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On a new constitutive equation for elastoviscoplastic fluid flows

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Abstract

From a thermodynamic theory, a new model for elastoviscoplastic fluid flow is presented. It extends the Bingham viscoplastic model and the Oldroyd viscoelastic model. Two fundamental flows are studied: the simple shear flow and the uniaxial elongation.

Sur une nouvelle équation constitutive pour les écoulements de fluides élastoviscoplastiques

Résumé – Nous présentons dans cette note un nouveau modèle de fluide élastoviscoplastique à partir d’une théorie thermodynamique. Il permet de retrouver le modèle viscoplastique de Bingham ainsi que le modèle viscoélastique d’Oldroyd. Nous étudions deux écoulements élémentaires : le cisaillement simple et l’élongation uniaxiale.

Key words: non-Newtonian fluid ; viscoelasticity ; viscoplasticity ; constitutive equation.

Mots-clés : fluide non newtonien ; viscoélasticité ; viscoplasticité ; loi de comportement.

Version française abrégée – De nombreux fluides d’intérêt pratique, tels les mousses, les émulsions, les suspensions de vésicules ou les écoulements du sang dans les artères, développent un comportement élastoviscoplastique : pour les faibles contraintes, les déformations sont élastiques, réversibles, tandis que pour des contraintes plus importantes, et passé un seuil, les déformations sont plastiques, irréversibles. Malgré une littérature très abondante concernant les expérimentations et les simulations, force est de constater qu’il n’existe pas de description théorique permettant de proposer un modèle (i) *objectif*, c’est-à-dire indépendant de l’observateur qui mesure les quantités physiques, et qui satisfasse (ii) *le second principe de la thermodynamique*.

Le but de cet article est de proposer un tel modèle, ainsi que de l’étudier pour les écoulements simples de cisaillement et d’élongation. Trois nombres sans dimensions apparaissent : We , le nombre de Weissenberg, exprimant l’effet de mémoire des contraintes au sein du matériau, Bi , le nombre de Bingham, exprimant l’effet de seuil de plasticité, et enfin Re , le nombre de Reynolds. Ce modèle permet de retrouver le modèle viscoplastique de Bingham pour $We = 0$, le modèle viscoélastique d’Oldroyd pour $Bi = 0$, et enfin les équations de Navier-Stokes pour $We = Bi = 0$.

Nous décrivons l’état du système en utilisant deux variables indépendantes : le tenseur des déformations totales ε et une variable interne, le tenseur des déformations élastiques ε_e . Nous avons $\varepsilon = \varepsilon_e + \varepsilon_m$ où ε_m représente les déformation plastiques. Les matériaux standards généralisés [3] sont caractérisés par l’existence d’une énergie libre spécifique \mathbb{E} et un potentiel de dissipation \mathbb{D} , qui sont des fonctions convexes

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de leurs arguments. Le modèle rhéologique représenté sur la Fig. 1, et combinant viscoélasticité et viscoplasticité, correspond à :

$$\begin{aligned}\mathbb{E}(\varepsilon, \varepsilon_e) &= \mu |\varepsilon_e|^2, \\ \mathbb{D}(\dot{\varepsilon}, \dot{\varepsilon}_e) &= \varphi(\dot{\varepsilon}) + \varphi_m(\dot{\varepsilon} - \dot{\varepsilon}_e)\end{aligned}\quad (1)$$

où $\mu > 0$ est le coefficient d'élasticité et où $|\cdot|$ désigne la norme matricielle, définie par la double contraction des indices : $|\varepsilon_e|^2 = \varepsilon_e : \varepsilon_e$. Les potentiels φ et φ_m sont donnés par :

$$\varphi(\dot{\varepsilon}) = \begin{cases} \eta |\dot{\varepsilon}|^2 & \text{si } \text{tr } \dot{\varepsilon} = 0 \\ +\infty & \text{sinon} \end{cases} \quad \varphi_m(\dot{\varepsilon}_m) = \begin{cases} \eta_m |\dot{\varepsilon}_m|^2 + \tau_0 |\dot{\varepsilon}_m| & \text{si } \text{tr } \dot{\varepsilon}_m = 0 \\ +\infty & \text{sinon} \end{cases}\quad (2)$$

