

Comparison between a stabilized mixed finite element formulation for Herschel-Bulkley fluid and regularized models

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Abstract. In this work, a mixed stabilized finite element formulation with continuous velocity and discontinuous pressure interpolations is used to approach pseudoplastic materials with yield stress, that is, nonlinear viscoplastics. Here, Herschel-Bulkley model and regularized ones for the apparent viscosity are considered. This formulation is based on two well succeeded stabilized methods, separately, one for pseudoplastic problems (nonlinear) without yield stress, and the other for linear problems with yield stress (ideal plastic) which are modeled by linear constitutive equations with inequality restriction. Regularized generalized alternatives (based on simple, Papanastasiou and Bercovier-Engelman schemes) are presented to deal with the discontinuity of the constitutive relations and results are presented showing their limitations. They are compared with the proposed stabilized formulation which allows obtaining stable results even with same interpolations, without the necessity of regularizations, applied directly to the Herschel-Bulkley constitutive relation.

Keywords: Fluid mechanics, Pseudoplasticity, Computation methods, Transport phenomena.

1 Introduction

Pseudoplasticity is one of the most encountered effect in non-Newtonian fluids and is characterized by a non linearity between shear stress and shear rate tensors and the most commonly used constitutive relation for this is a power-law equation, by its relative simplicity. Defining an apparent viscosity, it is possible to introduce it in the context of the generalized fluid theory and generate, for non convective case, a kind of generalized Stokes model, Bortoloti and Karam [1]. Due to the nonlinear character of this models, analytical solutions are very limited and the alternative is to use numerical methods. An additional difficulty, also present in the linear case, is the incompressibility constraint that can generate instabilities when using classical methods. To overcome these difficulties, Karam and Loula [2] proposed a stable mixed finite element method for the linear problem, accommodating equal order interpolations for the velocity and the pressure and Bortoloti and Karam [1] generalized it for pseudoplastic fluids, obtaining mathematically the range of stability by a discrete version of the Scheurer theorem Scheurer [3], which is a generalization of the Brezzi [4] one. Fluids that start to move when a critical value is reached are called fluids with yield stress, to which two regions can be possible: a flowing one (Newtonian or non-Newtonian) and a rigid one (moving or not) Skelland [5]. The oldest constitutive model to viscoplastics is the one by Bingham [6], having a discontinuity when the shear rate is zero. A common approach is to use a modified regularized function for the viscosity. However, several practical problems have properties that fit more to the Herschel-Bulkley model Skelland [5] which, differently from the Bingham one, takes into account pseudoplastic behaviour (nonlinear) after the yield limit. Herschel-Bulkley fluids present all the difficulties presented by pure pseudoplastics. In this work, based on the method of Bortoloti and Karam [1] for pseudoplastics, it is presented a stabilized formulation for the Herschel-Bulkley model, with the introduction of some regularizations into the apparent viscosity function. Numerical results are presented to show that this formulation accommodate equal order interpolations for velocity and pressure, comparing four regularization functions considered.

2 Model Problem

Let Ω be a domain in \mathbb{R}^n with smooth boundary. We consider the incompressible and stationary creeping flow problem governed by: $-\text{div } \boldsymbol{\sigma} = \mathbf{f}$ in Ω , where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, \mathbf{f} is the body force vector. The

governing equation is subjected to the incompressibility constraint: $\text{div } \mathbf{u} = 0$ in Ω , where \mathbf{u} is the velocity field. Here, we are interested in pseudoplastic materials, with the constitutive equation given by the Herschel-Bulkley model [7].

