Numerical prediction of the fiber orientation in steady flows

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RÉSUMÉ. *Cet article traite de la résolution numérique d'équations qui décrivent l'écoulement de suspensions de fibres dans un fluide newtonien (mise en forme de composites par extrusion). Ce modèle met en jeu une équation de Stokes généralisée aux fluides anisotropes et une équation dite d'orientation qui est hyperbolique. Nous montrons que le système de Stokes se résout sans difficulté par des méthodes standard pour fluides incompressibles et ce papier traite essentiellement de l'équation d'orientation. Nous comparons ici différentes techniques adaptées a priori aux équations hyperboliques (méthode des caractéristiques, SUPG et volumes finis discontinus)*

ABSTRACT. *Modelling fibers orientation induced by the flow of short fiber reinforced thermoplastic involves a classical anisotropic Stokes flow problem and a hyperbolic orientation equation. This paper aims to achieve a comparison between different solution techniques suited to the hyperbolicity of the orientation equation (viz. the method of characteristics, the SUPG method and the discontinuous finite volume method).*

MOTS-CLÉS : *écoulements de composites fibres courtes, équation de transport, méthode des caractéristiques, éléments finis SUPG, volumes finis discontinus*

KEY WORDS : *short fiber reinforced thermoplastic flow, transport equation, method of characteristics, SUPG finite elements method, discontinuous finite volumes*

1. Introduction

1.1. *Framework*

As a consequence of the increasing use of composite materials, there has been much work on constitutive equations and computational mechanics for short fiber composites. Since these materials are generally made of a matrix and fiber reinforcement, the mechanical properties of the conformed pieces depend greatly on the fibers orientation in the solid material. However, it turns out that this orientation is determined by the forming process, so that it is interesting to develop mathematical models for the flow during this conforming process and specific numerical strategies to solve the resulting equations.

The resulting system of equations involves the coupling of an elliptic boundary value problem with a convection-type equation. The elliptic problem is associated with the momemtum equations whereas the convection equation describes the time evolution of the anisotropic viscosity tensor. The second problem presents two difficulties: it is non-linear and hyperbolic. Therefore, it is not possible to apply the common Galerkin formulation which is inefficient on convection problems. In this paper, different techniques to obtain numerical solutions of the steady convection equation are discussed.

1.2. *State of the art*

Givler et al. [GIV 82], and others, have studied the orientation process of a fiber which moves along a streamline from a boundary condition imposed at the inflow gates. The velocity field used in the construction of the streamlines was obtained by assuming that the fibers do not disturb the flow. However, this model becomes inadequate when the flow is strongly affected (flow contractions).

Lipscomb et al. [LIP 88] simulate the flow with a finite element method which can be applied to complex domains. However, they assume the Evans hypothesis and impose the local alignment of the fibers with the velocity. Similar results are presented by Chiba et al. [CHB 90], who also assume the Evans hypothesis, and use an alternating direction implicit method to solve the momemtum equations.

There are also two-dimensional simulations coupling the motion and the orientation equations. Ausias [AUS 91] solves the two-dimensional coupled model with a finite element discretization of the motion equations, and with an integration of the orientation equations by the method of characteristics. Altan et al. [ALT 92] study the coupled model by means of the uncoupled fixed point strategy. The fourth order orientation equation is solved by the method of characteristics and the finite difference method is used to solve the momentum equations. Rosenberg et al. [ROS 90] uses the method of characteristics to simulate non-recirculating flows of dilute fibers suspensions.

Poitou et al. [POI 93] solve the two-dimensional steady state coupled model with an uncoupled strategy (fixed point), and use a SUPG finite element formulation to integrate the orientation equation. Convergence problems are detected for complex geometries. Chinesta et al. [CHI 95] analyze numerically the orientation in several recirculating flows. For general flows, they obtain the local alignment of the fibers with the flow, whose stability is proved numerically. Souloumiac [SOU 96] simulates the kinematic-orientation coupled model by means of an uncoupled fixed point strategy. To solve the orientation equation, he introduces the strain gradient tensor variable, and a Lesaint-Raviart technique (discontinuous Galerkin) for its discretization. Poitou et al. [POI 98] give a theoretical result concerning the uniqueness of the orientation equation solution in the steady state recirculating flows. This result makes it possible to use the method of characteristics in general flows, even with recirculating parts.

In this paper, section 2 introduces the governing equations. It describes the fixed point algorithm which has been used, leading to a classical anisotropic Stokes flow problem. Section 3 focuses on the orientation equation. It emphasizes the problems associated with the singularities and those related to the closed vortices in steady state regimes, and describes the three different techniques which are compared in this paper, viz. the method of characteristics, the SUPG method and the finite volume discontinuous method. Section 4 gives the results obtained on significative examples.

2. Mathematical modelling

The main feature of the anisotropic flow model related to the short fibers suspensions is the kinematic-orientation coupling. Kinematics depends directly on the orientations field, as the fibers orientation process is a function of the flow kinematics. The mathematical modelling of the anisotropic suspensions is achieved by a spatial homogenization and a statistical average procedure within a representative volume [BAT 70, HIN 75, HIN 76, HAN 62, MES 97].

2.1. *Governing equations*

— The momentum equation, without inertia and gravity contributions, has the following form

$$\mathrm{Div}\,\underline{\underline{\sigma}} = \underline{0} \qquad [1]$$

where $\underline{\underline{\sigma}}$ denotes the stress tensor.

— The incompressibility condition is

$$\mathrm{Div}\,\underline{v} = 0 \qquad [2]$$

with $\underline{v}$ the velocity vector.

