On the Fiber Orientation in Steady Recirculating Flows Involving Short Fibers Suspensions

Kunji Chiba, Amine Ammar, Francisco Chinesta

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Kunji Chiba [1], Amine Ammar [2] and Francisco Chinesta [3]

[1] *Faculty of Education, Shiga University,*

2-5-1 Hiratsu, Otsu, Shiga, 520-0862 Japan

kchiba@sue.shiga-u.ac.jp

[2] *Laboratoire de Rhéologie*

1301 rue de la piscine, BP 53 Domaine universitaire

38041 Grenoble Cedex 9, France

Amine.Ammar@ujf-grenoble.fr

[3] *LMSP (Laboratoire de Mécanique des Systèmes et des Procédés)*

UMR CNRS - ENSAM - ESEM

151 Boulevard de l'Hôpital, F-75013 Paris, France

francisco.chinesta@paris.ensam.fr

Abstract

In this work we present a new numerical strategy to treat the 3D Fokker-Planck equation in steady recirculating flows. This strategy combines some ideas of the method of particles, with a more original treatment of the periodicity condition, which characterizes the steady solution of the Fokker-Planck equation in steady recirculating flows, as usually encountered in some rheometric devices. Using this numerical technique the fiber orientation distribution can be computed accurately in any steady recirculating flow. The simulation results can be used to identify some rheological parameters of the suspension, using an inverse technique, as well as to analyze the validity of some simplified models widely used, which require a closure relation. Thus, in this paper several closure relations of the fourth order orientation tensor will be discussed in the context of a numerical example involving a steady recirculating flow.

Keywords: Short fiber suspensions; Fokker-Planck equation; Particle strategy; Steady recirculating flows; Closure relations

1. Introduction

Numerical modeling of non-Newtonian flows usually involves the coupling between equations of motion, which define an elliptic problem, and the fluid constitutive equation, which introduces an advection problem related to the fluid history. In short fiber suspensions (SFS) models, the extra-stress tensor depends on the fiber orientation whose evolution can be modeled from a transport problem. In all cases the flow kinematics and the fiber orientation are coupled: the kinematics of the flow governs the fiber orientation, and the presence and orientation of the fibers modify the flow kinematics. Thus, for example, in a contraction flow of a dilute suspension, large recirculating areas appear (Lipscomb et al. (1988)).

If one uses SFS flows in material forming processes, the final fiber orientation state depends on the process and exhibits flow-induced anisotropy. Thus, we need to compute the fiber orientation in order to predict the final mechanical properties of the composite parts, which depend strongly on the fiber orientation. Moreover, the numerical simulation of such flows becomes interesting if one want to identify their rheological parameters using some rheometric devices and an appropriate inverse technique.

The mechanical model governing the SFS flow is given by the following equations: (Batchelor (1970, 1971), Hand (1962), Hinch and Leal (1975, 1976), Meslin (1999))

- The momentum balance equation, when the inertia and mass terms are neglected, results

$$Div\underline{\underline{\sigma}} = \underline{0} \tag{1}$$

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

- The mass balance equation for incompressible fluids

$$Div\underline{v} = 0 \tag{2}$$

where $\underline{v}$ represents the velocity field.

- The constitutive equation for a dilute suspension of high aspect-ratio particles is given, with other simplifying assumptions (Tucker (1991)), by

$$\underline{\underline{\sigma}} = -p\underline{\underline{I}} + 2\eta\left\{\underline{\underline{D}} + N_p\left(\underline{\underline{\underline{\underline{a}}}} : \underline{\underline{D}}\right)\right\} \tag{3}$$

where p denotes the pressure, $\underline{\underline{I}}$ the unit tensor, η the viscosity which depends on the chosen model as discussed in Meslin (1999), $\underline{\underline{D}}$ the strain rate tensor, N_p a scalar parameter depending on both the fiber concentration and the fiber aspect ratio, ":" the tensorial product twice contracted (i.e. $\left(\underline{\underline{\underline{\underline{a}}}} : \underline{\underline{D}}\right)_{ij} = a_{ijkl}D_{kl}$) and $\underline{\underline{\underline{\underline{a}}}}$ the fourth order orientation tensor defined by

$$\underline{\underline{\underline{\underline{a}}}} = \int \underline{\rho} \otimes \underline{\rho} \otimes \underline{\rho} \otimes \underline{\rho}\, \psi(\underline{\rho})\, d\underline{\rho} \tag{4}$$

where $\underline{\rho}$ is the unit vector aligned in the fiber axis direction, "$\otimes$" denotes the tensorial product (i.e. $(\underline{\rho} \otimes \underline{\rho})_{ij} = \rho_i \rho_j$), and $\psi(\underline{\rho})$ is the orientation distribution function satisfying the normality condition

$$\int \psi(\underline{\rho})\, d\underline{\rho} = 1 \tag{5}$$

If $\psi(\underline{\rho}) = \delta(\underline{\rho} - \underline{\hat{\rho}})$, with $\delta(\,)$ the Dirac's distribution, all the orientation probability is concentrated in the direction defined by $\underline{\hat{\rho}}$, and the corresponding orientation tensor results $\underline{\underline{\underline{\underline{\hat{a}}}}} = \underline{\hat{\rho}} \otimes \underline{\hat{\rho}} \otimes \underline{\hat{\rho}} \otimes \underline{\hat{\rho}}$.

We can also define the second order orientation tensor as

$$\underline{\underline{a}} = \int \underline{\rho} \otimes \underline{\rho}\, \psi(\underline{\rho})\, d\underline{\rho} \tag{6}$$

It is easy to verify that if $\psi(\underline{\rho}) = \delta(\underline{\rho} - \underline{\hat{\rho}})$, the fourth order orientation tensor can be written as

$$\underline{\underline{\underline{\underline{a}}}} = \underline{\underline{a}} \otimes \underline{\underline{a}} \tag{7}$$

whose components are defined by $a_{ijkl} = a_{ij} a_{kl}$.

For general expressions of $\psi(\underline{\rho})$ the previous relation is not exact, and equation (7) becomes a closure approximation known as the quadratic closure relation: $a_{ijkl}^{quad} = a_{ij}a_{kl}$. However, other closure relations are usually applied (Advani and Tucker (1990), Dupret et al. (1998)), among them we can consider the linear closure relation

$$a_{ijkl}^{lin} = -\frac{1}{24}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{1}{6}(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{kl}\delta_{ij} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}) \quad (8)$$

the hybrid closure relation

$$a_{ijkl}^{hyb} = f\, a_{ijkl}^{quad} + (1-f)\, a_{ijkl}^{lin} \quad (9)$$

where $f = 1 - 4\det(\underline{\underline{a}})$; and finally, the natural closure relation (Dupret et al. (1998))

$$a_{ijkl}^{nat} = \frac{1}{6}\det(\underline{\underline{a}})(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{1}{3}(a_{ij}a_{kl} + a_{ik}a_{jl} + a_{il}a_{jk}) \quad (10)$$

The isotropic orientation state is defined by the uniform distribution function

$$\Psi(\underline{\rho}) = \frac{1}{4\pi} \quad (11)$$

and then, the second order orientation tensor related to that isotropic orientation state is

$$\underline{\underline{a}} = \frac{\underline{\underline{I}}}{3} \tag{12}$$

It is easy to verify that for isotropic orientation distributions (2D or 3D) the linear closure becomes exact.