Le potentiel φ exprime le comportement visqueux incompressible au niveau macroscopique à l'aide de la viscosité macroscopique $\eta > 0$, tandis que le potentiel φ_m exprime le comportement viscoplastique au niveau microscopique, associé à la viscosité microscopique $\eta_m > 0$, agissant sur la modification continue du réseau des contacts microscopiques, ainsi qu'au seuil de contrainte $\tau_0 \geq 0$ minimum pour que des modifications topologiques du réseau des contacts aient lieu. Le second principe de la thermodynamique est satisfait : dans le cadre des matériaux standards généralisés (cf. [3] et aussi [8,2]), cette propriété découle directement de la convexité de \mathbb{E} et \mathbb{D} .

Le reste de cet article s'organise comme suit : le premier paragraphe développe l'équation constitutive, le second, les équations régissant les mouvements d'un tel fluide, et enfin étudions deux écoulements fondamentaux : le cisaillement simple et l'élongation uniaxiale.

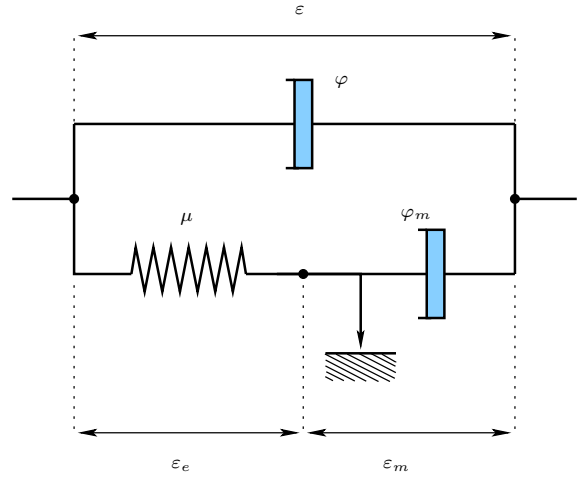


FIG. 1. The rheological model / Le modèle rhéologique.

1. The constitutive law

Let Ω be a bounded domain of \mathbb{R}^N , where $N = 1, 2, 3$. Since both φ and φ_m are non-linear and non-differentiable, the following manipulations involve subdifferential calculus from the convex analysis. The material constitutive laws write:

$$\sigma_{\text{tot}} \in \frac{\partial \mathbb{E}}{\partial \varepsilon} + \frac{\partial \mathbb{D}}{\partial \dot{\varepsilon}} \quad \text{and} \quad 0 \in \frac{\partial \mathbb{E}}{\partial \varepsilon_e} + \frac{\partial \mathbb{D}}{\partial \dot{\varepsilon}_e}$$

where σ_{tot} is the Cauchy's stress tensor. Using the definition (1) of \mathbb{E} and \mathbb{D} , we get:

$$\sigma_{\text{tot}} \in \partial \varphi(\dot{\varepsilon}) + \partial \varphi_m(\dot{\varepsilon} - \dot{\varepsilon}_e) \quad \text{and} \quad 0 \in 2\mu \varepsilon_e - \partial \varphi_m(\dot{\varepsilon} - \dot{\varepsilon}_e)\quad (3)$$