— The orientation equation, can be written, (i) neglecting the brownian effects, (ii) assuming that the particules have a quasi-infinite aspect ratio and (iii) using a quadratic closure approximation for the fourth-order orientation tensor

$$\frac{D\underline{\underline{a}}}{Dt} = \frac{\partial \underline{\underline{a}}}{\partial t} + (\underline{v}\,\mathrm{Grad})\,\underline{\underline{a}} = \mathrm{Grad}(\underline{v})\,\underline{\underline{a}} + \underline{\underline{a}}\,(\mathrm{Grad}(\underline{v}))^T - 2Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}} \qquad [3]$$

where $\underline{\underline{a}}$ represents the second-order orientation tensor, $\mathrm{Grad}(\underline{v})$ the velocity gradient tensor, and $\underline{\underline{d}}$ the deformation rate tensor.
The eigenvalues of the orientation tensor correspond to the probability to find the fibers in the direction of the corresponding eigenvectors.

— If the ambient fluid is Newtonian and if one chooses a quadratic closure approximation for the fourth order orientation tensor, then the anisotropic constitutive law can be written as

$$\underline{\underline{\sigma}} = -p\,\underline{\underline{I}} + 2\mu\{\underline{\underline{d}} + N_p\,Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}}\} \qquad [4]$$

where $\underline{\underline{I}}$ denotes the identity tensor, μ is the effective viscosity and N_p represents a non-negative scalar parameter ($N_p \geq 0$) depending on the fiber aspect ratio and the fiber volume fraction.

— The consistency conditions imposed on the orientation tensor are finally

$$\underline{\underline{a}} = \underline{\underline{a}}^T$$
$$Tr(\underline{\underline{a}}) = 1 \qquad [5]$$

with the eigenvalues λ_i of the orientation tensor $\underline{\underline{a}}$ verifying $0 \leq \lambda_i \leq 1$.

In the three-dimensional general case we obtain nine coupled partial differential equations with nine scalar fields as unknowns: the five independent components of the orientation tensor, the three components of the velocity vector and the pressure field. In the two-dimensional case, which will be treated in this work, we have two components of the orientation tensor, two components of the velocity vector and the pressure field.

To represent the orientation state we use the fact that an eigenvalue of the orientation tensor corresponds to the probability of finding the fibers in the direction of the corresponding eigenvector. In this form we will represent the orientation state in a point by means of an ellipse whose semiaxes correspond to the eigenvalues of the orientation tensor in this point and their directions correspond to their eigenvectors.

Instead of the second order orientation tensor, we can use the solution of the orientation equation (3) given by [MES 97]

$$\underline{\underline{a}} = \frac{\underline{\underline{F}}\,\underline{\underline{a}}^0\,\underline{\underline{F}}^T}{Tr(\underline{\underline{F}}\,\underline{\underline{a}}^0\,\underline{\underline{F}}^T)} \qquad [6]$$

where $\underline{\underline{a}}^0$ represents the initial orientation (boundary conditions in the steady state case), and $\underline{\underline{F}}$ is the deformation gradient solution of the convection problem

$$\frac{D\underline{\underline{F}}}{Dt} = \mathrm{Grad}(\underline{v})\,\underline{\underline{F}}$$
$$\underline{\underline{F}}(\underline{x} \in \Gamma_-) = \underline{\underline{I}} \qquad [7]$$

where the inflow boundary is denoted by Γ_-

$$\Gamma_- = \{\underline{x} \in \partial\Omega \equiv \Gamma,\ \underline{v}^T(\underline{x})\,\underline{n}\,(\underline{x}) < 0\} \qquad [8]$$

and $\underline{n}$ is the unit outwards vector, normal to the boundary at the point $\underline{x}$.

Obviously, this strategy to evaluate the orientation tensor can not be used in the recirculating parts of the flow. In this case, both the deformation gradient and the initial orientation state are *a priori* not defined.

2.2. *A fixed point strategy*

The determination of steady state solutions for this kind of constitutive relation presents similar difficulties to those found for viscoelastic fluids and more generally for all fluids with memory. Actually, the condition of steady flows is local only in eulerian variables. This is the reason why we use a velocitiy formulation. But in this case the constitutive relation is not local in space since it includes history effects. If some streamlines of a steady state flow are closed, the situation is qualitatively complex, because the initial conditions, that are essential in every problem depending on the history and which correspond to the boundary conditions on the inflow boundaries in eulerian variables, do not exist in this case. Due to this fact, we look for an orientation tensor periodic in time when one follows a particule along a closed trajectory.

We search for a numerical solution of a problem with zero traction on Γ_1 and with imposed velocity $\underline{v} = \underline{v}_g$ on Γ_2. The boundary Γ_2 is subdivided into Γ_- and Γ_0. Through Γ_- the material is introduced into the domain and we impose an orientation tensor $\underline{\underline{a}}^0$ and a velocity vector ($\underline{v}_g \neq \underline{0}$). The fluid leaves the domain through Γ_1 without any orientation condition being imposed. On the boundary $\Gamma_0 = \Gamma_2 - \Gamma_-$ we assume $\underline{v}_g = \underline{0}$ (no slip condition) and no orientation condition is required.