From a physical point of view, we can consider that the eigenvalues of the second order orientation tensor represent the probability of finding the fiber in the direction of the corresponding eigenvectors.

- If we consider spheroidal fibers immersed in a dilute suspension, we can describe the orientation evolution by means of the Jeffery equation (Jeffery (1922))

$$\frac{d\underline{\rho}}{dt} = \underline{\underline{\Omega}}\,\underline{\rho} + k\left(\underline{\underline{D}}\,\underline{\rho} - \left(\underline{\underline{D}} : \left(\underline{\rho} \otimes \underline{\rho}\right)\right)\underline{\rho}\right) \tag{13}$$

where $\underline{\underline{\Omega}}$ is the vorticity tensor, and k is a constant that depends on the fiber aspect ratio r (fiber length to fiber diameter ratio)

$$k = \left(r^2 - 1\right)/\left(r^2 + 1\right) \tag{14}$$

On the other hand the evolution of the fiber orientation distribution ψ is governed by the Fokker-Planck equation,

$$\frac{d\psi(\underline{\rho})}{dt} + \frac{\partial}{\partial \underline{\rho}}\left\{\psi(\underline{\rho})\frac{d\underline{\rho}}{dt}\right\} = 0 \tag{15}$$

where the material derivative is given by

$$\frac{d\psi}{dt} = \frac{\partial \psi}{\partial t} + \underline{v}\, Grad\psi \tag{16}$$

Now, taking into account equations (6), (13) and (15), the equation that governs the evolution of the second order orientation tensor can be deduced

$$\frac{d\underline{\underline{a}}}{dt} = \underline{\underline{\Omega}}\,\underline{\underline{a}} - \underline{\underline{a}}\,\underline{\underline{\Omega}} + k\left(\underline{\underline{D}}\,\underline{\underline{a}} + \underline{\underline{a}}\,\underline{\underline{D}} - 2\left(\underline{\underline{\underline{\underline{a}}}} : \underline{\underline{D}}\right)\right) \tag{17}$$

A similar equation can be derived for the evolution of the fourth order orientation tensor, which in this case involves the sixth-order orientation tensor.

To take account of fiber interaction effects in semi-concentrated suspensions Folgar and Tucker (1984) proposed the introduction of a diffusion term in the Fokker-Planck equation, i.e.

$$\frac{d\psi(\underline{\rho})}{dt} + \frac{\partial}{\partial \underline{\rho}}\left\{\psi(\underline{\rho})\frac{d\underline{\rho}}{dt}\right\} = \frac{\partial}{\partial \underline{\rho}}\left\{D_r \frac{\partial \psi(\underline{\rho})}{\partial \underline{\rho}}\right\} \tag{18}$$

Fiber interaction being taken into account, the equation governing the evolution of $\underline{\underline{a}}$ then yields

$$\frac{d\underline{\underline{a}}}{dt} = \underline{\underline{\Omega}}\,\underline{\underline{a}} - \underline{\underline{a}}\,\underline{\underline{\Omega}} + k\left(\underline{\underline{D}}\,\underline{\underline{a}} + \underline{\underline{a}}\,\underline{\underline{D}} - 2\left(\underline{\underline{\underline{\underline{a}}}} : \underline{\underline{D}}\right)\right) - 4D_r\left(\underline{\underline{a}} - \frac{\underline{\underline{I}}}{N}\right) \tag{19}$$

with

$$N = \begin{cases} 2 & \text{in } 2D \\ 3 & \text{in } 3D \end{cases} \tag{20}$$

The Fokker-Planck formalism circumvents the necessity of using closure relations, but it induces some difficulties related to its multidimensional character (the distribution function is defined in the physical and the configuration spaces) and moreover advection terms are defined in both spaces. By these reasons the number of works devoted to the treatment of the FP equation is relatively reduced.

In general we can solve the FP equation of its associated Ito stochastic differential equation for a large ensemble of realizations. The CONNFFESSIT method (Laso and Öttinger (1993)) was the first implementation of the stochastic approach. The Brownian Configuration Fields (Hulsen et al. (1997)) or the Lagrangian Particle Methods (Halin et al. (1998)) can be considered as some improvements of the CONNFFESSIT method (see Keunings (2003) for an excellent review about the micro-macro methods). However, the control of the statistical noise is a major issue in stochastic micro-macro simulations, problem that not arise in the deterministic Fokker-Planck approach.

The FP equation can be solved by using meshless particle techniques (Chorin (1973)) which requires a particle smoothing for treating the diffusive term in a proper way (Chaubal et al. (1997); Ammar and Chinesta (2003)). The main advantage of this Lagrangian meshless description is the possibility to represent accurately highly localized distribution functions without any remeshing. Other advantage of this kind of techniques is the accurate and natural treatment of the advection terms.

Other strategies have been successfully applied in the context of the fixed mesh techniques (Suen et al. (2003); Lozinski and Chauvière (2003); Chauvière and Lozinski (2004)). In these techniques, usually, to account for the multidimension of the FP equation, a time-splitting is often considered to decouple the advection problem in physical space and the advection-diffusion problem in the conformation space. The first problem can be solved by a numerical method appropriate for hyperbolic partial differential equations (discontinuous Galerkin, SUPG, …). The advection-diffusion problem can be treated using different implicit techniques (wavelets-Galerkin, spectral techniques, …) preserving stability, accounting for distribution relatively localized as well as periodic boundary conditions in the conformation space.

Finally, a mixed technique performing a multiscale simulation has also been proposed by Jendrejack et al. (2002). This technique combines the computation of the internal configuration evolution via stochastic simulation, with a convective updating of the distribution function in the physical space (using a fixed mesh) via an orthogonal polynomial representation of the microstructure state.

In this work, however, we focus on steady recirculating flows in the physical space, and we have noticed that the use of a polynomial or smooth particle representations of the microstructure configuration induces some difficulties in the imposition of the periodicity condition that the steady and recirculating character of the flow implies. Moreover, the diffusion in short fiber suspensions models can be very small, or some times simply neglected. In this case discretization techniques using particles seem to be more appropriate to solve the FP equation with a dominant advection character. By these reasons, we consider in this paper a statistical technique for solving the FP equation.

Sometimes, industrial or rheometric flows involve recirculating areas (Towsend and Walters (1993)), e.g. contraction flow in extruders; or recirculate themselves (plate-plate, cone-plate and other rheometric flows). In this case, and owing to the steady character of the flow, the resolution of advection equations becomes delicate, because neither initial nor boundary conditions are known. However, accurate solutions in those flows are required if one wants to identify accurately the rheological parameters of a complex fluid by using an inverse technique, or evaluate the accuracy of some assumptions involved in simplified flow models (e.g. closure relations analysis).