The combination of the two previous relations leads to $\sigma_{\text{tot}} - 2\mu \varepsilon_e \in \partial \varphi(\dot{\varepsilon})$. Then, by using the expression (A.3) of $\partial \varphi$ from the technical annex, and by introducing the pressure field p , we get the following

expression of the total stress tensor: $\sigma_{\text{tot}} = -pI + 2\eta\dot{\varepsilon} + 2\mu\varepsilon_e$ when $\text{tr}(\dot{\varepsilon}) = 0$. Then, the second relation in (3) is equivalent to $\dot{\varepsilon} - \dot{\varepsilon}_e \in \partial\varphi_m^*(2\mu\varepsilon_e)$ where φ_m^* is the dual of φ_m . Let us introduce the elastic stress tensor $\tau = 2\mu\varepsilon_e$. The expression (A.2) of $\partial\varphi_m^*$ in annex yields:

$$\lambda\dot{\tau} + \max\left(0, \frac{|\tau_d| - \tau_0}{|\tau_d|}\right) \tau = 2\eta_m\dot{\varepsilon} \quad (4)$$

where $\lambda = \eta_m/\mu$ is the relaxation time and $\tau_d = \tau - \frac{1}{N}\text{tr}(\tau)I$ denotes the deviatoric part of τ .

2. The system of equations

Since the material is considered in large deformations, we choose to use the Eulerian mathematical framework, more suitable for fluids flows computations. We assume that $\dot{\varepsilon} = D(\mathbf{v}) = (\nabla\mathbf{v} + \nabla\mathbf{v}^T)/2$ is the rate of deformation, while the material derivative $\dot{\tau}$ of the tensor τ in the Eulerian framework is expressed by the Gordon-Schowalter's derivative : $\overset{\square}{\tau} = \frac{\partial\tau}{\partial t} + \mathbf{v}\cdot\nabla\tau + \tau W(\mathbf{v}) - W(\mathbf{v})\tau - a(\tau D(\mathbf{v}) + D(\mathbf{v})\tau)$ where $W(\mathbf{v}) = (\nabla\mathbf{v} - \nabla\mathbf{v}^T)/2$ is the vorticity tensor. The material parameter $a \in [-1, 1]$ is associated to the Gordon-Schowalter's derivative. When $a = 0$ we obtain the Jaumann derivative of tensors, while $a = 1$ and $a = -1$ are associated to the upper and the lower convected derivatives, respectively.

The elastoviscoplastic fluid is then described by a set of three equations associated to the three unknowns (τ, \mathbf{v}, p) : the differential equation (4) completed with the conservation of momentum and mass:

$$\begin{cases} \lambda \overset{\square}{\tau} + \max\left(0, \frac{|\tau_d| - \tau_0}{|\tau_d|}\right) \tau - 2\eta_m D(\mathbf{v}) = 0 \\ \rho \left(\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} \right) - \mathbf{div}(-pI + 2\eta D(\mathbf{v}) + \tau) = \mathbf{f} \\ \mathbf{div}\mathbf{v} = 0 \end{cases}$$

where ρ denotes the constant density and \mathbf{f} some known external forces, such as the gravity. These equations are completed by some suitable initial and boundaries conditions in order to close the system. For instance the initial conditions $\tau(t=0) = \tau_0$ and $\mathbf{v}(t=0) = \mathbf{v}_0$ and the boundary condition $\mathbf{v} = \mathbf{v}_\Gamma$ on the boundary $\partial\Omega$ are convenient. The total Cauchy stress tensor writes $\sigma_{\text{tot}} = -pI + 2\eta D(\mathbf{v}) + \tau$. Notice that when $\tau_0 = 0$ the model reduces to the usual viscoelastic Oldroyd model [6] and when $\lambda = 0$ it reduces to the viscoplastic Bingham model [5]. When both $\tau_0 = 0$ and $\lambda = 0$ the fluid is Newtonian and the set of equations reduces to the classical Navier-Stokes equations associated to the total viscosity $\eta_0 = \eta + \eta_m$. Conversely, when both $\tau_0 \neq 0$ and $\lambda \neq 0$ the fluid is elastoviscoplastic.