The problem is then defined by: *Find* ($\underline{v}$, $\underline{\underline{\sigma}}$, $\underline{\underline{a}}$) *satisfying*

— Kinematic admissibility:

$$\begin{array}{ll} \underline{v} = \underline{v}_g & on\ \Gamma_2 \\ \mathrm{Div}\underline{v} = 0 & in\ \Omega \end{array} \quad [9]$$

— Static admissibility:

$$\begin{array}{ll} \underline{\underline{\sigma}}\,\underline{n} = \underline{0} & on\ \Gamma_1 \\ \mathrm{Div}(\underline{\underline{\sigma}}) = \underline{0} & in\ \Omega \end{array} \quad [10]$$

— Constitutive relation:

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + 2\mu\,\{\underline{\underline{d}} + N_p\, Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}}\,\}$$

$$\frac{D\underline{\underline{a}}}{Dt} - \mathrm{Grad}(\underline{v})\,\underline{\underline{a}} - \underline{\underline{a}}\,(\mathrm{Grad}(\underline{v}))^T = -\,2\,Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}} \quad [11]$$

$$\underline{\underline{a}} = \underline{\underline{a}}^0\ on\ \Gamma_-$$

For the solution of the coupled problem we introduce a fixed point algorithm and sucessively solve the following two steps until convergence:

Problem 1. In a first step, if the orientation tensor $\underline{\underline{a}}$ is known, the problem to be solved is expressed as a constrained minimization problem:

Find $\underline{v} \in \mathcal{U}$, so that $J(\underline{v})$ reaches a minimum

$$J(\underline{v}) = \int_\Omega \mu\,\{\,Tr(\underline{\underline{d}}(\underline{v})\,\underline{\underline{d}}(\underline{v})) + N_p\,Tr(\underline{\underline{a}}\,\underline{\underline{d}}(\underline{v}))^2\} \quad [12]$$

$$\mathcal{U} = \{\,\underline{v} \in R^2,\ \underline{v} \in (H^1(\Omega))^2,\ \mathrm{Div}(\underline{v}) = 0,\ \underline{v} = \underline{v}_g\ \ on\ \Gamma_2\,\} \quad [13]$$

Problem 2. In a second step, if the velocity field is known, the steady state orientation problem results in a convection-type problem, which can be expressed as:

Find $\underline{\underline{a}}$, with $\underline{\underline{a}} = \underline{\underline{a}}^T$ and $Tr(\underline{\underline{a}}) = 1$, verifying

$$(\underline{v}\,\mathrm{Grad})\,\underline{\underline{a}} - \mathrm{Grad}(\underline{v})\,\underline{\underline{a}} - \underline{\underline{a}}\,\mathrm{Grad}(\underline{v})^T =$$

$$= -\,2\,Tr(\underline{\underline{a}}\,\underline{\underline{d}}(\underline{v}))\,\underline{\underline{a}}\quad in\ \Omega \quad [14]$$

$$\underline{\underline{a}} = \underline{\underline{a}}^0 \qquad on\ \Gamma_- \quad [15]$$

The initialization of the algorithm is carried out using the newtonian solution $N_p = 0$. The efficiency of this fixed point scheme can be enhanced by using the following strategy: we calculate first the coupled solution for a low N_p value and then increment N_p step by step. The initialization of the fixed point algorithm at each step is carried out with the coupled solution of the previous one.

Velocity solver.

Problem 1 can be written:

Find $\underline{v} \in \mathcal{U}$ *such that*

$$\int_\Omega Tr\,(\underline{\underline{\sigma}}\,\underline{\underline{d}}^\star)\,d\Omega = 0 \qquad \forall\,\underline{v}^\star \in \mathcal{V} \qquad [16]$$

with

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + 2\mu\,\{\underline{\underline{d}} + N_p\,Tr\,(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}}\,\} \qquad [17]$$

and

$$\mathcal{V} = \{\,\underline{v}^\star \in R^2,\ \underline{v}^\star \in (H^1(\Omega))^2,\ \underline{v}^\star = \underline{0}\ on\,\Gamma_2\,\} \qquad [18]$$

where $H^1(\Omega)$ denotes the standard Sobolev space.

The discretization of the problem is carried out by the finite element method. In order to satisfy the Babuska Brezi's condition, the velocity is interpolated by P2 triangles and the pressure by consistent P1 triangles. If n is the number of nodes used in the velocity approximation and m in the pressure approximation, the discretization of the variational formulation leads (before imposing the velocity boundary conditions) to the algebraic equation system

$$\begin{array}{llll} \underline{\underline{A}}(\underline{\underline{a}}) & \underline{V} & +\underline{\underline{B}}^T\,\underline{P} & = \underline{0} \\ \underline{\underline{B}} & \underline{V} & & = \underline{0} \end{array} \qquad [19]$$

where $\underline{\underline{A}}(\underline{\underline{a}})$ is a matrix $2n \times 2n$ depending on the fiber orientation field, $\underline{\underline{B}}$ is a matrix $m \times 2n$, and $\underline{V}$, $\underline{P}$ denote the nodal velocities and pressures respectively.

If we know the fiber orientation, then $\underline{\underline{A}}(\underline{\underline{a}})$ is a symmetric and positive definite matrix. The symmetry is a consequence of the differential operator symmetry. To prove the positivity, the inequality $Tr(\underline{\underline{\tau}}\,\underline{\underline{d}}) > 0$ must be verified, where the extra-stress tensor $\underline{\underline{\tau}}$ is determined by the constitutive equation

$$\underline{\underline{\tau}} = 2\mu\,\{\underline{\underline{d}} + N_p\,Tr\,(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}}\,\} \qquad [20]$$

from which

$$Tr\,(\underline{\underline{\tau}}\,\underline{\underline{d}}) = 2\mu\{Tr(\underline{\underline{d}}\,\underline{\underline{d}}) + N_p\,(Tr(\underline{\underline{a}}\,\underline{\underline{d}}))^2\} \geq 0 \qquad [21]$$

and we can notice immediately that the equality is obtained only if $Tr(\underline{\underline{d}}^2) = 0$ (i.e. $\underline{\underline{d}} = \underline{\underline{0}}$).

The problem is solved by an augmented Lagrangian method [FOR 83].

Orientation problem.

Problem 2 is hyperbolic, and in consequence appropriate discretization techniques must be used. Moreover the orientation equation exhibits some specific difficulties associated with the existence of singularities and discontinuities in the solution. The main results concerning the steady recirculating flows have been presented in [POI 98], and now we will focus our analysis on the non-recirculating flows.