2. Steady recirculating flows involving short fibers suspensions

2.1. Imposing the solution periodicity along the closed streamlines.

In order to compute the fiber orientation distribution in this kind of flows, a first strategy consists of computing a finite element solution of the coupled problem (Azaiez et al. (1997)). However, in some cases the finite element solution can exhibit significant deviations from the exact one, as discussed in Chaidron and Chinesta (2001). Another strategy proposed by Chiba et al. (1998), in absence of diffusion effects, lies in the use of a statistical technique. Thus, several fibers with different initial orientations are introduced in a point inside the recirculating flow area. The fiber orientation evolution of each one can be computed by solving the Jeffery equation (13), and then the fiber orientation distribution can be evaluated. The evolution process is stopped when the steady regime is reached. Other alternative possibility lies in looking directly for a periodic solution (Chinesta et al. (2003)) of ψ when its evolution equation is integrated along a closed streamline.

From now on, we consider both a 3D flow and a 3D fiber orientation description. If we use the spherical coordinate system, $\underline{\rho}$ can be written as

$$\underline{\rho} = \begin{pmatrix} \sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta \end{pmatrix} \tag{21}$$

which introduced into Eq. (13) results in the fiber rotation velocity $\dot{\varphi}$ and $\dot{\theta}$.

We are going to summarize the algorithm used to compute this periodic solution described in deep Chinesta et al. (2002) for which only a turn is required. We define a discretisation of the unit sphere surface, i.e. we consider that we have $N \times M$ fibers, each one represented by a couple (i, j), all of them initially located at the point where the solution is searched, and aligned in the following directions:

$$Fiber\, i,j \rightarrow \begin{cases} \varphi_{i,j} = i \times h_{\varphi} \\ \theta_{i,j} = j \times h_{\theta} \end{cases} \tag{22}$$

with $0 \le i < N$, $1 \le j \le M$ and where $h_\varphi = 2\pi / N$ and $h_\theta = \pi /(M+1)$. We can notice that the singularities related to $\theta = 0$ and $\theta = \pi$ are avoided. Szeri and Leal (1994) prefer to consider a Cartesian representation of the sphere in order to avoid those singularities.

Now, we track the movement of each fiber, neglecting diffusion effects that will be introduced later, along the closed streamline. If we denote by $\left(x^0, y^0, z^0\right)$ the coordinates of the initial point (where the steady solution of the fiber orientation distribution is searched), an explicit integration by the method of characteristics results in

$$\begin{cases} x^{n+1} = x^n + \Delta t \times u(x^n, y^n, z^n) \\ y^{n+1} = y^n + \Delta t \times v(x^n, y^n, z^n) \\ z^{n+1} = z^n + \Delta t \times w(x^n, y^n, z^n) \\ \varphi_{i,j}^{n+1} = \varphi_{i,j}^n + \Delta t \times \dot{\varphi}\left(x^n, y^n, z^n, \varphi_{i,j}^n, \theta_{i,j}^n\right) \\ \theta_{i,j}^{n+1} = \theta_{i,j}^n + \Delta t \times \dot{\theta}\left(x^n, y^n, z^n, \varphi_{i,j}^n, \theta_{i,j}^n\right) \\ \qquad \forall i, j \end{cases} \tag{23}$$

Other semi-implicit or fully implicit strategies can be also applied. Effectively, after a complete turn, the departure point is reached. We note by the superscript T the final fiber orientation, i.e. $\left(\varphi_{i,j}^T, \theta_{i,j}^T\right)$ denotes the orientation after a complete turn of the fiber initially aligned on the direction defined by $\left(\varphi_{i,j}, \theta_{i,j}\right)$.

Now, we assume that the steady solution at point $\left(x^0, y^0, z^0\right)$ is defined by the fraction of fibers oriented in each direction $\left(\varphi_{i,j}, \theta_{i,j}\right)$, which will be denoted by α_{ij}. Thus, the fiber orientation distribution could be written in the form

$$\psi\left(x^0, y^0, z^0, \varphi, \theta\right) = \sum_i \sum_j \alpha_{ij} \delta\left(\varphi - \varphi_{i,j}\right) \delta\left(\theta - \theta_{i,j}\right) \tag{24}$$

The normality condition results

$$\int_0^{2\pi}\int_0^{\pi}\psi\left(x^0, y^0, z^0, \varphi, \theta\right)\sin\theta\, d\theta\, d\varphi = \sum_i \sum_j \alpha_{ij}\sin\theta_{i,j} = 1 \tag{25}$$

After a turn, the linearity and homogeneity of the Fokker-Planck equation being taken into account, the resulting fiber distribution can be written in the form

$$\psi^T\left(x^0, y^0, z^0, \varphi, \theta\right) = \sum_i \sum_j \alpha_{ij}\,\delta\left(\varphi - \varphi_{i,j}^T\right)\delta\left(\theta - \theta_{i,j}^T\right) \tag{26}$$

Now, the probability mass concentrated at the directions $\left(\varphi_{i,j}^T, \theta_{i,j}^T\right)$ can be transferred using appropriate weights to preserve the normality condition to the directions $\left(\varphi_{m,n}, \theta_{m,n}\right)$ related to the mesh used in the initial description. Thus, for example, if $\varphi_{m,n} < \varphi_{i,j}^T < \varphi_{m+1,n}$ and $\theta_{m,n} < \theta_{i,j}^T < \theta_{m,n+1}$, then the probability mass α_{ij} could be transferred to the following four directions: $\left(\varphi_{m,n}, \theta_{m,n}\right)$, $\left(\varphi_{m+1,n}, \theta_{m,n}\right)$, $\left(\varphi_{m+1,n}, \theta_{m,n+1}\right)$ and $\left(\varphi_{m,n}, \theta_{m,n+1}\right)$ (see Ammar et al. (2004) for a deep discussion on this projection). In this way, after a turn along the closed trajectory, the fiber orientation distribution (26) can also be written in the form

$$\psi^T\left(x^0, y^0, z^0, \varphi, \theta\right) = \sum_i \sum_j \beta_{ij}\,\delta\left(\varphi - \varphi_{i,j}\right)\delta\left(\theta - \theta_{i,j}\right) \tag{27}$$

where the coefficients β_{ij} depend linearly on the α_{ij}

$$\beta_{ij} = \sum_k \sum_l c_{ijkl} \, \alpha_{kl} \tag{28}$$

where the coefficients c_{ijkl} depend on the considered projection.