Dimensionless formulation – Let us introduce some classical dimensionless numbers:

$$We = \frac{\lambda U}{L}, \quad Bi = \frac{\tau_0 L}{\eta_0 U} \quad \text{and} \quad Re = \frac{\rho U L}{\eta_0}$$

where U and L are some characteristic velocity and length of the flow, respectively. We also use the retardation parameter $\alpha = \eta_m/\eta_0$. The problem reduces to find some dimensionless fields, also denoted by (τ, \mathbf{v}, p) such that:

$$\begin{cases} We \frac{\tau}{\tau} + \max\left(0, \frac{|\tau_d| - Bi}{|\tau_d|}\right) \tau - 2\alpha D(\mathbf{v}) = 0 \\ Re \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) - \mathbf{div} (-pI + 2(1 - \alpha)D(\mathbf{v}) + \tau) = \mathbf{f} \\ \mathbf{div} \mathbf{v} = 0 \end{cases} \quad (5)$$

where \mathbf{f} denotes some known dimensionless vector field. These equations are completed by the initial and boundaries conditions.

3. Examples

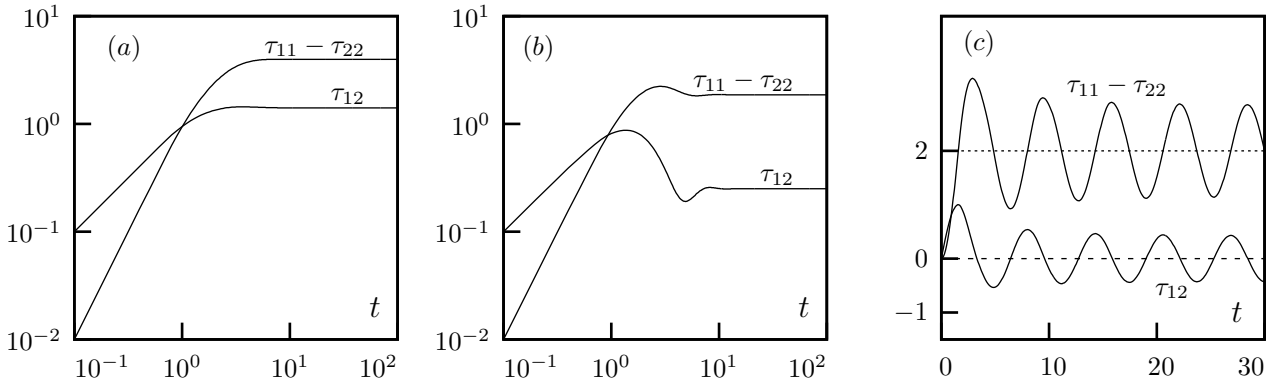


Figure 2. Simple shear flow for $We = 1$ and $\alpha = 1$: (a) $a = 1$ and $Bi = 1$; (b) $a = 0$ and $Bi = 1$; (c) $a = 0$ and $Bi = 2$ / *Écoulement en cisaillement simple pour $We = 1$ et $\alpha = 1$: (a) $a = 1$ et $Bi = 1$; (b) $a = 0$ et $Bi = 1$; (c) $a = 0$ et $Bi = 2$.*

3.1. Simple shear flow – The flow is bidimensional and the velocity gradient is constant: $\nabla \mathbf{v} = ([0, 1]; [0, 0])$. The problem reduces to find τ_{11}, τ_{22} and τ_{12} , from \mathbb{R}^+ to \mathbb{R} , such that

$$We \frac{d}{dt} \begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix} + We \begin{pmatrix} 0 & 0 & -(1+a) \\ 0 & 0 & 1-a \\ \frac{1-a}{2} & -\frac{1+a}{2} & 0 \end{pmatrix} \begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix} + \kappa \begin{pmatrix} \tau_{11} \\ \tau_{22} \\ \tau_{12} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \alpha \end{pmatrix} \quad (6)$$