In some flows we can find characteristics along which $\text{Grad}(\underline{v}) = \underline{\underline{0}}$, and as a consequence $\underline{\underline{d}} = \underline{\underline{0}}$. Along these characteristics there are no orientation effects and the fiber orientation remains invariant and keeps the initial value imposed on the inflow boundary. On the other hand, on characteristics located in the neighbourhood of the previous one, generally $\underline{\underline{d}} \neq \underline{\underline{0}}$, so the fibers rotate along these characteristics, which gives rise to a singularity. To illustrate this phenomenon, we can take as an example a rectangular domain $(x, y) \in [0, 0.1] \times [0, 0]$, on which we consider a Poiseuille flow defined by the following velocity field:

$$\begin{aligned} v_x &= v_x(y) = y(0.01 - y) \\ v_y &= 0 \end{aligned} \qquad [22]$$

If we impose on the inflow boundary ($x = 0$) an isotropic orientation ($\underline{\underline{a}}^0 = \frac{\underline{\underline{I}}}{2}$), the orientation evolution for different characteristics is represented in Fig. 1. We can notice that the time required for the fiber to align along the trajectories depends on the coordinate y. If we assume that the length of the domain is unbounded, and take into account two streamlines (the first one with $y = 0.005$, $\text{Grad}(\underline{v}) = \underline{\underline{0}}$ and $\underline{\underline{d}} = \underline{\underline{0}}$; and the second one with $y = 0.005 + \epsilon$, $\text{Grad}(\underline{v}) \neq \underline{\underline{0}}$ and $\underline{\underline{d}} \neq \underline{\underline{0}}$), then if ϵ is a very small parameter, we can conclude that:

$$\begin{aligned} &\forall\, \delta \in]0, \tfrac{1}{2}[,\ \exists x_c,\ \textit{so that}\ \forall x \geq x_c \\ &|\, \sup_i |\lambda_i(x, y = 0.005)| \ - \ \sup_i |\lambda_i(x, y = 0.005 + \epsilon)|\,| \ \geq \ \delta \end{aligned} \qquad [23]$$

where $\lambda_i(x, y)$ are the eigenvalues of the orientation tensor at the point (x, y).

However, we can prove the continuity in the orientation tensor, with respect to (x,y). More precisely, it is easy to note that

$$\begin{aligned} &\forall\, \gamma > 0,\ \textit{and}\ x_c > 0,\ \exists \eta\ \textit{so that}\ \forall x \leq x_c \\ &|\, \sup_i |\lambda_i(x, y = 0.005)| \ - \ \sup_i |\lambda_i(x, y = 0.005 + \eta)|\,| \ \leq \ \gamma \end{aligned} \qquad [24]$$

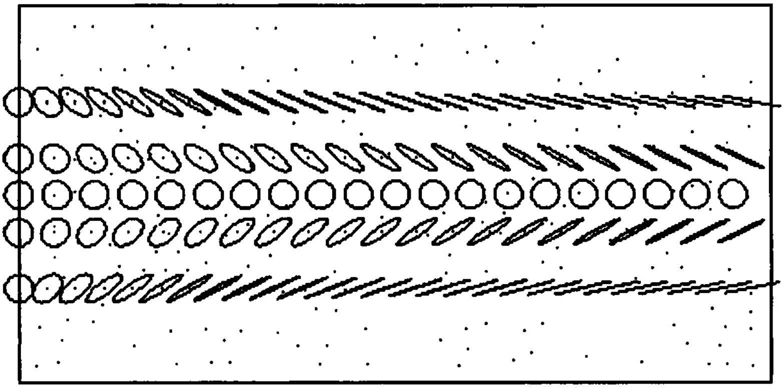

Figure 1. *Orientation solution for a Poiseuille flow*

The position of the singularity is *a priori* known in the preceeding example. Thus we can expect that the effects of the singularity could be removed by means of a local remeshing. However, the difficulty increases when the position of these singularities is unknown.

The only discontinuities in the orientation solution result from the orientation discontinuities on the inflow boundary. Due to the hyperbolic character of the equation, these eventual discontinuities are propagated inside the domain.

3. Orientation solver

3.1. *The method of characteristics*

In this section, the velocity field is assumed to be given and we wish to solve the orientation equation (*Problem 2*)

$$(\underline{v}\,\mathrm{Grad})\,\underline{\underline{a}} = \mathrm{Grad}(\underline{v})\,\underline{\underline{a}} + \underline{\underline{a}}\,(\mathrm{Grad}(\underline{v}))^T - 2Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}} \qquad [25]$$

with an orientation condition on the inflow boundary

$$\underline{\underline{a}}|_{\Gamma_-} = \underline{\underline{a}}^0 \qquad [26]$$

Even for a given velocity field, this equation is non-linear due to the term $Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}}$.

The characteristics are determined by

$$\frac{dt}{1} = \frac{dx}{v_x} = \frac{dy}{v_y} \qquad [27]$$

which are the streamlines for the steady state regimes.

If we define the tensor $\underline{\underline{c}}$ as

$$\underline{\underline{c}} = Grad(\underline{v})\,\underline{\underline{a}} + \underline{\underline{a}}\,(Grad(\underline{v}))^T - 2Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}} \quad [28]$$

by applying the method of the characteristics to the orientation equation (Eq. 3), we will obtain

$$\frac{dt}{1} = \frac{dx}{v_x} = \frac{dy}{v_y} = \frac{d\underline{\underline{a}}}{\underline{\underline{c}}} \quad [29]$$

and taking into account the initial and/or the boundary conditions, we will have

$$x = x(t); \qquad y = y(t); \qquad \underline{\underline{a}} = \underline{\underline{a}}(t) \quad [30]$$

A fourth order Runge-Kutta scheme with control step has been used in the integrations. At each point where we want to know the orientation, the characteristic must be reconstructed until it reaches Γ_-, from where we must follow the flow in integrating the orientation equation from the boundary condition until returning to the starting point.

