A case study on the evolution of rigid zones within the permanent two-dimensional Herschel-Bulkley fluid flow

Um estudo de caso sobre a evolução de zonas rígidas dentro do fluxo de fluido permanente bidimensional Herschel-Bulkley

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ABSTRACT
The formation and development of undeformed regions during the flow of viscoplastic fluids can significantly affect fluid flow behaviour. They can impair the efficiency and effectiveness of industrial operations that use viscoplastic fluids. This paper uses numerical analysis to examine the emergence of rigid zones during non-stationary Herschel-Bulkley fluid flow across a square plate. The impact of pressure and yield stress on the behaviour of rigid zones over time is explored, and the development of the rigid zone area is shown. This work produced mathematical correlations that describe the relationship between the area of rigid zones and both the time of flow and the yield stress, as well as the area of rigid zones and the stagnation time.

Keywords: pressure, laminar flow, Herschel-Bulkley fluid, non-stationary flow,
rigid zones.

RESUMO
A formação e desenvolvimento de regiões não deformadas durante o fluxo de fluidos viscoplastícios podem afetar significativamente o comportamento do fluxo de fluido. Elas podem prejudicar a eficiência e eficácia das operações industriais que utilizam fluidos viscoplastícios. Este artigo utiliza análise numérica para examinar o surgimento de zonas rígidas durante o fluxo não estacionário de fluido Herschel-Bulkley através de uma placa quadrada. O impacto da pressão e do limite de escoamento no comportamento das zonas rígidas ao longo do tempo é explorado, e o desenvolvimento da área da zona rígida é mostrado. Este trabalho produziu correlações matemáticas que descrevem a relação entre a área das zonas rígidas e tanto o tempo de fluxo quanto o limite de escoamento, assim como a área das zonas rígidas e o tempo de estagnação.

Palavras-chave: pressão, fluxo laminar, fluido Herschel-Bulkley, fluxo não estacionário, zonas rígidas.

1 INTRODUCTION
The behavior of non-Newtonian fluids is showcased in natural processes such as processing concrete, petroleum, printing inks, paints, mud, polymers, and lava flows. They can also be found in biological fluids like blood and internal medicine. In addition, non-Newtonian fluids are used in personal care products like toothpaste and household products like foodstuffs. These fluids follow a nonlinear model that relates shear stress with the shear rate [1, 2]. The non-Newtonian fluids can be divided into several types, including viscoplastic. Viscoplastic fluids, like toothpaste, exhibit a fascinating behavior. They behave as solids when weak forces are applied but transition into fluid-like flow when subjected to stronger forces beyond the yield stress threshold. This unique characteristic sets them apart from traditional viscous fluids, emphasizing the need to understand viscoplastic fluids’ distinct behavior and practical applications [3]. The Herschel-Bulkley model is the most used to describe the materials obeying the viscoplastic behaviour [4]. This model has garnered significant attention and is becoming increasingly popular, as evidenced by its growing usage (for example, see [5,6]). The Herschel-Bulkley fluid and non-Newtonian fluids generally combine rigid-like and fluid-like behaviours.

The material behaves like a solid when the imposed stress is below the yield limit. It resists deformation and maintains its shape, exhibiting little or no flow. The
material's internal structure is strong enough to withstand the applied stress, preventing any significant flow. The material transitions and flows like a fluid once the applied stress exceeds the yield limit. At this point, the material's internal structure breaks down or rearranges, allowing it to flow and deform under the applied stress. The material loses its rigidity and behaves more like a conventional fluid. In this fluid-like behavior the deformation rate is close to zero, and the viscosity tends to infinity, which poses numerical difficulties during the simulation of this scenario. An exponentially regularized model has been proposed by Papanastasiou to overcome these difficulties [7]. The regularization parameters of this model have been the subject of several studies. For example, the m parameter called the stress growth exponent measures how the fluid is close to the ideality; in [8], the authors postulate that when the fluid is ideal while Mitsoulis and al. have [9] have recommended m<100 to get accurate results for viscoplastic materials. A numerical flow study was done for the authors in [10] to determine yield stress's effect on the Herschel-Bulkley fluid's effective viscosity. The Herschel-Bulkley fluids have the following particularity when the particle concentration of the mixture is very high, and the viscosity is large, the forces generated by the interaction and collision of particles lead the fluid to become pasty and indicate the creation of rigid zones. Many researchers in the literature investigate how different parameters affect the performance of rigid zones. Mossaz et al. [11,12] have studied the effect of the Oldroyd number and the power law index on the unyielded zones.