Now, if we impose the periodicity of the solution

$$\psi\left(x^0, y^0, z^0, \varphi, \theta\right) = \psi^T\left(x^0, y^0, z^0, \varphi, \theta\right) \tag{29}$$

using a collocation technique, we obtain

$$\alpha_{ij} = \beta_{ij} = \sum_k \sum_l c_{ijkl} \, \alpha_{kl} \tag{30}$$

Eq. (30) and the normality condition (25) allow us to determine the different α_{ij}, and consequently from Eq. (24), the steady fiber orientation distribution at point $\left(x^0, y^0, z^0\right)$.

In Ammar et al. (2004) we have proved that for usual projections, Eq. (30) has one and only one solution. This result is not in conflict with the one stated by Leal and Hinch (1971), which establishes that in absence of diffusion the 3D Fokker-Planck equation, defined in a 3D simple shear flow, has not a steady solution. In our case, the small amount of diffusion - $\Theta(h)$ - induced by the projection step, makes possible the existence of a steady solution as discussed later.

2.2. Taking account of diffusion effects

The previous numerical technique can be extended in the context of a random walk strategy for treating problems involving diffusion effects (Chinesta el al. (2003)). Thus, we can consider F fibers initially aligned in each direction $(\varphi_{i,j},\theta_{i,j})$, with a weight of $1/F$ each one. Now, the movement of each one of these fibers is subjected to three actions:

I. The flow advection that only changes the position of the center of mass of each fiber

$$\begin{cases} x^{n+1} = x^n + \Delta t \times u(x^n, y^n, z^n) \\ y^{n+1} = y^n + \Delta t \times v(x^n, y^n, z^n) \\ z^{n+1} = z^n + \Delta t \times w(x^n, y^n, z^n) \\ \qquad\qquad \forall i, j \end{cases} \tag{31}$$

II. Due to the flow kinematics each fiber rotates according to the Jeffery equation:

$$\begin{cases} \varphi_{i,j,f}^{n+1/2} = \varphi_{i,j,f}^n + \Delta t \times \dot{\varphi}\left(x^n, y^n, z^n, \varphi_{i,j,f}^n, \theta_{i,j,f}^n\right) \\ \theta_{i,j,f}^{n+1/2} = \theta_{i,j,f}^n + \Delta t \times \dot{\theta}\left(x^n, y^n, z^n, \varphi_{i,j,f}^n, \theta_{i,j,f}^n\right) \\ \qquad\qquad \forall i, j, f \end{cases} \tag{32}$$

where the index f refers to the fiber $f \in [1, \cdots, F]$ considered.

III. The diffusion effects induce another angular rotation which results from a random process:

$$\begin{cases} \varphi_{i,j,f}^{n+1} = \varphi_{i,j,f}^{n+1/2} + \beta(0, 2D_r\Delta t) \\ \theta_{i,j,f}^{n+1} = \theta_{i,j,f}^{n+1/2} + \beta(0, 2D_r\Delta t) \\ \qquad \forall i, j, f \end{cases} \tag{33}$$

where $\beta(0, 2D_r\Delta t)$ is a Gaussianly distributed random variable with zero mean and variance $2D_r\Delta t$.

Diffusion effects can be also introduced in a deterministic framework, which allows to reduce significantly the computation time, and whose accuracy and efficiency was proved in a former work (Ammar and Chinesta (2003)). In this way, the particle technique just described was adapted to consider smooth particles instead "Dirac" distributions, which allows computing the fiber distribution derivatives involved in the diffusion term.

3. Numerical example

3.1. Checking the accuracy

Before to analyze steady recirculating flows, that is the main aim of this paper, it seems important to check the accuracy of the proposed strategy by comparing their predictions with some known exact solution. Leal and Hinch (1971) proved that in a simple shear flow, the 3D Fokker-Planck equation for $D_r = 0$ has no solution. In fact there are infinite solutions, and a particular solution can be done as soon as the probability distribution for each Jeffery orbit is fixed (Ammar et al. (2004)). In the Leal and Hinch paper a simple shear flow is assumed, and they derive the steady solution of the fiber orientation distribution by introducing a very small (as small as desired) diffusion term. Now, imposing that the net flux of particles is zero across any Jeffery orbit, the analytic expression of the orientation distribution is obtained (see the Leal and Hinch paper for more details). This behavior is not found in the 2D case, deeply analyzed in Chinesta et al. (2003), where it can be proved that a steady solution exists when the diffusion is neglected.

In order to compute the steady solution in a simple 3D shear flow, when diffusion vanishes, using our strategy, we impose that the searched solution ψ^0 must remains unchanged, that is $\psi(t) = \psi^0, \forall t$, where $\psi(t)$ is computed from ψ^0 using the particle technique described in the previous section. Of course, the computed solution is in excellent agreement with the Leal and Hinch solution, and the convergence can be reached by decreasing time step and increasing number of particles (which implies the reduction of h, and in consequence the numerical diffusion introduced in the projection step). This behavior proves that: (*i*) the numerical diffusion related to the projection step allows to compute, and then the existence, of a steady solution; and (*ii*) the Leal and Hinch solution is reached by reducing diffusion, that is, increasing number of particles.

3.2. Computing the 3D fiber orientation distribution neglecting diffusion effects

The first simulation is concerned with the shear recirculating flow defined by the following velocity field

$$\underline{v} = \begin{pmatrix} -y\sqrt{x^2+y^2} \\ x\sqrt{x^2+y^2} \\ 0 \end{pmatrix} \tag{34}$$

This kinematics has not a rheological interest, but its simplicity allows us to compute exact solutions with the possibility of concluding about the numerical strategies accuracy. In spite of the simplicity of the flow considered, the numerical technique proposed and illustrated in this work can be obviously applied to any steady recirculating flow.

In this example the diffusion effects are neglected $(D_r = 0)$ and the fibers have different aspect ratios: $k = 0.4, 0.5, 0.65$ and 0.85 in Figure 1, respectively. These figures depict the fiber orientation distribution at point $(x^0, y^0) = (1,0)$. We can notice that the highest orientation probability concentrates around the plane xy $(\theta \approx \pi/2)$ and the angles $\varphi \approx \pi/2$ and $\varphi \approx 3\pi/2$. This situation corresponds to a fiber orientation concentrating around the flow direction at the considered point.

We can also notice in these figures that the intensity of the fibers concentration around the flow direction increases with the fiber aspect ratio. This result is in agreement with the theoretical result given in Poitou et al. (2000) for planar orientation problems. Moreover, we can verify the following symmetry condition:

$$\psi(\varphi, \theta) = \psi(\varphi + \pi, \pi - \theta) \tag{35}$$

3.3. Taking account of diffusion effects

Figure 2 depicts the fiber orientation distribution for fibers with *k*=0.85 and two different diffusion coefficients: $D_r = 0$ and $D_r = 0.1$. The numerical solution involving diffusion effects has been computed by means of the particle stochastic technique described in section 2.2.