3.2. *SUPG finite elements formulation*

If we want to be able to use a fully coupled (kinematics-orientation) Newton-type algorithm, we need to use a eulerian formulation of the orientation equation. A possible technique for the discretization of the variational formulation of the orientation equation is the finite elements method. However, due to the non-linear hyperbolic character of this equation, the Galerkin formulation can not be applied. We use a SUPG formulation (streamline upwind Petrov Galerkin) combined with a Newton-Raphson algorithm for the treatment of the non-linearity.

3.2.1. *Variational formulation*

The orientation equation in the two-dimensional case consists of two independent scalar equations which in a steady state regime, are expressed in the cartesian system of coordinates as

$$\begin{aligned} v_x \frac{\partial a_{11}}{\partial x} + v_y \frac{\partial a_{11}}{\partial y} &= c_{11}(a_{11}, a_{12}) \\ v_x \frac{\partial a_{12}}{\partial x} + v_y \frac{\partial a_{12}}{\partial y} &= c_{12}(a_{11}, a_{12}) \end{aligned} \quad [31]$$

where $\underline{\underline{c}}$ is defined here by

$$\underline{\underline{c}} = \mathrm{Grad}(\underline{v})\,\underline{\underline{a}} + \underline{\underline{a}}\,(\mathrm{Grad}(\underline{v}))^T - 2\,Tr(\underline{\underline{a}}\,\underline{\underline{d}})\,\underline{\underline{a}} \quad [32]$$

This equation is satisfied in the domain $\Omega \subset R^2$, whose boundary is denoted by $\partial\Omega$. The orientation on the inflow boundary is given by

$$\underline{\underline{a}} = \underline{\underline{a}}^0 \quad on\, \Gamma_- \qquad [33]$$

with

$$\Gamma_- = \{\, \underline{x} \in \partial\Omega \;:\; \underline{v}^T \underline{n} < 0 \,\} \qquad [34]$$

The Newton-Raphson method enables us to obtain the linearization of the set of equations (31)

$$\begin{aligned} v_x \frac{\partial \delta a_{11}}{\partial x} + v_y \frac{\partial \delta a_{11}}{\partial y} - \frac{\partial c_{11}}{\partial a_{11}} \delta a_{11} - \frac{\partial c_{11}}{\partial a_{12}} \delta a_{12} &= - R_1(a_{11}, a_{12}) \\ v_x \frac{\partial \delta a_{12}}{\partial x} + v_y \frac{\partial \delta a_{12}}{\partial y} - \frac{\partial c_{12}}{\partial a_{11}} \delta a_{11} - \frac{\partial c_{12}}{\partial a_{12}} \delta a_{12} &= - R_2(a_{11}, a_{12}) \end{aligned} \qquad [35]$$

with the components of the residue vector $\underline{R}$, R_1 and R_2, defined by

$$\begin{aligned} R_1 &= v_x \frac{\partial a_{11}}{\partial x} + v_y \frac{\partial a_{11}}{\partial y} - c_{11}(a_{11}, a_{12}) \\ R_2 &= v_x \frac{\partial a_{12}}{\partial x} + v_y \frac{\partial a_{12}}{\partial y} - c_{12}(a_{11}, a_{12}) \end{aligned} \qquad [36]$$

If we take into account the flow incompressibility, the variational formulation of the problem (Eq. 35) is

$$\begin{aligned} &\int_\Omega \delta a_{11}^\star \, \underline{v}^T \, \mathrm{Grad}(\delta a_{11}) \, d\Omega - \\ &\quad - \int_\Omega \frac{\partial c_{11}}{\partial a_{11}} \delta a_{11} \, \delta a_{11}^\star \, d\Omega - \int_\Omega \frac{\partial c_{11}}{\partial a_{12}} \delta a_{12} \, \delta a_{11}^\star \, d\Omega = \\ &\qquad = - \int_\Omega \delta a_{11}^\star \, \underline{v}^T \, \mathrm{Grad}(a_{11}) \, d\Omega + \int_\Omega c_{11} \, \delta a_{11}^\star \, d\Omega \end{aligned} \qquad [37]$$

and

$$\begin{aligned} &\int_\Omega \delta a_{12}^\star \, \underline{v}^T \, \mathrm{Grad}(\delta a_{12}) \, d\Omega - \\ &\quad - \int_\Omega \frac{\partial c_{12}}{\partial a_{11}} \delta a_{11} \, \delta a_{12}^\star \, d\Omega - \int_\Omega \frac{\partial c_{12}}{\partial a_{12}} \delta a_{12} \, \delta a_{12}^\star \, d\Omega = \\ &\qquad = - \int_\Omega \delta a_{12}^\star \, \underline{v}^T \, \mathrm{Grad}(a_{12}) \, d\Omega + \int_\Omega c_{12} \, \delta a_{12}^\star \, d\Omega \end{aligned} \qquad [38]$$

3.2.2. *Discretization*

The discretization is carried out with a weighted residual technique, over the triangularization T_j of finite elements. A linear C^0 approximation is used for the interpolation of the second-order orientation tensor components. The test functions $\delta a_{ij}^\star$ are interpolated in each triangle according to

$$\delta a^{\star}_{ij} = \delta a^{\star}_{ij}{}^{1}\,\overline{N}_1 + \delta a^{\star}_{ij}{}^{2}\,\overline{N}_2 + \delta a^{\star}_{ij}{}^{3}\,\overline{N}_3 \qquad [39]$$

and $\overline{N}_j$ are obtained in a SUPG formulation from

$$\overline{N}_j = N_j + \frac{\beta \overline{h}}{2\|\underline{v}\|}\left(v_x \frac{\partial N_j}{\partial x} + v_y \frac{\partial N_j}{\partial y}\right) \qquad [40]$$

where N_j are the standard shape functions and $\overline{h}$ is the average length of the element in the convection direction. In a SUPG formulation of the convection-diffusion equation, β is a function of the Peclet number. In our case we consider $\beta = 1$.

