Numerical solutions for the fluid flow and the heat transfer of viscoplastic-type non-Newtonian fluids

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Abstract. The aim of this work is to provide numerical solutions for the fluid flow and the heat transfer generated in closed systems containing viscoplastic-type non-Newtonian fluids. A lid driven cavity (LDC) and a differentially heated cavity (DHC) are used as test cases. These numerical solutions can be an appropriate tool for verifying CFD codes which have been developed or adapted to deal with this kind of non-Newtonian fluids. In order to achieve this objective, an in-house CFD code has been implemented and correctly verified by the method of manufactured solutions and by some numerical solutions too. Furthermore, a high-performance CFD code (Termo Fluids S.L.) has been adapted and properly verified, by the corresponding numerical solutions, to deal with this kind of non-Newtonian fluids.

The viscoplastic behaviour of certain non-Newtonian fluids will be generated from a viscous stress which has been defined by a potential-type rheological law. The pseudoplastic and dilatant behaviours will be studied. On this matter, the influence of different physical aspects on the numerical simulations will be analysed, e.g. different exponent values in the potential-type rheological law and different values of the non-dimensional numbers. Moreover, the influence of different numerical aspects on the numerical simulations will also be analysed, e.g. unstructured meshes, conservative numerical schemes and more efficient and parallel algorithms and solvers.

1. Introduction
In most of the engineering applications the more relevant non-Newtonian characteristics are those associated with the viscoplastic behaviour of non-Newtonian fluids. Furthermore, to this kind of non-Newtonian fluids CFD simulations in complex geometries are of special interest due to the increase of their applications in the biotechnological industry, food processing industry, smelting industry; among many others.

Several authors have used specific rheological laws in the generalized Newtonian model to analyse the flow of non-Newtonian fluids which exhibit stresses exclusively viscous with plastic effects (viscoplastic fluids).

Brent C. Bell and Karan S. Surana [1] used a power-type rheological law to analyse the flow of some non-Newtonian fluids in different geometrical configurations. Among which, on the one hand, some configurations were analysed as isothermal systems: parallel plates without relative motion (Hagen-Poiseuille flow), 2:1 symmetric sudden expansion and cavity with a sliding lid (lid-driven cavity); and, on the other hand, other configurations were analysed as non-isothermal systems: parallel plates with relative motion (Couette flow) and 4:1 symmetric sudden contraction.

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K.A. Pericleous [2] studied the fluid flow and the heat transfer in the case of a differentially heated cavity using a power-type rheological law, in order to characterize the pseudoplastic and dilatant behaviour of certain non-Newtonian fluids. This case is of special interest because it has important applications in biotechnology, areas where the heat transfer in fine suspensions are required, etc..

Nevertheless, from our point of view, few numerical solutions for viscoplastic-type non-Newtonian fluids have been provided, despite its growing presence in the field of CFD simulations.

2. Mathematical analysis

First of all, the equations describing the non-Newtonian behaviour of the infinitesimal elements which form a continuum medium (from a point of view external to them) will be presented together with the corresponding hypothesis. It is assumed a fluid with constant thermophysical properties ($\rho$, $c_p$, $\lambda$) and with negligible effects of viscous dissipation.

Continuity equation: Law of conservation of mass.

$$\nabla \cdot \mathbf{v} = 0$$ (1)

Linear momentum equation: Newton’s second law.