with the initial condition $\tau(0) = 0$ and where $\kappa = \max(0, 1 - Bi/|\tau_d|)$ and $|\tau_d|^2 = (1/2)(\tau_{11} - \tau_{22})^2 + 2\tau_{12}^2$. The solution is represented in Fig. 2 for $a = 1$ and $a = 0$. Since $\tau(0) = 0$ and $\tau(t)$ is continuous, there exists $t_0 > 0$ such that when $t \in [0, t_0]$ we have $|\tau_d| \leq Bi$ and thus $\kappa = 0$: this is the linear flow regime. The eigenvalues of the system are 0 and $\pm i\sqrt{1-a^2}$. At $t = t_0$, $|\tau_d|$ reaches Bi . Then, for $t > t_0$, the non-linear factor $\kappa > 0$ occurs: the corresponding term amortizes the grown of the solution, that remains bounded. When $a = 1$ (see Fig. 2.a, where $\tau_{22} = 0$) and when $|a| < 1$ and Bi (see Fig. 2.b, where $\tau_{22} = -\tau_{11}$) is small enough, the solution tends to a constant. When $|a| < 1$ and Bi becomes large, instabilities appear, while the solution remains bounded (see Fig. 2.c).

3.2. *Uniaxial elongation* – The flow is tridimensional and $\nabla \mathbf{v} = \text{diag}(1, -1/2, -1/2)$. The problem reduces to find τ_{11}, τ_{22} and τ_{33} such that

$$\begin{cases} We \frac{d\tau_{11}}{dt} + (\kappa - 2aWe)\tau_{11} = 2\alpha \\ We \frac{d\tau_{kk}}{dt} + (\kappa + aWe)\tau_{kk} = -\alpha, \quad k = 2, 3 \end{cases}$$

with the initial condition $\tau(t=0) = 0$ and where $\kappa = \max(0, 1 - Bi/|\tau_d|)$. As above, since $\tau(0) = 0$ and $\tau(t)$ is continuous, there exists $t_0 > 0$ such that when $t \in [0, t_0]$ we have $|\tau_d| \leq Bi$ and thus $\kappa = 0$: this is the linear flow regime. The eigenvalues of the system are $-2aWe$ and aWe . For $t > t_0$, the case $\kappa > 0$ occurs. Since $\kappa \leq 1$, when $aWe > 1/2$ the solution is no more bounded, as shown on Fig. 3.a. This drawback is still true when $Bi = 0$, i.e. for the Oldroyd viscoelastic model. In the context of viscoelastic models, some alternate constitutive equations that extends the Oldroyd model has been proposed. Let us consider the following constitutive equation:

$$We \overset{\square}{\tau} + (1 + \xi \text{tr} \tau) \max\left(0, \frac{|\tau_d| - Bi}{|\tau_d|}\right) \tau - 2\alpha D(\mathbf{v}) = 0 \quad (7)$$

where $\xi \geq 0$ is a new material parameter. For $Bi = 0$ we obtain the viscoelastic Phan-Thien and Tanner model (see e.g. [7]). For $\xi = 0$ we obtain the previous elastoviscoplastic model (5) while for any $\xi > 0$ the solution remains bounded, as shown on Fig. 3.b for $We = 0.75$.