3.3. *Discontinuous finite volume formulation*

Another scheme well adapted to the convection equations is the discontinuous finite volume method. We consider a conforming P^1 triangulation and for each node i the cell V^i formed by the mid point of the element edges joining at node i, as well as the barycentre of all the elements containing the node i [PIR 89]. In this way we relate the generic function f_h, which is a piecewise polynomial of degree one and continuous over the triangulation, to a function $\tilde{f}_h$ with a constant value in each volume V^i

$$\tilde{f}_h|_{V^i} = \frac{1}{|V^i|}\int_{V^i} f_h(\underline{x})\, d\Omega \qquad [41]$$

The discontinuous Galerkin method allows us to write for each cell V^i

$$- \int_{\partial V^i_-} [\widetilde{\delta a_{11h}}]\, \underline{v}^T \underline{n}\, dS - \int_{V^i} \frac{\partial c_{11}}{\partial a_{11}}\, \widetilde{\delta a_{11h}}\, d\Omega - \int_{V^i} \frac{\partial c_{11}}{\partial a_{12}}\, \widetilde{\delta a_{12h}}\, d\Omega =$$

$$= \int_{\partial V^i_-} [\widetilde{a_{11h}}]\, \underline{v}^T \underline{n}\, dS + \int_{V^i} c_{11}\, d\Omega \qquad \forall\, V^i \qquad [42]$$

$$- \int_{\partial V^i_-} [\widetilde{\delta a_{12h}}]\, \underline{v}^T \underline{n}\, dS - \int_{V^i} \frac{\partial c_{12}}{\partial a_{11}}\, \widetilde{\delta a_{11h}}\, d\Omega - \int_{V^i} \frac{\partial c_{12}}{\partial a_{12}}\, \widetilde{\delta a_{12h}}\, d\Omega =$$

$$= \int_{\partial V^i_-} [\widetilde{a_{12h}}]\, \underline{v}^T \underline{n}\, dS + \int_{V^i} c_{12}\, d\Omega \qquad \forall\, V^i \qquad [43]$$

where ∂V^i_- represents the inflow boundary of the cell V^i and $[f_h]$ represents the jump of the function f_h across the inflow boundary ∂V^i_-

$$[f_h](\underline{x}) = lim_{\epsilon \to 0^+}(f_h(\underline{x} + \epsilon \underline{v}(\underline{x})) - f_h(\underline{x} - \epsilon \underline{v}(\underline{x}))\,,\ \forall \underline{x} \in \partial V^i_-) \qquad [44]$$

3.3.1. *Aspects related to the Newton method*

In this case, as for the upwind scheme of finite elements, the convergence of the fixed point algorithm is a difficult matter since:

1. The convergence rate depends on the arbitrary initial orientation considered.
2. In the first step of the iteration algorithm, an extremely small correction parameter is required in order to insure convergence.

For this reason, we propose a globally convergent Newton's scheme to solve the non-linear orientation equation. This method converges towards the minimum of the residual, but it sometimes stops at a local minimum. In this situation, we propose a strategy with physical and heuristic basis, assuming that there is only one fiber orientation solution with physical sense. Thus, when the globally convergent Newton's method reaches a minimum with non-zero residual (local minimum), the eigenvalues of the orientation tensor in each node are calculated, and when their values do not verify the conditions

$$\begin{array}{ll} sup\,\lambda_i & \leq 1 \\ inf\,\lambda_i & \geq 0 \end{array} \qquad [45]$$

then the orientation at the node is substituted by the isotropic orientation $\underline{\underline{I}}/2$, and the minimization process is started again.

3.3.2. *The deformation gradient variable*

The previous method may be applied to solve the convection problem associated with the deformation gradient $\underline{\underline{F}}$, $Eq.(7)$, in order to obtain the orientation tensor from Eq. (6).

In this case the system is linear, and from Eq. (7) we obtain the following system of convection-type scalar equations

$$\begin{array}{lll} v_x \frac{\partial F_{11}}{\partial x} + v_y \frac{\partial F_{11}}{\partial y} & = & (\text{Grad}\underline{v})_{11}F_{11} + (\text{Grad}\underline{v})_{12}F_{21} \\ v_x \frac{\partial F_{21}}{\partial x} + v_y \frac{\partial F_{21}}{\partial y} & = & (\text{Grad}\underline{v})_{21}F_{11} + (\text{Grad}\underline{v})_{22}F_{21} \\ v_x \frac{\partial F_{12}}{\partial x} + v_y \frac{\partial F_{12}}{\partial y} & = & (\text{Grad}\underline{v})_{11}F_{12} + (\text{Grad}\underline{v})_{12}F_{22} \\ v_x \frac{\partial F_{22}}{\partial x} + v_y \frac{\partial F_{22}}{\partial y} & = & (\text{Grad}\underline{v})_{21}F_{12} + (\text{Grad}\underline{v})_{22}F_{22} \end{array} \qquad [46]$$

We can notice that the two first equations are decoupled with the two last ones. Moreover, the two resultant problems are identical except for the boundary conditions on Γ_- ($\underline{\underline{F}}(\underline{x} \in \Gamma_-) = \underline{\underline{I}}$). This fact and the linear character of the problem simplify notably the numerical solution.