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \nabla \cdot (\mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot (\eta \nabla \mathbf{v}) + \nabla \cdot (\eta \nabla^T \mathbf{v}) + \rho \mathbf{g}$$ (2)

Thermal energy equation: First law of Thermodynamics.

$$\rho \frac{\partial T}{\partial t} + \rho \nabla \cdot (\mathbf{v} T) = \frac{\lambda}{c_p} \nabla^2 T$$ (3)

These equations are expressed in matrix form (see ref. [3]) as:

$$M_c[f_c(\mathbf{v}) \cdot \mathbf{n}]_f = 0 \quad \text{where} \quad f_c(\mathbf{v}) = \mathbf{v}$$ (4)

$$\rho_3c \frac{\partial \mathbf{v}_c}{\partial t} \Omega_3c + C_3c \mathbf{v}_c = -G_c p_c + D_3c \mathbf{v}_c + M_3c[f_c(\mathbf{v}) \cdot \mathbf{n}]_f + B_3c \mathbf{g} \quad \text{where} \quad f_c(\mathbf{v}) = \eta \nabla^T \mathbf{v}$$ (5)

$$\rho_c \frac{\partial T_c}{\partial t} \Omega_c + C_c T_c = D_c T_c$$ (6)

Where $c \equiv \text{center}$ and $f \equiv \text{face}$. Furthermore: $\mathbf{v}_c \in \mathbb{R}^{3n}$, $p_c \in \mathbb{R}^n$, $M_c \in \mathbb{R}^{n,m}$, $G_c \in \mathbb{R}^{3n,n}$, $D_3c \in \mathbb{R}^{3n,3n}$, $D_c \in \mathbb{R}^{n,n}$, $C_3c \in \mathbb{R}^{3n,3n}$ and $C_c \in \mathbb{R}^{n,n}$; here $n$ and $m$ applies for the total number of control volumes and control faces of the discretised domain, respectively.

In the second place, the equations generating the non-Newtonian behaviour of the infinitesimal elements that form a continuous medium (from a point of view internal to them) will be analysed (see ref. [4]).

Due to the nature of the fluid model (viscoplastic type) to be analysed, a rheological model known in the specialized literature as generalized Newtonian model will be developed. This rheological model will allow dealing with a fluid model without memory and, therefore, the principle of determinism of the stresses may be ignored.

$$\mathbf{\sigma} (X, t) = \mathcal{F} [D (X, t)]$$ (7)

Where X is the reference of any material element of the continuous medium. In addition, the fluid to be analysed must be isotropic. It means there is no prevailing direction in the physical
properties. Therefore, the main coordinate system of the strain rate tensor match up with the corresponding of the extra stress tensor. Thereby, the previous tensor relationship is reduced to a scalar relationship between the main values of the $\sigma$ and $D$ tensors.

\[ \sigma_i = \phi_1 + \phi_2 D_i + \phi_3 D_i^2 \] (8)

Finally, the following expression, general and reasonable, for the stress tensor of a viscoplastic fluid (assuming incompressible fluid) is obtained:

\[ \boxed{\sigma(D) = -p\delta + 2\eta(\dot{\gamma})D} \] (9)

Consequently the viscosity of a non-Newtonian fluid will vary with a metric of the shear rate tensor. Therefore, the viscosity not have a value only and exclusively defined from the pressure and temperature at which it is, unlike what happen in the case of Newtonian fluids.

In this study, the pseudoplastic and dilatant behaviours will be defined from a potential-type rheological law (Ostwald-de Waele rheological law).

\[ \eta(\dot{\gamma}) = k\dot{\gamma}^{n-1} \] where \[ \dot{\gamma} = \sqrt{\frac{1}{2}(\dot{\gamma} : \dot{\gamma})} \] (10)

3. Test Cases

3.1. Lid driven cavity (LDC)

The physical problem consists of the laminar flow of an incompressible fluid confined in a cubic cavity whose upper lid moves along its own plane, with a uniform velocity, and tangential to the flow, while the rest of the walls remain motionless [5, 1].