2.1 Herschel-Bulkley model

The Herschel-Bulkley model describes certain non-Newtonian fluids and has a nonlinear stress-rate dependence in the flow region. This constitutive model predicts that a minimum level of shear stress is required to start flowing. This is a generalization of the Bingham model taking into account the changes in apparent viscosity with the rate of deformation by means of a Power-law behavior. It can be thought of as a hybrid between Bingham and Power-law models. Thus, we have the following Herschel and Bulkley model

$$\boldsymbol{\tau}(\mathbf{u}) = \tau_y + K_H \dot{\gamma}(\mathbf{u})^{\alpha-1}, \quad \text{if } |\boldsymbol{\tau}(\mathbf{u})| > \tau_y, \quad (1)$$

$$\dot{\gamma}(\mathbf{u}) = 0, \quad \text{if } |\boldsymbol{\tau}(\mathbf{u})| \leq \tau_y. \quad (2)$$

Thus, there is a nonlinear relation between shear stress and shear rate, and apparent viscosity, $\mu_a(\dot{\gamma}(\mathbf{u}))$, given by

$$\mu_a(\dot{\gamma}(\mathbf{u})) = \frac{\tau_y}{\dot{\gamma}(\mathbf{u})} + K_H \dot{\gamma}(\mathbf{u})^{\alpha-2}, \quad \text{if } |\boldsymbol{\tau}(\mathbf{u})| > \tau_y, \quad (3)$$

where τ_y is the yield stress, K_H is the consistency parameter and α is the power-law index. It is worth mentioning that $|\boldsymbol{\tau}(\mathbf{u})| \leq \tau_y$ the viscosity $\mu_a(\dot{\gamma}(\mathbf{u})) \rightarrow \infty$ and direct calculations are not possible. Therefore, the reduced stress tensor can be rewritten as: $\boldsymbol{\tau}(\mathbf{u}) = \tau_y \mathbf{I} + \mu_a(\mathbf{u}) \boldsymbol{\epsilon}(\mathbf{u})$, with $\mu_a(\mathbf{u})$ obtained from:

$$\boldsymbol{\tau}(\mathbf{u}) = \left(\frac{\tau_y}{|\boldsymbol{\epsilon}(\mathbf{u})|} + K_H |\boldsymbol{\epsilon}(\mathbf{u})|^{\alpha-2} \right) \boldsymbol{\epsilon}(\mathbf{u}) = \mu_a(\mathbf{u}) \boldsymbol{\epsilon}(\mathbf{u}), \quad (4)$$

where $\mathbf{I} \in \mathbb{R}^n \times \mathbb{R}^n$ is the identity tensor, $\boldsymbol{\epsilon}(\mathbf{u}) = (\nabla \mathbf{u} + \nabla^T \mathbf{u})/2$ the symmetric part of $\nabla \mathbf{u}$. We recall that for $\alpha = 2$ the fluid is newtonian and when $1 < \alpha < 2$, power-law it is *Pseudoplastic*.

2.2 Generalized Stokes Problem for Herschel-Bulkley

From the above consideration, the Generalized Stokes problem in the context of pseudoplastic flows using the Herschel-Bulkley model is obtained as:

Problem PG. Let \mathbf{f} and $\bar{\mathbf{u}}$ given, find $\{\mathbf{u}, p\}$ such that

$$-\text{div}(\mu(\mathbf{u}) \boldsymbol{\epsilon}(\mathbf{u})) + \nabla p = \mathbf{f} \quad \text{in } \Omega, \quad (5)$$

$$\text{div } \mathbf{u} = 0 \quad \text{in } \Omega, \quad (6)$$

$$\mathbf{u} = \bar{\mathbf{u}} \quad \text{on } \Gamma. \quad (7)$$

where $\bar{\mathbf{u}}$ is the value of \mathbf{u} on the boundary; p is the hydrostatic pressure; $\boldsymbol{\epsilon}(\mathbf{u})$ is the strain rate tensor; $\mu_a(\mathbf{u}) = \mu(\mathbf{u})$ is the apparent viscosity. For this fluids when $|\boldsymbol{\tau}(\mathbf{u})| < \tau_y$ there is no flow, meaning that the system has infinite viscosity. The behavior of Bingham or Herschel-Bulkley materials near the yield stress is not at all smooth and differential in a mathematical sense, with a singularity that is also a difficult to be solved. These problems can lead to inconsistencies in the numerical modeling in complex geometries, and difficulties in defining the boundaries between the non-deformable ‘‘solid’’ zone and the flowing ‘‘liquid’’ zone. Alternatives to avoid the singularity are the methods of viscosity regularization, although they do not solve alone in case of classical numerical methods.