The discretization scheme in this case takes the form

$$- \int_{\partial V_-^i} [\widetilde{F_{1kh}}] \, \underline{v}^T \underline{n} \, dS \; - \; \int_{V^i} (\mathrm{Grad}\underline{v})_{11} \, \widetilde{F_{1kh}} \, d\Omega \; - \\ - \int_{V^i} (\mathrm{Grad}\underline{v})_{12} \, \widetilde{F_{2kh}} \, d\Omega \; = \; 0 \qquad \forall \, V^i \quad [47]$$

$$- \int_{\partial V_-^i} [\widetilde{F_{2kh}}] \, \underline{v}^T \underline{n} \, dS \; - \; \int_{V^i} (\mathrm{Grad}\underline{v})_{21} \, \widetilde{F_{1kh}} \, d\Omega \; - \\ - \int_{V^i} (\mathrm{Grad}\underline{v})_{22} \, \widetilde{F_{2kh}} \, d\Omega \; = \; 0 \qquad \forall \, V^i \quad [48]$$

for $k = 1$ and $k = 2$.

This strategy can not be applied to treat steady state vortex flows, where neither the deformation gradient $\underline{\underline{F}}$ nor the initial orientation $\underline{\underline{a}}^0$ are defined.

4. Results and discussion

In Table 2, we compare the numerical and the theoretical solutions of the orientation in the middle point of the outflow boundary for a Poiseuille flow between two parallel plates when we impose an isotropic orientation at the inflow boundary. These results are obtained by using the discontinuous finite volume method to solve the orientation equation with the second order orientation tensor as unknown variable. The theoretical solution of this problem is shown in Fig. 1. Obviously, we find a non-physical orientation of the fibers on the characteristic line with zero deformation rate, and this non-physical effect is due to a numerical diffusion in the normal direction of the characteristics, and also to the non-consistent interpolation of the second order orientation tensor. The SUPG formulation in finite elements gives us similar results.

Mesh: dof	a_{11}^{exac}	a_{12}^{exac}	a_{11}^{num}	a_{12}^{num}
1500	0.5	0.0	0.9349	0.00380
3400	0.5	0.0	0.9290	-0.0023
12600	0.5	0.0	0.8925	-0.0045

Figure 2. *Poiseuille flow: orientation in the mid point at the outflow boundary*

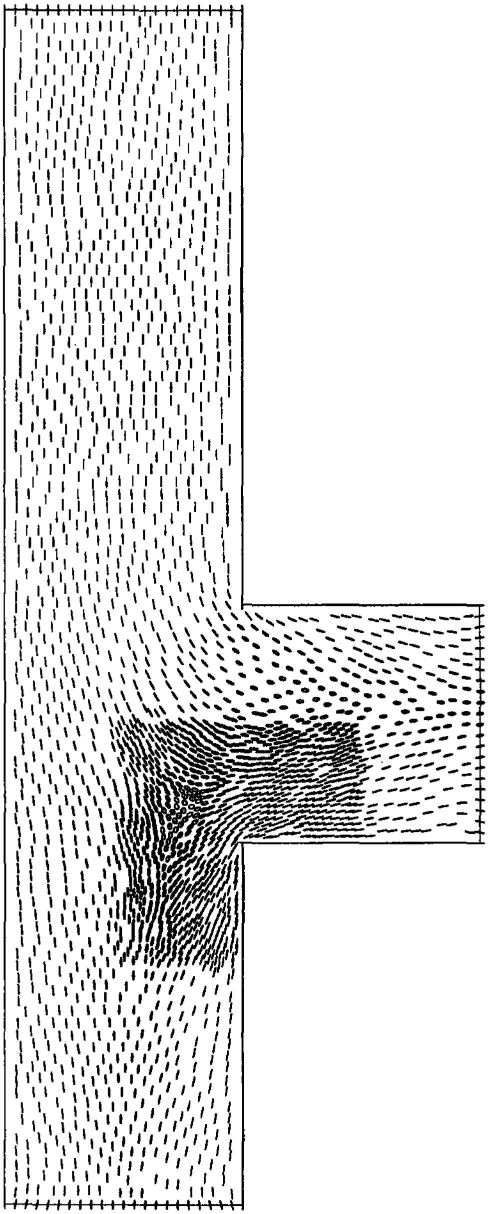

Figure 3. *Numerical solution: formulation with the orientation tensor as unknown variable*

We can also see in Table 2, that this diffusion can not be removed by remeshing, because it is not justified to use so many degrees of freedom to solve such a simple problem. To understand the problems associated with the orientation interpolation, we can consider the interpolation of two orientations defined at two points by ($a_{11}^1 = 1$, $a_{12}^1 = 0$) and ($a_{11}^2 = 0$, $a_{12}^2 = 0$). The standard interpolation at a mid point located between the previous ones, gives us the isotropic orientation ($a_{11} = \frac{1}{2}$, $a_{12} = 0$). Thus, from a perfect alignment of the fibers in both cases, we obtain an isotropic interpolated orientation. We can conclude that the fiber orientation probability is modified by the interpolation of the second order orientation tensor. More physical solutions are obtained by the interpolation of eigenvalues and eigenvectors, that gives us the alignment of the fibers in the direction making 45^0 with the x-direction ($a_{11} = \frac{1}{2}, a_{12} = \frac{1}{2}$).

It is easy to prove that interpolations of the deformation gradient do not change the orientation probability in the preceeding way. If we solve the equation that governs the evolution of the deformation gradient in order to calculate the orientation, we obtain the results shown in Table 4, where the discontinuous finite volume method is used to solve the convection problem associated with the strain gradient variable. Another advantage of using this variable is that then the convection problem is linear, and no iteration scheme is required.