The mathematical model is formed by a set of equations which has its origin in the transport equations (equations 1, 2 and 3) and which is closed from a non-Newtonian behaviour of viscoplastic type with a viscous stress defined according to a potential-type rheological law (equation 10). Furthermore, a fluid with constant thermophysical properties ($\rho$) and with negligible effects of viscous dissipation is assumed. It is also assumed two-dimensional case. The dimensionless variables have been defined from: $l_o = L$, $t_o = l_o/v_o$, $v_o = v_L$, $\Delta p_o = \rho v_o^2$, $\eta_{ao} = k(v_o/l_o)^{n-1}$. Therefore, the parameters $L$ and $v_L$ are the characteristic values of the problem. Moreover, the test case is completely defined by just two dimensionless numbers: $n$ and $Re$, where the latter is defined as follows: $Re = (\rho v_o l_o)/\eta_{ao}$. Thus, the results presented below correspond to a Reynolds number of 100.

The kind of mesh used to discretize the domain is uniform.

The boundary conditions adopted to close the domain are the following: for the fixed boundaries the velocity is set at zero, whereas for the sliding cover the velocity is set at a certain value. Regarding the pressure, this has been extrapolated from the inner values of the domain.

The aim of this test case is take a first step towards the verification of the terms involved in the generation of non-Newtonian behaviour, which will allow to consider the case of viscoplastic fluid flow and, at the same time, to generate numerical solutions for this test case.

The characteristic values of the numerical solutions are presented on the table 1. On the left hand side of Table 1 some of these characteristic values provided by other authors (Bell and Surana [5] and Guide et al. [1]) are shown. Together with the characteristic velocities, a mass flow balance through their corresponding plane is also provided in percentages. As can be seen, the maximum value of this mass flow balance is less than 1 %. On the right hand side of this table, the obtained characteristic values of the numerical solutions are also provided, together with the relative deviation in percentages respect to the corresponding solution provided by another author, if any. For the studied non-Newtonian fluids, this deviation has been always
kept at less than 3%, except when the exponent value of the potential-type rheological law has become equal to or less than 0.25. In the latter case, the velocity profiles acquire some very small velocity values and, therefore, the relative error becomes very large and is not significant. In order to obtain these results, it has been necessary to use a mesh of 41x41 control volumes, except for the two cases with an exponent value of the potential-type rheological law of 0.5 and 0.75. For the latter cases, the velocity profiles of the velocity component \( W \) have been obtained with a mesh of 81x81 control volumes.

### Table 1: Characteristic values for the LDC

| \( Re \) | Present results | Other authors |
|---|---|---|
| | \( n \) | \( \frac{U_{\text{max},1/2}}{Z} \) | \( \frac{W_{\text{max},1/2}}{X} \) | \( Z \) | \( \frac{W_{\text{max},1/2}}{X} \) | From |
| 0.25 | 0.055106 | 0.597561 | 0.030397 | 0.817073 | 0.047620 | Bell and Surana [1] |
| | (13.588) | (1.086) | (8.605) | (-0.196) | (0.671) | |
| 0.50 | 0.117749 | 0.500000 | 0.141987 | 0.833333 | -0.114674 | Bell and Surana [1] |
| | (2.611) | (1.744) | (2.623) | (0.194) | (0.448) | |
| 0.75 | 0.176058 | 0.451220 | 0.222248 | 0.829988 | 0.114674 | Bell and Surana [1] |
| | (0.401) | (1.509) | (0.856) | (0.247) | (0.513) | |
| 1.00 | 0.210535 | 0.451220 | 0.251234 | 0.817073 | 0.210933 | Guia et al. [5] |
| | (-0.173) | (-0.417) | (2.356) | (1.514) | (0.004) | |
| 1.25 | 0.228748 | 0.451220 | 0.263465 | 0.792683 | -0.245331 | |
| 1.50 | 0.238379 | 0.475610 | 0.269580 | 0.792683 | -0.235054 | Bell and Surana [1] |
| | (1.395) | (1.390) | (0.018) | (0.019) | (0.506) | |
| 1.75 | 0.245705 | 0.475610 | 0.273348 | 0.792683 | -0.224151 | |
| | (0.029) | | | | | |