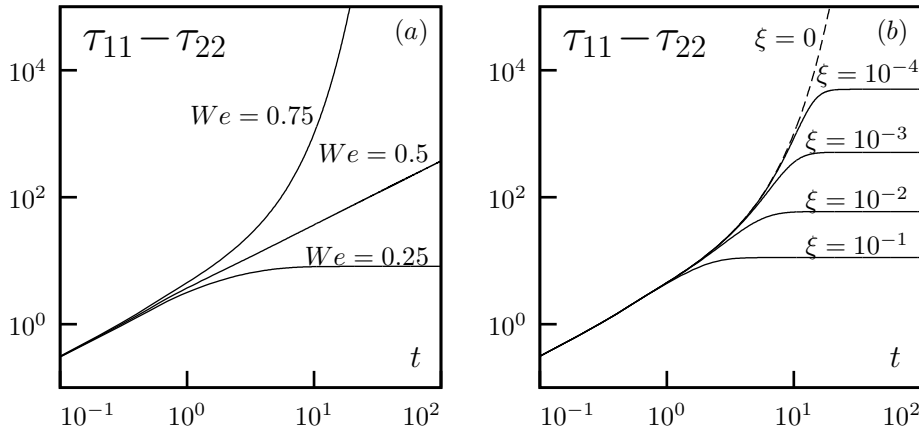


Figure 3. The uniaxial elongation for $Bi=1, a=1$ and $\alpha=1$: (a) influence of We for $\xi=0$; (b) influence of ξ for $We=0.75$ / *Élongation uniaxiale pour $Bi = 1, a = 1$ et $\alpha = 1$: (a) influence de We pour $\xi = 0$; (b) influence de ξ pour $We = 0.75$.*

Conclusion

A new model for elastoviscoplastic fluid flows that is objective and satisfies the second principle of the thermodynamic is presented. A variant of this model is also introduced in equation (7) in order to enforce finite extensional properties of the material. This model and its variant are good candidates for the numerical simulation of elastoviscoplastic in multidimensional geometries. Future works will compare such computations with experiments measurements [4,1] on elastoviscoplastic flows.

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Appendix A. Subdifferential calculus

A.1. *The φ_m function* – The subgradient $\partial\varphi_m$, as introduced in (2), is defined for any tensor D by:

$$\begin{aligned}\partial\varphi_m(D) &= \{\tau, \tau : (H - D) \leq \varphi_m(H) - \varphi_m(D), \forall H\} \\ &= \{\tau, j_m(D) \leq j_m(H), \forall H \text{ with } \text{tr}(H) = 0 \text{ and } \text{tr}(D) = 0\}\end{aligned}$$

with the notation $j_\tau(H) = \eta_m|H|^2 + \tau_0|H| - \tau : H$. When the minimizer D of j_τ over the kernel of the trace operator $\text{Ker}(\text{tr})$ is non vanishing, it satisfies, from the theory of Lagrange multipliers:

$$\nabla j_\tau(D) - p.\nabla\text{tr} = 0 \quad \text{and} \quad \text{tr}(D) = 0$$

where p is the Lagrange multiplier. Then $2\eta_m D + \tau_0 \frac{D}{|D|} - \tau - p.I = 0$ and $\text{tr}(D) = 0$. Thus the subgradient finally writes:

$$\partial\varphi(D) = \begin{cases} \{\tau, |\tau_d| \leq \tau_0\} & \text{when } D = 0 \\ \left\{ \tau, \tau = -p.I + 2\eta_m D + \tau_0 \frac{D}{|D|} \right\} & \text{when } D \neq 0 \text{ and } \text{tr}(D) = 0 \\ \emptyset & \text{otherwise} \end{cases} \quad (\text{A.1})$$

where τ_d denotes the deviatoric part of τ . The dual φ_m^* of φ_m is then characterized by the Fenchel identity, that is, for any $\tau \in \partial\varphi_m(D)$, by $\varphi_m^*(\tau) = \tau : D - \varphi_m(D)$. Moreover, $\tau \in \partial\varphi_m(D)$ is equivalent to $D \in \partial\varphi_m^*(\tau)$. From $\tau + p.I = (2\eta_m + \tau_0/|D|)D$ we get $|\tau_d| = 2\eta_m|D| + \tau_0$ and thus $|D| = (|\tau_d| - \tau_0)/(2\eta_m)$. Finally:

$$\partial\varphi_m^*(\tau) = \left\{ D, D = \frac{1}{2\eta_m} \max\left(0, \frac{|\tau_d| - \tau_0}{|\tau_d|}\right) \tau_d \right\} \quad (\text{A.2})$$

A.2. *The φ function* – The function φ , as introduced in (2), is a particular case of φ_m with $\eta_m := \eta$ and $\tau_0 := 0$. From (A.1), the subgradient writes:

$$\partial\varphi(D) = \begin{cases} \{\tau, \tau = -p.I + 2\eta D\} & \text{when } \text{tr}(D) = 0 \\ \emptyset & \text{otherwise} \end{cases} \quad (\text{A.3})$$