3.4. Evaluating the accuracy of the closure relations in a planar orientation problem solved by using the Fokker-Planck equation

In this case we consider the steady recirculating flow defined by Eq. (34) and a planar orientation state, i.e. the fibers are assumed on the plane *xy*, because the exact solutions of the Fokker-Planck equation can be easily calculated from the flow symmetry (see Chinesta et al. (2003) for more details). In this case, an excellent accuracy of the particle technique used to compute numerically the fiber orientation distribution can be noticed. Figure 3 shows the fiber orientation distribution at the point $(x, y) = (0,1)$ for fibers with different aspect ratios when the diffusion coefficient vanishes, i.e. $D_r = 0$.

Now, the steady solution of the fiber orientation distribution being known, the fourth and second order orientation tensors can be computed using Eqs. (4) and (6). These tensors will be considered as the reference solutions and they will be denoted by $\underline{\underline{\underline{\underline{a}}}}^{ref}$ and $\underline{\underline{a}}^{ref}$ respectively. Moreover, from the expression of the second order orientation tensor we can obtain also the expressions of the fourth order orientation tensor using different closure relations: quadratic closure $\underline{\underline{\underline{\underline{a}}}}^{quad}$, linear closure $\underline{\underline{\underline{\underline{a}}}}^{lin}$, hybrid closure $\underline{\underline{\underline{\underline{a}}}}^{hyb}$ and the natural closure $\underline{\underline{\underline{\underline{a}}}}^{nat}$. Figure 4 depicts the error in the evaluation of the different components of the fourth order orientation tensor for the different closure relations and fiber aspect ratios. This error is defined as the positive relative difference between the reference value of the considered component and the one obtained using each closure relation. Also in Figure 4, picture (d), a global error, defined by Eq. (36) is depicted.

$$Error = \frac{\sqrt{\sum_i \sum_j \sum_k \sum_l \left(a_{ijkl}^{ref} - a_{ijkl}^{clos.rel.}\right)^2}}{\sqrt{\sum_i \sum_j \sum_k \sum_l \left(a_{ijkl}^{ref}\right)^2}} \qquad (36)$$

Now, we are going to introduce the diffusion effects through different values of the parameter D_r for fibers with $k = 0.6$ and $k=0.95$. Figure 5 shows the fiber orientation distributions for different diffusion coefficients.

Figure 6 depicts the error in norm associated to each closure relation. We can conclude from these results that the lowest value of *k* produces rather small variation of the fiber orientation distribution (compare Figures 5(a) and 5(b)), which induces a very low accuracy of the quadratic closure relation. So, we can expect that for low values of the fiber aspect ratio or for high diffusion coefficients the quadratic closure relation will be the worst one. Although the quadratic closure relation becomes rather accurate as the value of *k* is further increased, it remains to be the worst among the closure relations considered in this numerical example for $k \leq 0.95$.

3.5. Evaluating the accuracy of the closure relations in a planar orientation by solving the equation governing the evolution of the second order orientation tensor

If the solution of Eq. (19), for the kinematics defined in equation (34), is computed at point (0,1) using the closure relations given by equations (7), (8), (9) and (10) and the numerical algorithms proposed in Chinesta and Chaidron (2001) and Chaidron and Chinesta (2002), the resulting second order orientation tensors for both k=0.6 and k=0.95 are shown in Figure 7.

Figure 8 depicts the error using the norm defined by equation (37) when the different numerical solutions shown in Figure 7 are compared with the exact one, that is very close to the one computed by using the stochastic simulation presented in previous section.

$$Error = \frac{\sqrt{\sum_i \sum_j \left(a_{ij}^{ref} - a_{ij}^{num.}\right)^2}}{\sqrt{\sum_i \sum_j \left(a_{ij}^{ref}\right)^2}} \tag{37}$$

These results introduce some new and unexpected evidences. From figure 8 we can conclude that when the quadratic closure relation is introduced in the equation governing the evolution of the second order orientation tensor, the error associated with the computed steady solution decreases as the diffusion coefficient increases, despite the fact that the accuracy of the quadratic closure relation has, as proved in figure 6 the inverse tendency. Moreover, for a given diffusion coefficient, the error associated with the use of the quadratic closure relation seems to be slightly higher for the most elongated fibers (k=0.95).

4. Conclusions

A new numerical strategy to compute steady solutions of the fiber orientation distribution in steady recirculating flows involving short fiber suspensions have been applied to compute 2D and 3D steady solutions of the Fokker-Planck equation. This technique uses some of the ideas of the particle method, in combination with the periodicity condition imposed by the steady and recirculating character of the flow. The highly accurate solutions can be used in rheological applications as well as to analyse some simplified models obtained using closure relations in the orientation averages.

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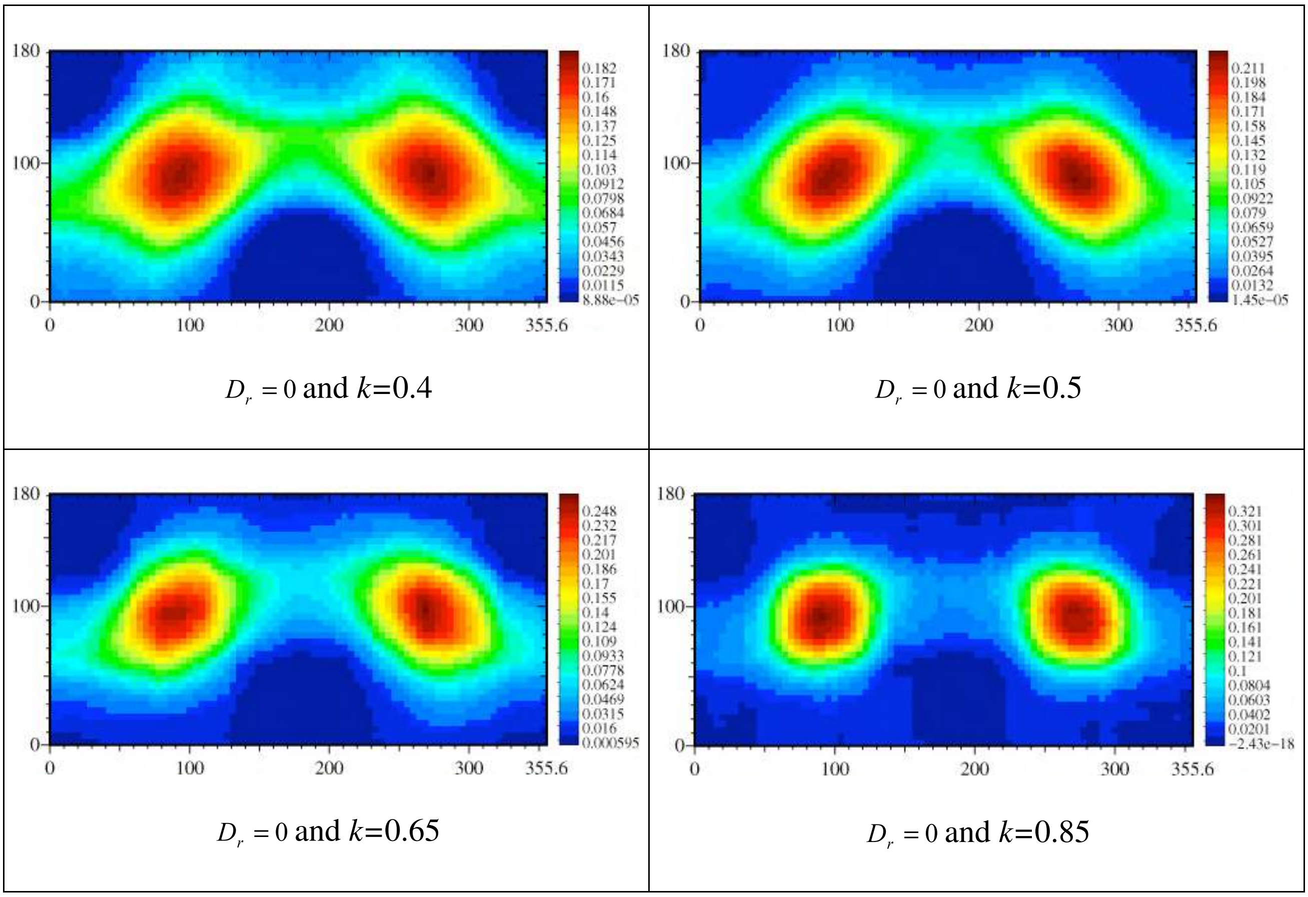