Similarly, in [13], the influence of Oldroyd numbers on the rigid zones is studied. Using mathematical arguments, Messelmi [14] has proved that as yield stress rises, the rigid zones grow, and the flow may be wholly blocked. This work aims to scout the development of rigid zones during the unsteady flow of Herschel-Bulkley fluid in two-dimensional domain to show the evolution of these rigid zones and its behavior under pressure and yield stress. Additionally, the correlation between the measure of rigid zones with yield stress and pressure in the case of non-stationary flow is proposed. The study utilized numerical simulations performed with the COMSOL Multiphysics 6.0 software, in which the regularized Papanastasiou model is implemented. The paper is structured as follows: The second section presents the problem statement. The mathematical equations are presented in the third section with the regularization parameters used in this study.
The validation of numerical simulations and the grid study are shown in the fourth section. The fifth section is consecrated to the obtained results with discussions to conclude the present paper by conclusions.

2 PROBLEM DESCRIPTION

The present work studies the behavior of rigid zones during Herschel-Bulkley fluid's unsteady, laminar, and isothermal flow. The concrete in its fresh state obeys the Herschel-Bulkley model, where its rheological properties are as follows [15], the density is $\rho = 1370$ kg/m$^3$, the consistency $k = 2.42$ Pa s, the power law index is $n = 0.552$, and the yield stress is $\tau_y = 5$ Pa. A two-dimensional (2D) square-shaped plate is studied using COMSOL Multiphysics 6.0. An imposed $x$-pressure governs the flow in the inlet boundary $p_{in} = 15$ Pa with an initial value of velocity $u_{in} = 0.001$ m/s. The no-slip condition and a null velocity in the outlet boundary are adopted at the walls.

3 MATHEMATICAL FORMULATION

The flow is governed by the continuity equations and momentum equations given sequentially, as follows:

$$\nabla \cdot U = 0 \quad (1)$$

$$\rho \frac{\partial U}{\partial t} + \rho (U \cdot \nabla) U = \nabla[-pI + \tau] + f \quad (2)$$

The shear stress is given by the Herschel-Bulkley model [16]:

$$\tau = \max(\tau_y, \frac{\tau_s}{\beta} \frac{\dot{\gamma}}{\dot{\gamma}_0}^{n-1})$$

where $\dot{\gamma}$ is the shear rate, $\dot{\gamma}_0$ is the reference shear rate, and $\beta$ is the consistency index.
\[
\begin{cases}
\tau = \left( k |\dot{\gamma}|^{n-1} + \frac{\tau_y}{|\dot{\gamma}|} \right) |\dot{\gamma}| \\
|\dot{\gamma}| = 0
\end{cases}
\] for \(|\tau| > \tau_y\)  \\
\text{for } |\tau| \leq \tau_y
\] (3)

Where:

\(\tau_y\) is the yield stress, \(\gamma\) is the shear rate tensor, and \(|\gamma|\) is its magnitude.

The following relations give the shear rate:

\[
\dot{\gamma} = \frac{1}{2} [\nabla U + (\nabla U)^T]
\] (4)

\[
|\dot{\gamma}| = \sqrt{2 \dot{\gamma} : \dot{\gamma}}
\] (5)

In the Herschel-Bulkley viscoplastic model, the fluid behaves in two ways; when the applied stress to the fluid exceeds its yield limit, the fluid will flow and show pseudo-plastic behavior. However, if the stress does not reach the yield point, the fluid will not flow and behave like a solid; in this case, the viscosity goes to infinity. Therefore, the rigid zones appear and begin to change measure, form, and location with time. The rigid zones are defined mathematically, wherein the shear rate vanishes [14].

\[
\Omega_r = \{ x \in \Omega, t \geq 0 : |\dot{\gamma}(U(x,y,t))| = 0 \}
\] (6)