The implicit correction method (SIMPLEC) implemented in the in-house CFD code has turned out to be robust and accurate, although it was suspected that its efficiency should be far from the optimum. Reason why different methods for treating the coupling between velocity and pressure have been studied by a more general CFD code (Termo Fluids S.L. [6]). This CFD code has been extended to deal with this kind of non-Newtonian fluids (see Figure 1) and it has also been properly verified by means of the corresponding numerical solutions. Regarding the conclusions obtained from each one of the studied methods, firstly, the implicit Euler method has turned out not to be robust when a large time discretization step is imposed. Secondly, the explicit projection method has turned out not to be efficient, since it requires a very small time discretization step. For the last two reasons an implicit projection method has been implemented in the Termo-Fluids CFD code. It has turned out to be robust and accurate, with an efficiency that appears to be much closer to the optimum than that corresponding to the implicit correction method (SIMPLEC). The correct running of these methods is shown in Figure 1.

### 3.2. Differentially heated cavity (DHC)

The physical problem consists of a fluid flow which is driven by the buoyancy of the fluid itself when it is subjected to the temperature difference that exists between the two vertical and confronted walls of the cubic cavity in which it is confined [7, 8].

The mathematical model consists of a set of equations which has its origin in the transport equations (equations 1, 2 and 3) and which is closed from a non-Newtonian behaviour of viscoplastic type with a viscous strain defined by a potential-type rheological law (equation 10). Furthermore, it is assumed a fluid with constant thermophysical properties \((\rho, c_p, \lambda)\), negligible effects of viscous dissipation and the Boussinesq approximation. It is also assumed two-dimensional case. The corresponding dimensionless variables have been defined from: \( l_o = L \).
\[ t_o = l_o/v_o, \quad v_o = \lambda/(\rho c_p l_o), \quad \Delta p_{ho} = \rho v_o^2, \quad \eta_{ao} = k (v_o/l_o)^{n-1}, \quad T_o = (T_h + T_c)/2 \quad \text{and} \quad \Delta T_o = T_h - T_c. \]

Therefore, the parameters \( L, T_h \) and \( T_c \) are the characteristic values of the problem. Moreover, the test case is completely defined by just three dimensionless numbers: \( n, \text{Pr, Ra} \); where the last two are defined as follows: \( \text{Pr} = (c_p \eta_{ao}/\lambda) \) and \( \text{Ra} = (g \beta \Delta T_o l_o^3)/(\nu_{ao} \alpha) \), for which \( \nu_{ao} = \eta_{ao}/\rho \) and \( \alpha = \lambda/(\rho c_p) \). Thus, the results presented below correspond to a Rayleigh number of \( 1 \times 10^5 \) and a Prandtl number of 0.71.

The kind of mesh used to discretize the domain is not uniform and has been concentrated by a hyperbolic-tangent function (see ref. [3]).

The boundary conditions adopted to close the domain are the following: for all the fixed boundaries the velocity is set at zero and the pressure has been extrapolated from the inner domain. Furthermore, the cavity walls are kept isotherms at different temperature, while its base and cover are kept adiabatic.

The aim of the DHC with viscoplastic fluids is to generate some numerical solutions of the same form as those obtained for the LDC.

A brief overview of the most important characteristic values are provided in Table 2. The average Nusselt number increases considerably when the exponent value of the potential-type rheological law decreases. Furthermore, the balance of the convective heat flow has been also gathered in Table 3. As can be seen, for values of \( n \) below 0.75 it is difficult to obtain a permanent numerical solution.