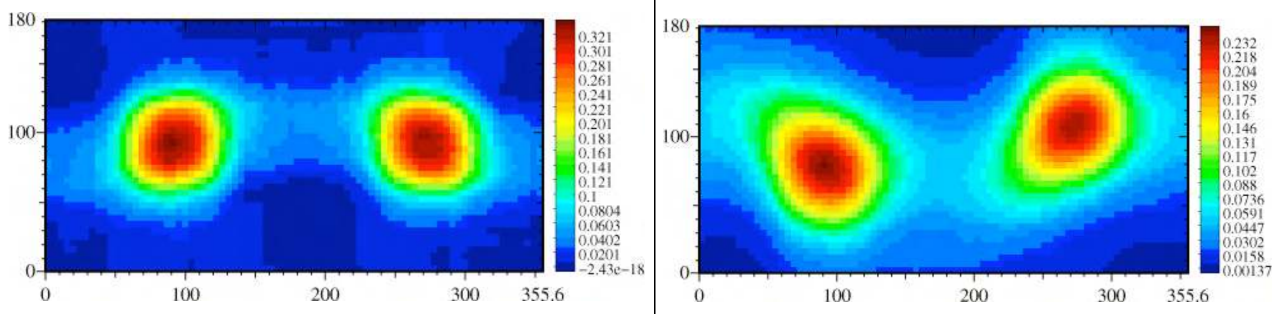
$D_r = 0$ and k=0.4

$D_r = 0$ and k=0.5

$D_r = 0$ and k=0.65

$D_r = 0$ and k=0.85

Figure 1. Fiber orientation distribution at point (1,0)



$D_r = 0$ and k=0.85

$D_r = 0.1$ and k=0.85

Figure 2. Fiber orientation distribution at point (1,0)

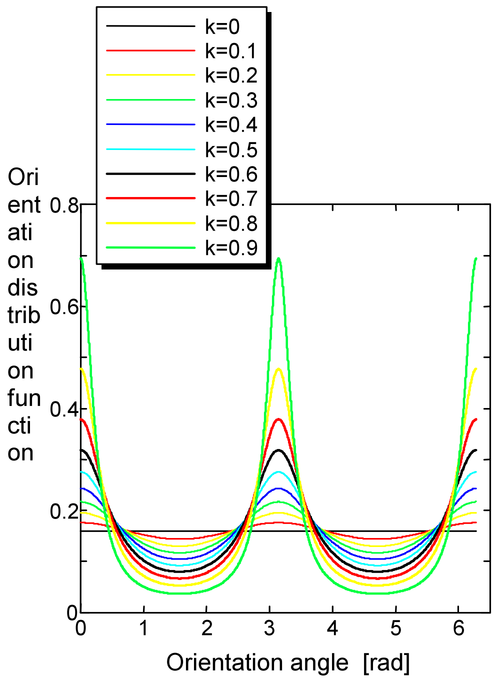


Figure 3. Fiber orientation distribution for fibers with different aspect ratios and $D_r = 0$.