The null value of the shear rate leads to a singularity in the constitutive model of the Herschel-Bulkley fluid, which poses difficulties in numerical simulations of this behavior. Thus, regularization methods are presented in the literature to avoid this discontinuity (see [19,20,21]). The regularized Papanastasiou model is adopted in this work, for which the Herschel Bulkley model becomes as follows: [7,22].
\[ \tau = k|\dot{\gamma}|^{n-1} + \frac{\tau_y}{|\dot{\gamma}|} \left[ 1 - \exp(-m|\dot{\gamma}|) \right] \dot{\gamma} \]  

(7)

and the viscosity takes the formula:

\[ \mu(\dot{\gamma}) = k|\dot{\gamma}|^{n-1} + \frac{\tau_y}{|\dot{\gamma}|} \left[ 1 - \exp(-m|\dot{\gamma}|) \right] \]  

(8)

As the introduction mentions, the regularization parameter \( m \) is called the stress growth exponent, which determines how the Herschel-Bulkley model is close to the ideality. In this study, it is chosen as \( m = 10 \text{ s} \). The critical shear rate in the regularized model \( \dot{\gamma}_c \) significantly affects the rigid zones in terms of location and measure. Based on the previous works, the critical shear rate adopted in this work is parameter \( \dot{\gamma}_c = 0.01 \text{ s}^{-1} \) [23]. Therefore, in the regularization technique, the rigid zones are defined wherein the shear rate \( \dot{\gamma} \) is less than or equal to the critical shear rate \( \dot{\gamma}_c \), i.e. \( \dot{\gamma} \leq \dot{\gamma}_c \) [8]. The mathematical definition of rigid zones becomes as follows:

\[ \Omega_r = \left\{ x \in \Omega, t \geq 0 : \left| \dot{\gamma}(U(x,y,t)) \right| \leq \dot{\gamma}_c \right\} \]  

(9)

4 VALIDATION AND GRID STUDY

Ensuring the steady-state solution is accurate is crucial because it is the starting point for simulating unsteady flow. The CFD predictions of the velocity field were compared with the exact analytical solutions obtained through theoretical calculations to confirm the accuracy of the steady-state solution. Consider a flow in a rectangular domain with the dimensions \( \Omega = [0; L] \times [0; H] \) that is moving at a constant velocity. \( u^* \) is the non-dimensional velocity in the horizontal direction such that the velocity is given by \( U = Vu^*(y) \vec{e}_x \) where \( V \) is the reference velocity. The following relations give the analytical solution Eq. (10) of this flow [24]:
\[ u^* = \frac{1}{M} f^* \left\{ \begin{array}{c} \left( \frac{y_0}{H} \right)^M - \left( \frac{y}{H} \right)^M \\ \left( \frac{y_0}{H} \right)^M - \left( \frac{y - (H - y_0)}{H} \right)^M \end{array} \right\} \]

Where:

\[ 1 + 1/n f^* = \left( \frac{f H}{K} \right)^{\frac{1}{n}} \times \frac{H}{V} \]

is the non-dimensional gradient force and \( y_0 = \frac{H}{2} - \frac{\tau y}{f} \).

The theoretical velocity profile obtained by the analytical relations has been compared with the horizontal velocity profile obtained numerically at \( x = H/2 \) using COMSOL Multiphysics 6.0. The velocity profiles obtained numerically and analytically are presented in Fig. 2. As shown in the Fig, the agreement between the two profiles validates the numerical simulations using COMSOL Multiphysics 6.0. To ensure the accuracy of the results, it is essential to select the grid for the numerical simulations carefully. In this study, a regular mapped mesh was generated and tested to determine the appropriate mesh size. The axial velocity profiles for three different mesh sizes are shown in Fig. 3 along the fluid’s direction. It can be observed that the axial velocity profiles for Grid 2 and Grid 3 are very similar. Based on this, Grid 2 was chosen for all simulations presented in the remainder of the paper. This ensures that the simulations are accurate and reliable for further analysis and interpretation.