3 Regularized Models

Currently, viscosity regularization methods are probably the most popular for linear and nonlinear viscoplastic fluid flows. These methods replace eq. (4) by an approximation of the following form: $\boldsymbol{\tau}(\mathbf{u}) =$

$\mu_\eta(\dot{\gamma}(\mathbf{u}))\dot{\gamma}(\mathbf{u})$ with $\eta < 1$, where η is the regularization parameter, such that $\mu_\eta(\dot{\gamma}(\mathbf{u})) \rightarrow \mu_a(\dot{\gamma}(\mathbf{u}))$ when $\eta \rightarrow 0$ and $\mu_\eta(\dot{\gamma}(\mathbf{u}))$ is well defined when $(\dot{\gamma}(\mathbf{u})) \rightarrow 0$ for all $\eta > 0$ fixed, approximating the viscosity to a finite value even when the strain rate tends to zero. There is a multitude of adaptable functions for regularizing the viscosity. Probably the simplest one is the following, called *Simple Model*,

$$\mu_\eta(\mathbf{u}) = K_H(\dot{\gamma}(\mathbf{u}))^{n-2} + \frac{\tau_y}{\eta + \dot{\gamma}(\mathbf{u})}. \quad (8)$$

Another two of the most popular have been the *Bercovier-Engleman Model*, [8],

$$\mu_\eta(\mathbf{u}) = K_H(\dot{\gamma}(\mathbf{u}))^{n-2} + \frac{\tau_y}{\sqrt{\eta^2 + \dot{\gamma}(\mathbf{u})^2}}, \quad (9)$$

and the *Papanastasiou Model*, [9],

$$\mu_\eta(\mathbf{u}) = K_H(\dot{\gamma}(\mathbf{u}))^{n-2} + \frac{\tau_y}{\dot{\gamma}(\mathbf{u})}(1 - e^{-\dot{\gamma}(\mathbf{u})/\eta}). \quad (10)$$

Bercovier and Engleman [8] proposed this model based on the mathematical studies of Glowinski et al. [10], and Papanastasiou [9] approximated the experimental results observed in simple experiments with rheological fluids.

Figure 1 below shows the graphs of shear stress and apparent viscosity by shear rate for eqs. (8), (9), (10).

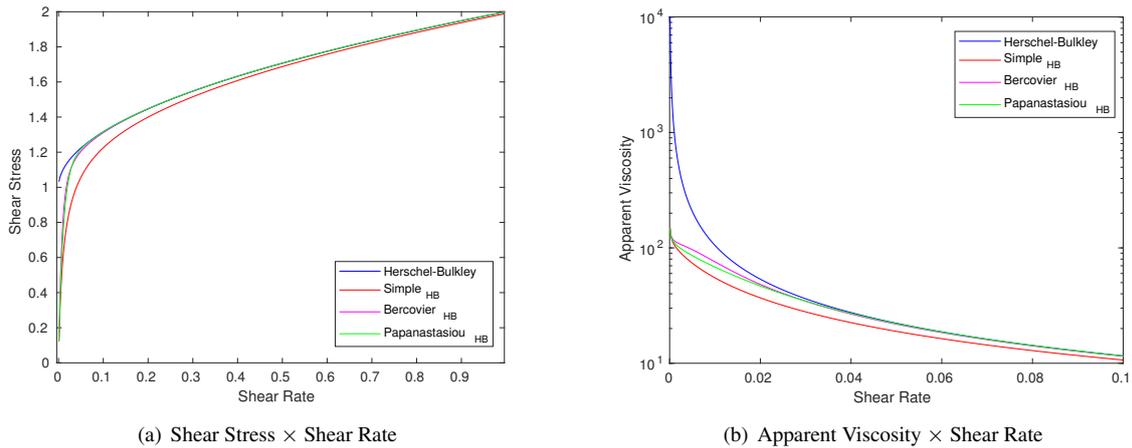


Figure 1. Regularized models compared with the Herschel-Bulkley model for $\tau_y = 1.0$ and $\eta = 0.01$

It can be seen that when $\dot{\gamma} \rightarrow 0$, the regularized models tend towards the Herschel-Bulkley model, Fig.(a), and the viscosity takes on finite values, Fig.(b). In all cases, our simulations considered $\eta < 1$, since the aim is to approximate the Herschel-Bulkley model. It is worthy to mention that non of these regularization work with classical method for equal order interpolation for \mathbf{u} and p .