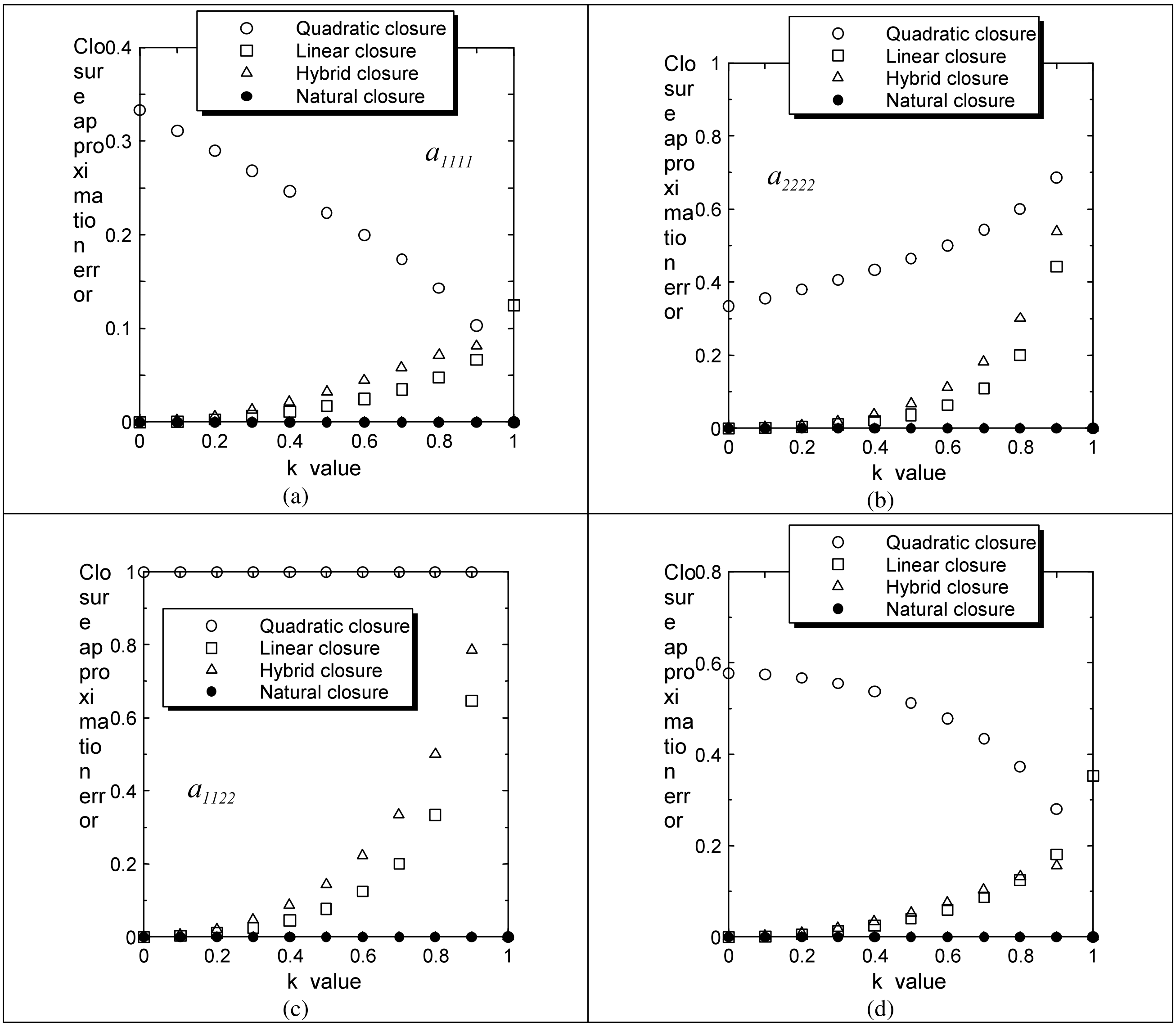


Figure 4. Closure approximation errors: (a) a_{1111} ; (b) a_{2222} ; (c) a_{1122} and (d) global error, for $D_r = 0$

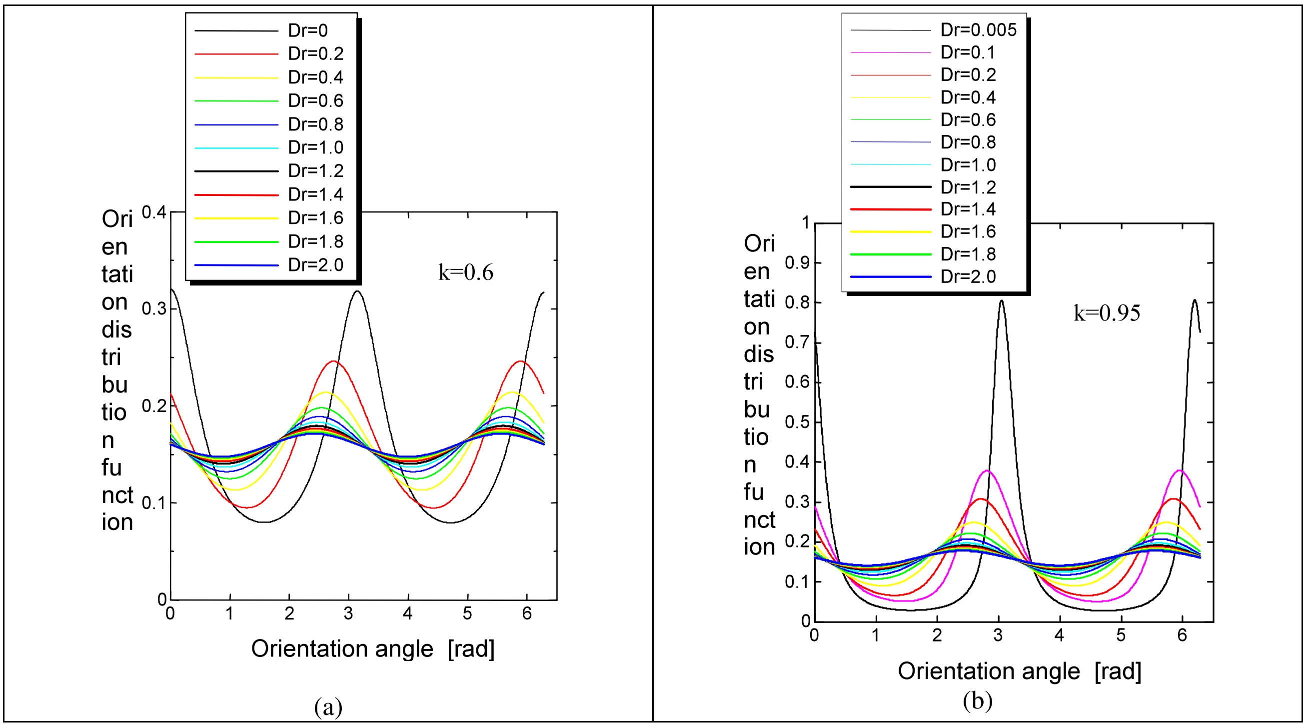


Figure 5. Orientation distribution for different diffusion coefficients; (a) $k = 0.6$; (b) $k = 0.95$.

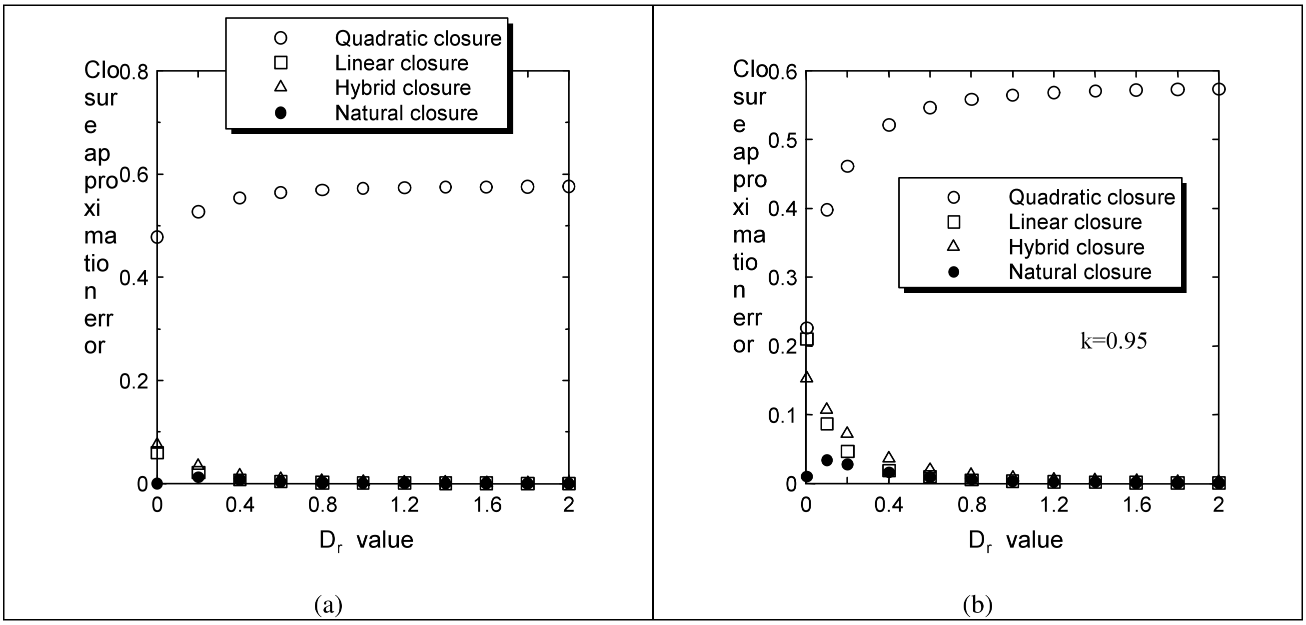


Figure 6. Error in norm of the fourth order orientation tensor for different closure approximations; (a) *k*=0.6; (b) *k*=0.95.