Figure 2. Comparison of velocity magnitude predicted numerically with the theoretical velocity profiles
5 RESULTS AND DISCUSSION

5.1 EFFECT OF YIELD STRESS ON THE EVOLUTION OF RIGID ZONES

Figure 4 shows the growth of the rigid zone area with respect to flow time for various yield stress values. It is observed, for all yield stress values, the measure of the rigid zones grows slowly over time as the flow develops. However, at some point, the area of rigid zones starts to rise until it reaches a maximum amount rapidly. After that, the measure of the rigid zones stabilizes and remains constant. Otherwise, as shown in Fig. 4, in the case of lesser yield stress, the measure of the rigid zones takes small values compared to the other cases wherein the yield stress is more significant. For example, for a yield stress $\tau_y = 10$ Pa, the maximal value of the rigid zones area is $A = 1.24 \times 10^{-5}$ m$^2$ while it reaches $A = 9.99 \times 10^{-5}$ m$^2$ for the yield stress of $\tau_y = 5$ Pa.
The blocking property describes what happens to the flow domain when the yield stress is increased; specifically, the area of the stiff zones grows until it reaches a maximum value corresponding to the complete solidification of the flow domain. The results can be summarized in a three-dimensional curve, which shows the evolution of the rigid zone area according to the time and the yield stress. Based on Fig. 4, a correlation is proposed to identify the rigid zone area at any given moment and yield stress value. If we consider, A the rigid zones area, the correlation can be given as follows:

$$A = Z_0 + at + b\tau_y$$  \hspace{1cm} (11)

According to the findings mentioned earlier, as the yield stress value increases in Herschel-Bulkley fluids, it causes the particles or components within the fluid aggregate or clump together, resulting in coagulation. Conversely, the components become more dispersed when the yield stress value decreases, leading to a diluted fluid. Therefore, yield stress can be regarded as a parameter to measure the fluid's liquidity degree. In other words, the higher the yields stress, the less liquid the fluid becomes, and the lower the yield stress, the more liquid the fluid becomes.

Figure 5 presents the contours explaining the scenario and distribution of rigid zones according to flow time for different yield stress values. As discussed previously, the rigid zone area increases over time until they reach its final shape, and then it stabilizes.
Figure 5. Scenario of rigid zone formation with time for various yield stress values

<table>
<thead>
<tr>
<th>a. (\tau_y = 10) Pa</th>
<th>b. (\tau_y = 20) Pa</th>
<th>c. (\tau_y = 50) Pa</th>
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<tbody>
<tr>
<td>(t = 0) s</td>
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<td>(t = 0.005) s</td>
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Figure 6 demonstrates the relationship between the stagnation time and the size of rigid zones for different yield stress values. The figure reveals a nonlinear, inverse relationship between the yield stress and the stagnation time. In other words, as the value of yield stress increases, the stagnation time decreases. Moreover, as the yield stress increases, the area of the rigid zones also increases. This may be attributed to increased particle concentration and interaction forces between them, forming larger rigid zones. Since stagnation time is required for forming solid regions, it is reasonable to expect solidification time to be reduced with increased yield stress. This is due to the larger and faster formation of rigid zones, as observed in Fig. 6. Therefore, the yield stress is crucial in determining the stagnation time. The correlation between the area of rigid zones and stagnation time can be expressed as follows:

\[ t_{\infty} = c(1 + A)^q \]  

(12)
5.2 EFFECT OF PRESSURE ON THE RIGID ZONES

The study examines the effect of pressure on the measure of rigid zones by imposing different pressure values on the flow domain. The results are presented in Fig. 7, which shows the evolution of the rigid zone area with respect to time for different pressure values at fixed yield stress. It is observed that, as expected, the area of the rigid zones decreases with increasing pressure. However, for low values of yield stress and each value of pressure, as depicted in Fig. 7. (a) and Fig. 7. (b), the area of the rigid zones initially increases slowly over time as the flow develops. Then it grows pseudo-linearly until it reaches a maximum value, beyond which it remains constant. On the other hand, for high-yield stress values, as shown in Fig. 7. (c), the measure of the rigid zones is constant for low-pressure values, and the decrease in this area starts after reaching a high-pressure value, unlike the two other cases.
By analyzing the behaviour of the Herschel-Bulkley fluid under different pressure values, it was observed that when the applied pressure exceeds the yield stress, the rigid zones in the fluid will start to completely break down, causing the fluid to move freely with a uniform velocity. It was noted that at this limit, the Herschel-Bulkley fluid behaves like a power law fluid. The extent of the rigid zones' breakdown depends on the pressure magnitude. Therefore, the higher the pressure, the greater the deformation and breakdown of the rigid zones. Moreover, it was found that an increase in the yield stress value necessitates a corresponding increase in the pressure value to ensure its effect on the flow. This implies that higher yield stress values require higher pressure values to cause a breakdown of the rigid zones and initiate the flow movement.