Regarding physical aspects, in the shear-thinning or pseudoplastic regime the boundary layer generated by the isotherm walls was getting thinner and moving faster as the exponent value of the potential-type rheological law was reduced. This fact implies that efforts introduced by buoyancy forces tend to be concentrated in this boundary layer region and that the inner region of the cavity stays increasingly stagnant. As a consequence of this behaviour, the main double vortex associated with the Newtonian behaviour tends to expand and disappear from the cavity center. By contrast, in the shear-thickening or dilatant regime the boundary layer generated by the isotherm walls was getting wider and moving more slowly as the exponent value of the potential-type rheological law was increased. This fact means that efforts introduced by buoyancy forces tend to propagate towards the inner region of the cavity and that the
latter becomes increasingly active. As a consequence of this behaviour, the main double vortex associated with the Newtonian behaviour tends to concentrate and appear as a single vortex in the center of the cavity. Thus, the viscous stresses generated by the buoyancy forces, appearing in the cavity through the isotherms walls, were better concentrated towards the outermost region for the pseudoplastic fluids than for the Newtonian fluids. By the contrary, such stresses were better propagated towards the innermost region for the dilatant fluids than for the Newtonian fluids. The last fact reduces the efficiency with which the heat transfer by convection was produced, which is reflected in a decrease of the average Nusselt number when the exponent value of the potential-type rheological law \((n)\) is increased. In summary, pseudoplastic fluids seem to transport heat energy better than Newtonian fluids and, conversely, dilatant fluids seem to transport it worse.

4. Discussion

Regarding numerical aspects, the mesh resolution required to properly reproduce the numerical solutions of reference (Guia et al. [5], Bell and Surana [1] and Vahl Davis [7,8]) depends on the type of non-Newtonian fluid to be studied. For pseudoplastic fluids \((n < 1)\) exist the necessity of using mesh densities higher than that for a Newtonian fluid \((n = 1)\). This, that seems obvious, is not always taken into account in some of the consulted articles from the literature. For example, the mesh with 41x41 control volumes used in the LDC for a Newtonian fluid, that turns out to be appropriate to reproduce the numerical solution of Guia et al. [5], is not enough for the

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Table 2: Summary of the characteristic values

| \( Ra = 1 \times 10^3 \) | \( n \) | \( U_{\text{max,}1/2} \) | \( Z \) | \( W_{\text{max,}1/2} \) | \( X \) | \( N_{u_{\text{avg}}} \) | \( Z \) | \( N_{u_{\text{max}}} \) | \( Z \) | \( N_{u_{\text{min}}} \) | \( Z \) |
|----------------|------|----------------|-----|----------------|----|----------------|-----|----------------|-----|----------------|-----|
| 0.25 | 392.978 | 0.998 | 412.093 | 0.002 | 64.692 | 0.996 | 14.241 |
| 0.50 | 184.557 | 0.980 | 209.342 | 0.010 | 19.991 | 0.945 | 9.476 |
| 0.75 | 107.96 | 0.938 | 132.702 | 0.028 | 11.19 | 0.943 | 6.823 |
| 1.00 | 34.730 | 0.855 | 68.590 | 0.066 | 7.717 | 0.999 | 4.521 |
| VahlDavis [7, 8] | 34.730 | 0.855 | 68.590 | 0.066 | 7.717 | 0.999 | 4.521 |

Table 3: Balance of the convective heat flow

| Balance of the convective heat flow: \( N_{u_{\text{avg}}} - N_{u_{\text{max}}} \) | \( n \) | \( 21 \times 21 \) mesh | \( 41 \times 41 \) mesh | \( 81 \times 81 \) mesh | \( 21 \times 21 \) mesh | \( 41 \times 41 \) mesh | \( 81 \times 81 \) mesh | \( VahlDavis [7, 8] \) |
|--------------------------------|------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| \( 0.25 \) | 0.49 | no conv. ! | no conv. ! | no conv. ! | no conv. ! | --- | --- | --- |
| \( 0.50 \) | -0.09524 | -0.0335 | -0.01542 | no conv. ! | no conv. ! | --- | --- | --- |
| \( 0.75 \) | 0.0659 | 0.02357 | 0.00587 | 0.0211 | -0.00147 | 0.00012 | --- | --- |
| \( 1.00 \) | 0.01999 | -0.00577 | -0.00117 | 0.00941 | -0.00529 | -0.000074 | 0.01 | --- |
| \( 1.25 \) | -0.05455 | -0.02978 | -0.01511 | 0.00005 | -0.00001 | 0.00006 | --- | --- |
| \( 1.50 \) | -0.07564 | -0.04462 | -0.02349 | 0.02797 | 0.00651 | 0.00162 | --- | --- |
| \( 1.75 \) | -0.09188 | -0.05612 | -0.03124 | 0.04615 | 0.01169 | 0.00248 | --- | --- |
| \( 2.00 \) | -0.10105 | -0.06015 | -0.03348 | 0.03763 | 0.01054 | 0.00235 | --- | --- |
analysed pseudoplastic fluids. Similarly, the mesh with 81x81 control volumes used in the DHC for a Newtonian fluid, that turns out to be appropriate to reproduce the numerical solution provided by Vahl Davis [7, 8], is only sufficient for pseudoplastic fluids with values of $n \geq 0.75$. However, in both test cases the used meshes for a certain Newtonian fluid have been enough for the dilatant fluids ($n > 1$) analysed.

