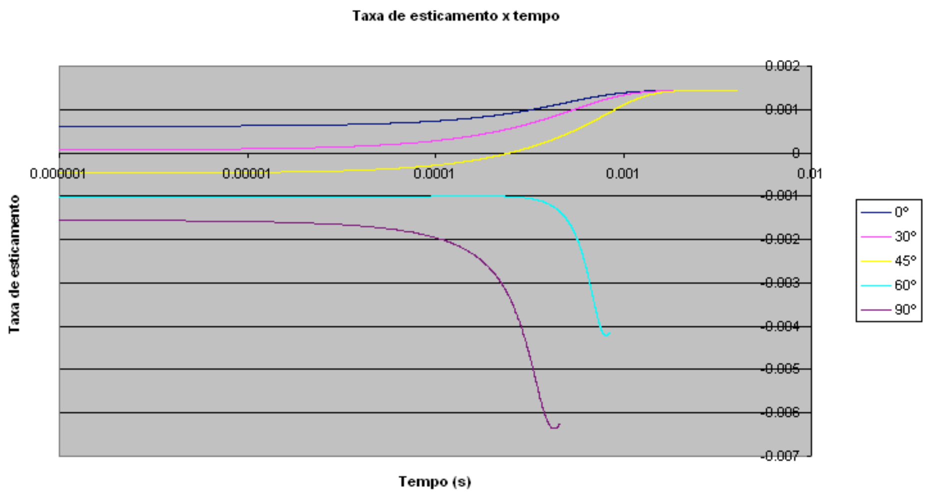


Figure 5. Evolution in time of the rate of stretching of five differently oriented drops in an extensional flow.

Figure 6 shows the two principal directions of the rate-of-strain as seen by the micro-element. In blue is the principal direction using the velocity gradient as suggested by Olbritch et al. (1982). In red the one of the present approach. This is for the case of the drop which is at the orientation of $\pi/6$.

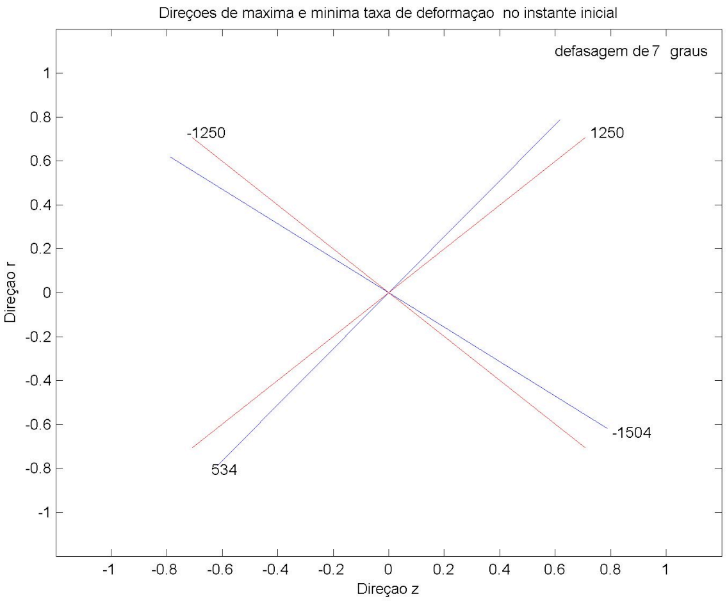


Figure 6. Difference between the principal directions of the deformation rate considering Olbritch et al. (1982), in blue and the present work, in red.

5. ACKNOWLEDGEMENTS

We would like to aknowledge CNPq and FAPERJ for financial support.

6. REFERENCES

Astarita, G.; "Objective and generally applicable criteria for flow classification", Journal of Non-Newtonian Fluid Mechanics, 6 (1979) 69-76.

Doshi, S.R. and Dealy, J.M.; "Exponential shear: a strong flow", Journal of Rheology, 31 (1987) 563-582.

Khakhar, D.V. and Ottino, J.M.; "A Note on the Linear Vector Model of Olbricht, Rallison, and Leal as Applied to the Breakup of Slender Axisymmetric Drops" , Journal of Non-Newtonian Fluid Mechanics, 21 (1986) 127-131.

Olbricht, W. L., Rallison, J.M, and Leal, L.G; " Strong Flow Criteria Based on Microstructure Deformation", Journal of Non-Newtonian Fluid Mechanics, 10 (1982) 291-318.

Tanner, R.I. and Huilgol, R.R., On a classification scheme for flow fields", Rheologica Acta, 14 (1975) 959-962.

Tanner, R.I.; "A test particle approach to flow classification for viscoelastic fluids", A.I.Ch.E.J., 22 (1976) 910-918.

Thompson, R. L. E Souza Mendes, P. R.; "Persistence of straining and flow classification"; Int. Journal of Eng. Sci., 43 (2005) 79-105.

Thompson, R. L. e Souza Mendes, P. R.; "Further remarks on persistence-of-straining and flow classification" Int. Journal of Eng. Sci., 45 (2007) 504-508.

Thompson, R. L.; "Some perspectives on the dynamic history of a material element". Int Journal of Eng. Sci., 46 (2008) 524-549.

5. RESPONSIBILITY NOTICE