The rigid zones area, with respect to time and pressure at yield stress, values $\tau_y = 10 \text{ Pa}$, $\tau_y = 50 \text{ Pa}$, and $\tau_y = 100 \text{ Pa}$, can be estimated using the correlation shown in Fig.7. It is written in the following order:

$$A = N + B \times \exp\left(- \exp\left(\frac{S-t}{D}\right)\right) + E \times \exp\left(- \exp\left(\frac{F-p}{G}\right)\right) + J \times \exp\left(- \exp\left(\frac{S-t}{D}\right) - \exp\left(\frac{F-p}{G}\right)\right)$$

$$A + Z + \frac{g}{\left(1 + \left(\frac{t}{R}\right)^{-i}\right)\left(1 + \left(\frac{P}{F}\right)^{-y}\right)}$$

$$A = W + Lt + hp$$
6 CONCLUSION

In the present study, 2D simulation is performed using COMSOL Multiphysics 6.0 in a non-stationary condition where the concrete fluid flows in a laminar condition. It was discussed how the rigid zones develop over time, with a change in the yield stress value each time. It was found that the rigid zone area increases with time and with the increase in the yield stress value until it reaches the upper limit. Mathematically, a correlation was extracted from a three-dimensional curve to calculate the rigid zone area at any moment and under any yield stress value. To reach the right level of liquidity in the fluid, the value of the yield stress should be taken into consideration, as the increase in the value of the yield stress leads to coagulation, and the decrease of it leads to the dilution of the fluid. The results show that the larger the area of the rigid zones is at its final form, and the greater the value of the yield stress, the shorter the stagnation time. A correlation has been extracted to calculate the stagnation time as a function of the area of the rigid zones. The results also show that the increase in pressure affects the rigid zones clearly, especially when the value of the yield stress is small; additionally, the effect of the pressure on the rigid zones only occurs at high values of pressure, given that the value of the yield stress is high. It is found that the particle bonds of the rigid zones of the Herschel-Bulkley fluid are broken at its pressure yield limit, diminishing the rigid zones within it, and the Herschel-Bulkey fluids behave like power-law fluids. Yield stress, pressure, and time all heavily affect the rigid zones.
REFERENCES


NOMENCLATURE

A \hspace{5mm} \text{area of the rigid zones} [m^2]

f \hspace{5mm} \text{external body forces}

f^* \hspace{5mm} \text{non-dimensional gradient force}

H, L \hspace{5mm} \text{dimensions of domain}

I \hspace{5mm} \text{unit tensor}

k \hspace{5mm} \text{consistency [Pa]}

M, y_0 \hspace{5mm} \text{constants of theoretical velocity}

n \hspace{5mm} \text{the power law index}

p \hspace{5mm} \text{pressure [Pa]}

p_{in} \hspace{5mm} \text{Inlet pressure}

\tau_{\infty} \hspace{5mm} \text{stagnation time [s]}

t \hspace{5mm} \text{time of flow [s]}

\text{u^*} \hspace{5mm} \text{non-dimensional velocity}

U \hspace{5mm} \text{velocity field [m/s]; } u \text{ in the x-direction and } v \text{ in the y-direction}

\text{u_{in}} \hspace{5mm} \text{Inlet velocity}

V \hspace{5mm} \text{reference velocity}

(x, y) \hspace{5mm} \text{point coordinates}

GREEK SYMBOL

\mu \hspace{5mm} \text{viscosity [Pa.s^n]}

\rho \hspace{5mm} \text{density [kg/m^3]}

\tau \hspace{5mm} \text{deviator shear stress [Pa]}

\tau_y \hspace{5mm} \text{yield stress [Pa]}

(\nabla U)^T \hspace{5mm} \text{transpose}

\dot{\gamma}_c \hspace{5mm} \text{critical shear rate [s^{-1}]}\n
\nabla U \hspace{5mm} \text{velocity gradient}

\Omega \hspace{5mm} \text{flow domain}

\Omega_r \hspace{5mm} \text{rigid zones}

\dot{\gamma} \hspace{5mm} \text{shear rate tensor}