4 Variational Formulation

To generate the proposed finite element method, the following definitions will be used. Let the space $L^2(\Omega) = \left\{ u \mid u \text{ measurable and } \int_{\Omega} |u|^2 d\Omega < \infty \right\}$, with the usual inner product $(u, v) = \int_{\Omega} uv d\Omega$, $\forall u, v \in L^2(\Omega)$. Let the space $H_0^1(\Omega) = \{u \in H^1(\Omega); u = 0 \text{ on } \Gamma\}$, with $H^1(\Omega) = \{u \in L^2(\Omega) \mid \nabla u \in L^2(\Omega)\}$ and usual norms. Let V and W be the spaces for velocity and pressure defined by: $V = \{v \in H_0^1(\Omega) \times H_0^1(\Omega)\}$ and $W = \{p \in L^2(\Omega), (p, 1) = 0\}$, with their respective norms, $\|v\|_V = \|v\|_1$ and $\|p\|_W = \|p\|_0$. Let Ω be a polygonal domain discretized by a classical uniform finite element mesh with N_e elements. Let $S_h^k(\Omega)$ be the finite element space of continuous polynomials in Ω of degree k , class C^0 , and $Q_h^l(\Omega)$ is the finite element space of discontinuous polynomials in Ω of degree l , class C^{-1} , we define the approximation spaces, $\mathbf{V}_h^k = (S_h^k(\Omega) \cap H_0^1(\Omega))^n$ and $\mathbf{W}_h^l =$

$Q_h^l(\Omega) \cap L^2(\Omega)$, for the velocity \mathbf{u}_h with continuous interpolations and for the pressure p_h with discontinuous interpolations, respectively.

Thus, based on the stabilized formulation of Bortoloti and Karam [1] for the nonlinear Stokes problem without yield stress and the regularization models, we have constructed the following consistent regularized stabilized discontinuous variational formulation for the nonlinear model problem with yield stress:

Problem PG_{hb}: Given \mathbf{f} in the dual space of $H^1(\Omega)$, find $\{\mathbf{u}_h, p_h\} \in \mathbf{V}_h^k \times \mathbf{W}_h^l$ such that

$$(A_h(U_h), V_h) + B_h(p_h, \mathbf{v}_h) = F_h(V_h) \quad \forall \{\mathbf{v}_h, q_h\} \in \mathbf{V}_h^k \times \mathbf{W}_h^l, \quad (11)$$

$$B_h(q_h, \mathbf{u}_h) = 0 \quad \forall q_h \in \mathbf{W}_h^l, \quad (12)$$

where

$$(A_h(U_h), V_h) = (\mu(\mathbf{u}_h)\epsilon(\mathbf{u}_h), \epsilon(\mathbf{v}_h)) + \delta_2 \vartheta (\operatorname{div} \mathbf{u}_h, \operatorname{div} \mathbf{v}_h) + \frac{\delta_1 h^2}{\vartheta} (-\Delta_\mu \mathbf{u}_h + \nabla p_h, -\Delta_\mu \mathbf{v}_h + \nabla q_h)_h, \quad (13)$$

$$B_h(q_h, \mathbf{u}_h) = -(q_h, \operatorname{div} \mathbf{u}_h)_h, \quad F_h(V_h) = \mathbf{f}(\mathbf{v}_h) + \frac{\delta_1 h^2}{\vartheta} (\mathbf{f}, -\Delta_\mu \mathbf{v}_h + \nabla q_h)_h, \quad (14)$$