Variable	a_{11}^{exac}	a_{12}^{exac}	a_{11}^{num}	a_{12}^{num}
$\underline{\underline{a}}$	0.5	0.0	0.9349	0.00380
$\underline{\underline{F}}$	0.5	0.0	0.5048	0.07325

Figure 4. *Poiseuille flow: orientation in the mid point at the outflow boundary*

However, for more complex geometries, the difficulty increases even when we use the deformation gradient as variable. Fig. 3 shows the orientation solution in a T domain with the second order orientation tensor as a variable and 5300 dof. Since the orientation condition imposed on the inflow boundary is the local alignment of the fibers with the flow, and since this orientation is a local solution of the orientation problem, we can conclude that the local alignment of the fibers with the flow is the solution at each point in the domain. This solution is shown in Fig. 5. As we can notice from the comparison of Figs. 3 and 5, the problems associated with the interpolation of $\underline{\underline{a}}$ subsist, and they are propagated due to the convective character of the equation.

If we look for the error associated with solutions obtained with different meshes from the theoretical solution (local alignment of the fibers with the flow), we can prove that the error decreases slowly with the remeshing.

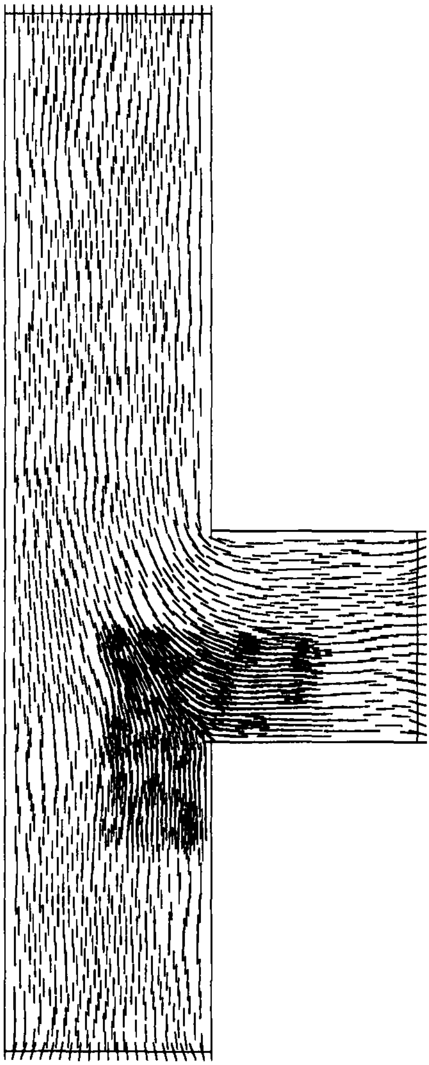

Figure 5. *Reference solution: local alignment of the fibers with the flow*

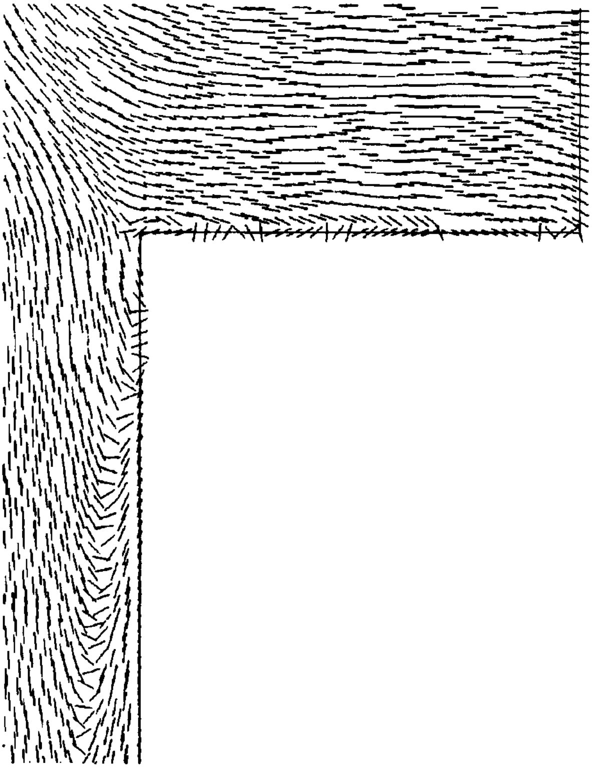

Figure 6. *Numerical solution: formulation with the deformation gradient as unknown variable. Zoom in the neighborhood of the corner*

Moreover, if we change the variable of the model, taking into account the better interpolation properties of the deformation gradient, the problems still remain. In this case, the singularities located in the corners of the boundary introduce a distortion in the fiber orientation that is convected by the flow, and the singularity persists with remeshing. Fig. 6 shows the solution in the corner neighborhood with 15100 dof. For this reason, the convergence rate to the reference solution is very slow, and it is not possible to avoid the singularities with the introduction of extra-boundary conditions due to the singularity of the deformation gradient in the boundaries with zero velocity. However if we work with the variable $\underline{\underline{a}}$, these problems may be removed by imposing local alignment of the fibers with the boundary, which also improves the convergence rate of the non-linear iteration scheme.

5. Conclusions

Different discretization techniques well adapted to the convection problems have been analyzed, and we have pointed out their limitations for the resolution of the orientation field in certain flows with industrial interest. From this analysis, we can conclude, like many authors working in the field of hyperbolic equations, that the method of characteristics is the most accurate for this type of problems [POI 98]. After [POI 98] this method may also also applied in the case of steady recirculating flows. In the same work we have shown that SUPG or discontinuous finite volumes techniques fail to give even approximated solutions in recirculating flows, and now other problems associated with the functional approximations, the treatment of the non linearities, and the existence of singularities in the fiber orientation solution, are pointed out. Another difficulty concerns the use of fully coupled schemes to solve the coupled model kinematic-orientation, which usually requires the use of a eulerian formulation of the orientation problem. With regard to the other techniques, we must continue with the study of the limitations in order to identify those that are inherent and those that could be removed with an appropriate remeshing or with better models, interpolations and discretization techniques.

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