Moreover, on the one hand, it is important to note that for values of $n$ below 0.5 the pressure correction of the SIMPLEC segregated algorithm has had to be relaxed increasingly. This fact might have its origin in a numerical or physical problem. To tackle the latter problem we are working on the following topics: unstructured meshes in order to have a high mesh concentration in certain domain regions (boundary layers), conservative numerical schemes to reproduce correctly the physics implicit in the continuous mathematical operators by the discrete mathematical operators, implicit projection methods to obtain at the same time the advantages of implicit correction and explicit projection methods. Regarding the last topic, an implicit projection method has been implemented in the Termo-Fluids CFD code. It has turned out to be robust and accurate, with an efficiency that appears to be much closer to the optimum than that corresponding to the SIMPLEC method (implicit correction method). On the other hand, it is interesting to observe how in the DHC the SMART numerical scheme tends to act as an UPWIND when approaching to $n = 2.0$. In addition, for the last test case, an improved version of the Pressure Weighted Interpolation Method (PWIM, A. Pascau in 2009 [9]) has been used in order to obtain a numerical solution independent of the relaxation factor and the temporal discretization step.
Regarding physical aspects, in the pseudoplastic fluids the generated strain tends to concentrate in form of a boundary layer region which is increasingly thin and fast, whereas in the dilatant fluids it tends to propagate in form of a boundary layer region which is increasingly wide and slow. Thus, the viscous stresses appearing in the cavity are better concentrated towards the outermost region for the pseudoplastic fluids than for the Newtonian fluids. By the contrary, such stresses are better propagated towards the innermost region for the dilatant fluids than for the Newtonian fluids. In this way, in the DHC the last fact reduces the efficiency with which is produced the heat transfer by convection, which is reflected in a decrease of the average Nusselt number when the exponent value of the potential-type rheological law (n) is increased. The latter fact was also appreciated by K.A. Pericleous in one of his articles [2]. Therefore, pseudoplastic fluids seem to transport heat energy better than Newtonian fluids and, conversely, dilatant fluids seem to transport it worse.

5. Conclusions
In this work it is provided numerical solutions for the fluid flow and the heat transfer generated in closed systems containing viscoplastic-type non-Newtonian fluids. The last ones are expected to serve as a reference for the verification of those CFD codes that have been developed or adapted to deal with the last kind of non-Newtonian fluids. Furthermore, during the development of this work, it has been observed different numerical and phenomenological aspects.

Whereas flow configuration is similar for all types of non-Newtonian fluids studied in the LDC, such configuration presents major changes in the DHC. For the pseudoplastic fluids in the last test case, the numerical solutions for the permanent regime are achieved except when the exponent value of the potential-type rheological law is equal to or less than 0.5. Therefore, the used pseudotransient process not allow to achieve the numerical solution corresponding to the permanent regime, if any. It could also be possible that the permanent regime does not exist and that the transient regime leads to a periodic or an aperiodic unsteady state. Consequently, more effort is needed to clarify this point.

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