with $(\psi, \phi)_h = \sum_{i=1}^{N_e} \int_{\Omega^e} \psi \cdot \phi \, dx$, where N_e is the number of mesh elements, h the mesh parameter, δ_1 and δ_2 positive constants as stability parameters and ϑ a dimensional parameter. The norm induced by the inner product $(\cdot, \cdot)_h$ will be defined as $\|\cdot\|_h$. Note that when $\delta_1 = \delta_2 = 0$ the Problem PG_{hb} is reduced to the Galerkin formulation which can exhibit velocity locking and spurious pressure oscillations. For Galerkin's method, k and l must have different orders, Fortin [11], Hughes [12]. To easily fulfil the LBB condition, Brezzi [4], the discontinuous pressure can be rewritten as: $p_h = p_h^* + \bar{p}_h$, with $p_h^* \in \mathbf{W}_h^{*l} = \left\{ p_h^* \in L^2(\Omega) : \int_{\Omega^e} p_h^* \, d\Omega^e = 0; \nabla p_h^e = \nabla p_h^{e*} \right\}$, where

\mathbf{W}_h^{*l} is the pressure subspace with null mean in each element and $\bar{p}_h \in \bar{\mathbf{W}}_h^l = \left\{ \bar{p}_h \in L^2(\Omega) : \nabla \bar{p}_h^e = 0, \bar{p}_h^e = \int_{\Omega^e} p_h^e \, d\Omega^e / \int_{\Omega^e} d\Omega^e \right\}$, where $\bar{\mathbf{W}}_h^l$ is the subspace of the piecewise constant function, where p_h^e is the restriction of p_h on the element Ω^e . Thus, we can write the Problem PG_{hb}*:

Problem PG_{hb}*: Given $\mathbf{f} \in \mathbf{V}'$, find $\{\mathbf{u}_h, p_h^*, \bar{p}_h\} \in \mathbf{V}_h^k \times \mathbf{W}_h^{*l} \times \bar{\mathbf{W}}_h^l$, such that

$$(A_h^*(U_h^*), V_h^*) + B_h(\bar{p}_h, \mathbf{v}_h) = F_h^*(V_h^*) \quad \forall \{\mathbf{v}_h, q_h^*\} \in \mathbf{V}_h^k \times \mathbf{W}_h^{*l}, \quad (15)$$

$$B_h(\bar{q}_h, \mathbf{u}_h) = 0 \quad \forall \bar{q}_h \in \bar{\mathbf{W}}_h^l, \quad (16)$$

$$\text{where} \quad (A_h^*(U_h^*), V_h^*) = (\mu(\mathbf{u}_h)\epsilon(\mathbf{u}_h), \epsilon(\mathbf{v}_h)) + B_h(p_h^*, \mathbf{v}_h) + \delta_2 \vartheta (\operatorname{div} \mathbf{u}_h, \operatorname{div} \mathbf{v}_h) + B_h(q_h^*, \mathbf{u}_h) + \frac{\delta_1 h^2}{\vartheta} (-\Delta_\mu \mathbf{u}_h + \nabla p_h^*, -\Delta_\mu \mathbf{v}_h + \nabla q_h^*)_h, \quad (17)$$

$$B_h(p_h^*, \mathbf{v}_h) = -(p_h^*, \operatorname{div} \mathbf{v}_h)_h, \quad B_h(\bar{p}_h, \mathbf{v}_h) = -(\bar{p}_h, \operatorname{div} \mathbf{v}_h)_h, \quad (18)$$

$$F_h^*(V_h^*) = \mathbf{f}(\mathbf{v}_h) + \frac{\delta_1 h^2}{\vartheta} (\mathbf{f}, -\Delta_\mu \mathbf{v}_h + \nabla q_h^*)_h, \quad (19)$$