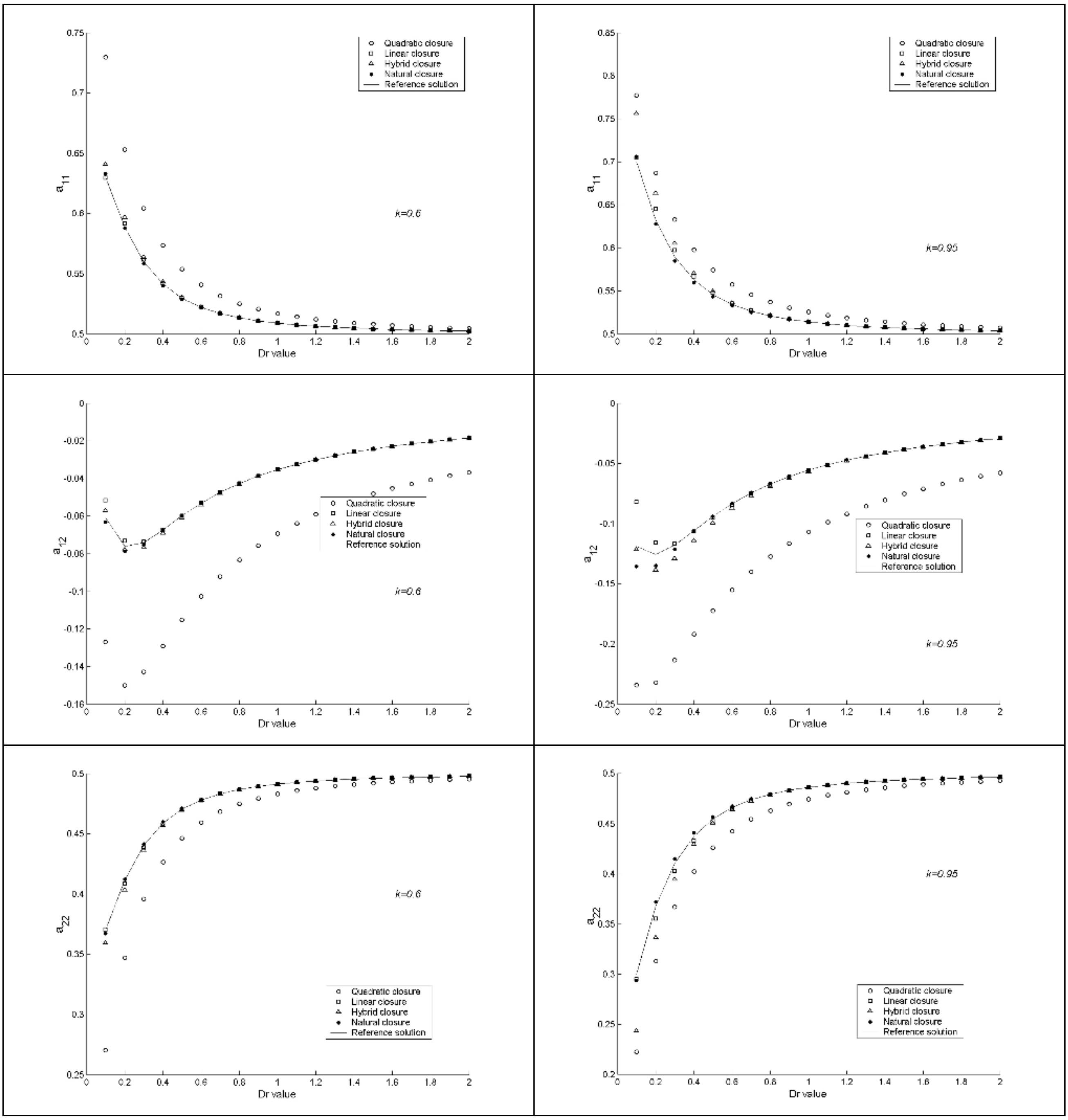


Figure 7. Second order orientation tensor computed by solving the equation governing its evolution and different closure relations for *k*=0.6 and *k*=0.95.

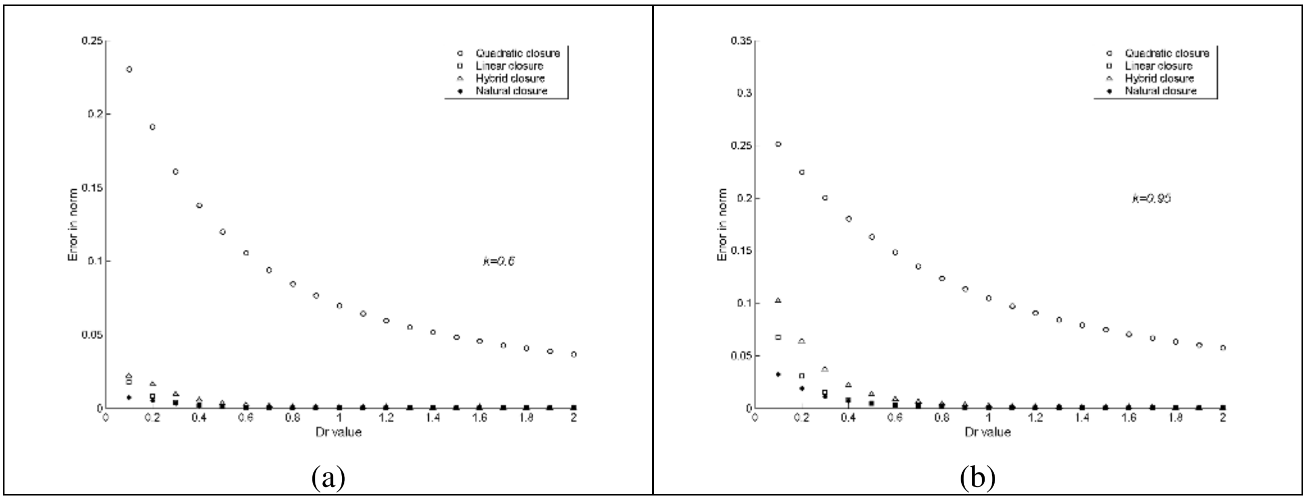


Figure 8. Error in norm of the second order orientation tensor for different closure approximations; (a) *k*=0.6; (b) *k*=0.95.