with $(\psi, \phi)_h = \sum_{i=1}^{N_e} \int_{\Omega^e} \psi \cdot \phi \, dx$, h the mesh parameter, $\delta_1, \delta_2 > 0$ as stability parameters and ϑ a dimensional parameter. To simplify the notation, the following definition was used: $\Delta_\mu \mathbf{u} = \operatorname{div}(\mu(\mathbf{u})\epsilon(\mathbf{u}))$, where $\mu(\mathbf{u})$ is not constant. Note that, again, when $\delta_1 = \delta_2 = 0$ the Problem PG_{hb} is reduced to the Galerkin formulation which can exhibit velocity locking and spurious oscillations of the pressure. For Galerkin's method, k and l must have different orders, Fortin [11]. The non-linearity of this problem is introduced by the viscosity law given by a continuous and limited function, $\mu: \mathbb{R}^+ \rightarrow \mathbb{R}^+$, com $\mu_\infty \leq \mu(s) \leq \mu_0$, where μ_0 and μ_∞ are positive reals that limit the apparent viscosity at low and high shear rates, respectively.

5 Numerical Results

The numerical results below show the behaviour of the formulation for a Herschel-Bulkley fluid with the regularizations. The example used was the cavity problem in a unit square domain with $\mathbf{u}(x, 1) = (1, 0)$ for

$x \in [0, 1]$ and $\mathbf{u} = 0$ on the other boundaries. We adopted a uniform mesh with 17×17 nodes and continuous biquadratic interpolation functions for velocity and discontinuous biquadratic interpolation functions for pressure. For the regularized models, the parameter was $\eta = 0.1$, the values used were $\tau_y = 1.0$ Pa and $\tau_y = 5.0$ Pa as shown in the figures. The following graphs show the velocity field and pressure rises obtained with the stabilization parameters set as $\delta_1 = 1.0$ and $\delta_2 = 10.0$ for the Herschel-Bulkley models with regularizations in the viscosity term of the following types: Simple, Bercovier-Engleman and Papanastasiou.

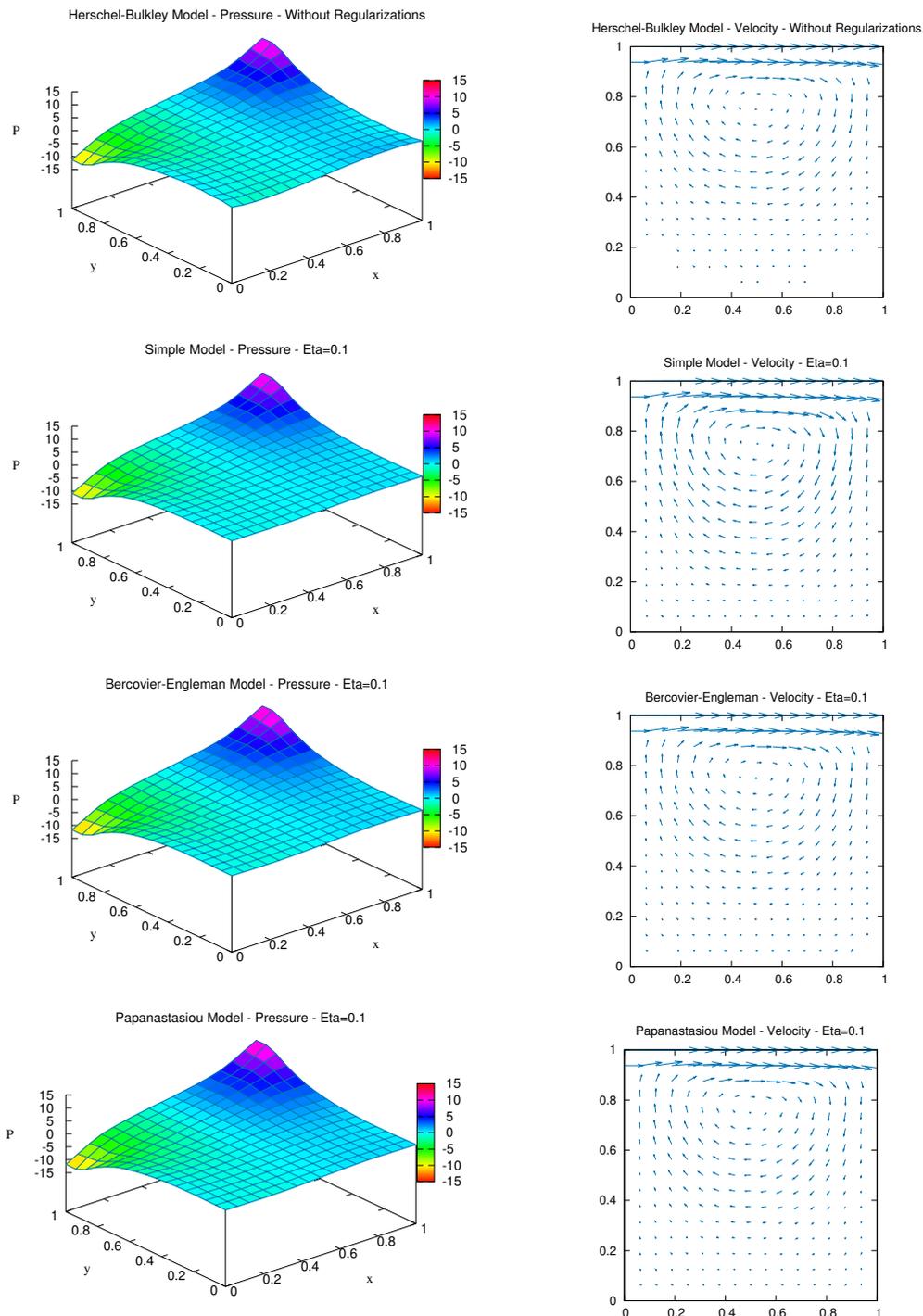


Figure 2. Velocity and pressure fields for the cavity problem using discontinuous pressure for $\tau_y = 1.0$

The graphs in Fig. 2 and Fig.3 show results for a stabilized mixed finite element formulation for solving pseudoplastic fluid flow problems with yield stress, where regularization was considered in the apparent viscosity term. Although the discontinuous interpolations resulted in greater accuracy of the results, even in regions of

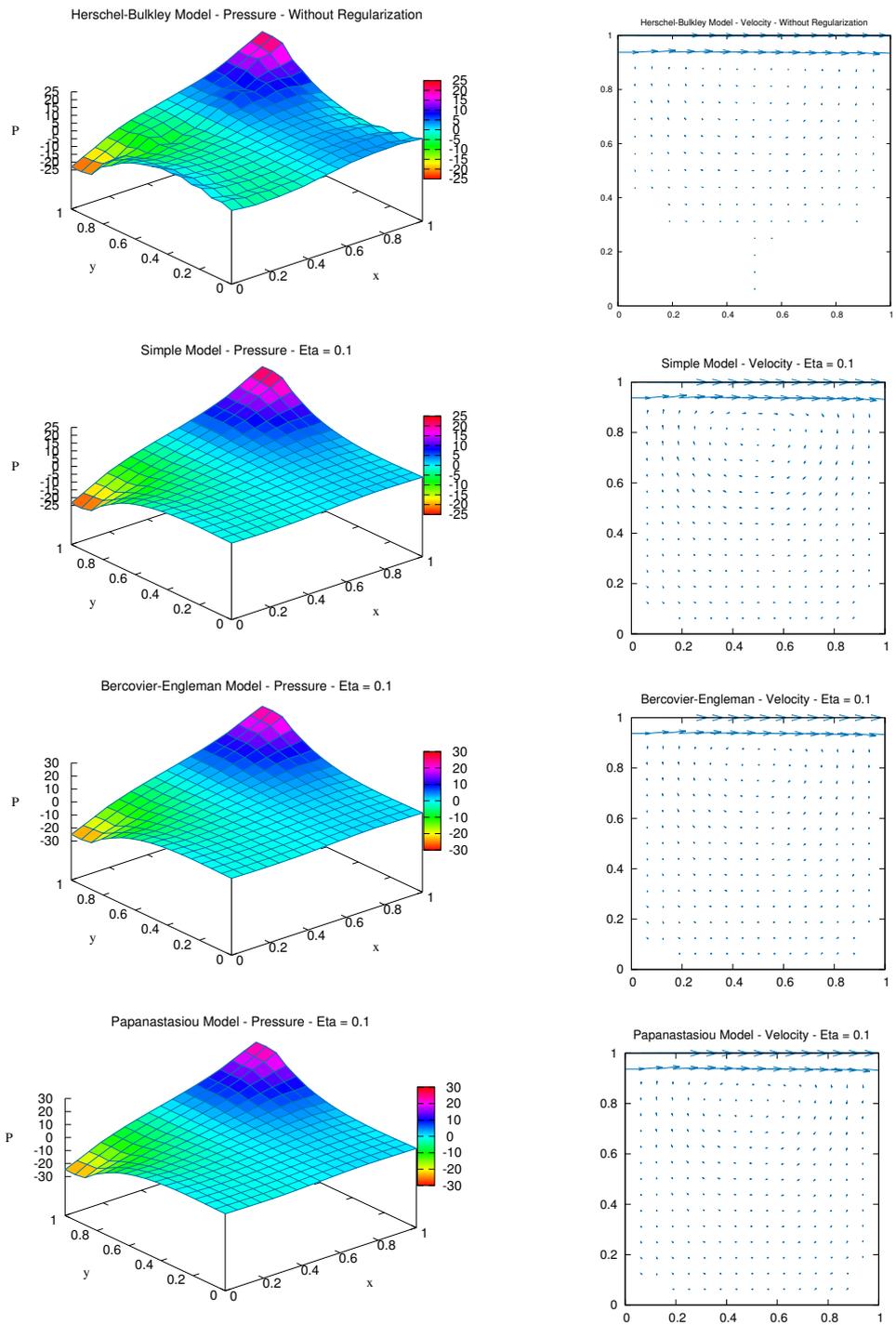


Figure 3. Velocity and pressure fields for the cavity problem using discontinuous pressure for $\tau_y = 5.0$

higher pressure gradients, we found that as the value of the yield stress increases, the solutions lose stability. Three regularized constitutive models were compared: the Simple, the Bercovier and the Papanastasiou models. When $\eta \rightarrow 0$, regularization methods invariably have the same computational problems as pure the Herschel-Bulkley model. It is necessary to associate a small finite value of η for the computational calculations and, in order to select it in a consistent way, one must understand whether and how the solution of the regularized problem converges to the exact problem.

Remark 1. As expected, as τ_y increases the velocities at the core are smaller (greater velocity gradients relative to the upper boundary), since the resistance to flow is bigger for the same kinetic energy applied on the boundary.

Remark 2. Above the 17×17 mesh presented, no variations have been obtained in the results, in all the cases.

Remark 3. $\tau_y = 1.0$ and 5.0 (Pa) correspond to dilute and more concentrated carbopol in water solution, respectively.

Remark 4. Since only the velocity is prescribed on the boundaries, of course the pressures on the boundaries vary as a function of the yield stress and other data.

6 Conclusions

This paper presents a stabilized and regularized mixed finite element formulation, with continuous interpolation for velocity and discontinuous interpolation for pressure, for a stationary incompressible nonlinear flow problem that models pseudoplastic fluids with yield stress governed by the constitutive relations of the Herschel-Bulkley model (nonlinear viscoplastic). The main mathematical difficulties, apart from the complexity of non-linearity, that are present in such flows are: the inequality constraint of the Herschel-Bulkley constitutive model, which makes it challenging to obtain stable solutions; and the internal incompressibility constraint, which makes it impossible to use some interpolations when classical methods are applied. To avoid these difficulties, the formulations were built based on the method used in [1], where a stabilized mixed formulation for nonlinear problems without boundary stress with discontinuous interpolation for pressure was able to deal with incompressibility and allowed interpolations of the same order for velocity and pressure. Numerical results are presented comparing four regularization functions considered and even the cases where this stabilized formulation is stable when applied directly to the Herschel-Bulkley constitutive relation without the need of regularizations.

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