Direct Simulation of the motion of rigid fibers in viscous fluid

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Introduction (1)

- Injection of thermoplastic

- Injection of fiber-reinforced polymer
  - use the same process as classical thermoplastic
  - complex composite products with improved mechanical properties
  - mechanical properties depend on fiber orientation
Introduction (2)

- Fiber orientation in flow motion

Shear flow

Elongational flow
Background & Motivations

- **Macroscopic modelling**
  - Dilute suspension → **Jeffery’s equation** [Jeffery 1922]
    Newtonian fluid – slender body theory
    \[
    \frac{dp}{dt} = \Omega p + \lambda \left( \hat{\varepsilon} p - \left( \hat{\varepsilon} : [p \otimes p] \right) p \right)
    \]
    \(f(\beta = \text{aspect ratio})\)
  - Semi-concentrated suspension → **Folgar and Tucker's equation** [Folgar 1984]
    Population of fiber:
    \[
    a_2 = \int \psi(p) p \otimes p \, dp = \frac{1}{N} \sum_{k=1}^{N} p_k \otimes p_k
    \]
    \[
    \frac{D a_2}{Dt} = \Omega a_2 - a_2 \Omega + \lambda \left( \dot{\varepsilon} a_2 + a_2 \dot{\varepsilon} - 2 \hat{\varepsilon} : [a_2] \right) + 2 C I_{d} \dot{\varepsilon} \left( I_d - 3a_2 \right)
    \]

- **Closure approximation, Ci**?
Objectives: Micromechanic modelling approach

Micromechanic approach → Direct simulation

Simulate directly the motion of a dense population of fiber in a REV

Particle interactions are given by a fluid-structure coupling

Gives macroscopic informations on tensor $a_2$ and rheological properties
Numerical Procedure

1. Computation of velocity field with Rem3D
   finite element method for the Stokes equation with multi-domain approach
   (no inertia, no gravity)

2. Update particle position
   particle method

3. Computation of characteristic functions associated to each domain
   voxelisation method

- Numerical approach similar to Glowinski & Joseph’s modelling [Glowinski 1999]
  (Fictitious domain method for particulate flows)
Computation of Velocity field (1)

1) Characteristic function

\[ l_{\Omega_j}(x, t) = \begin{cases} 
1 & x \in \Omega_j \\
0 & x \notin \Omega_j 
\end{cases} \]

\( j = \text{fluid or solid (fibers)} \)

\( \Omega = \Omega_1 \cup \Omega_s \)

\( \Omega_s = \bigcup_{i=1}^{n} \Omega_{s_i} \)

2) Velocity field

\[ \nabla \cdot \sigma = 0 \]

\[ \int_{\Omega} 2 \eta \varepsilon(u) : \varepsilon(v) \, d\Omega + \int_{\Omega_s} r \varepsilon(u) : \varepsilon(v) \, d\Omega \]

\[ -\int_{\Omega} p \nabla \cdot v \, d\Omega = 0 \]

\[ \nabla \cdot u = 0 \]

\[ -\int_{\Omega} q \nabla \cdot u \, d\Omega = 0 \]

Penalization \( \sim 10^3 \eta \)

\( \varepsilon(u) = 0 \)

Shear rate
Update fiber position and orientation (2)

Particle method

Rigid motion

\[ X_i(t + \Delta t) = X_i + V_{X_i} \Delta t \]

Langrangian updating of the position of the two extremities of each fiber

Advantages

- Perfect rigid motion of each fiber
- Conservation of the length
- No numerical diffusion
Computation of Characteristic Function (3)

Voxelisation method

Cavity mesh

Voxelisation

Add fiber mesh

switch on pixels

Get values
Single Fiber Motion in shear flow

Shear flow, Periodic Cell
aspect ratio $\beta=10$

Find Jeffery's orbit for a shear flow

$$T = \frac{2\pi}{\gamma} \left( \beta + \frac{1}{\beta} \right)$$
Hydrodynamical Interactions

It is not necessary to have an explicit form (as in [Yamane 1994], [Fan 1998])

- drag forces
- lubrication forces (short range interactions)

→ An example of hydrodynamical interactions

The central particle moves due to hydrodynamical interactions

Spherical particles in Couette Flow
Fiber – Wall interaction (1)

- Fiber initially perpendicular to the wall
Fiber – Wall interaction (2)

- Fiber initially parallel to the wall

Fiber migration and alignment near the wall
Statistical studies - 3D example -

- Aspect ratio $\beta = 12$, concentrated suspension
- Shear flow

Get $a_2$ and $a_4$ on time

$$a_2 = \frac{1}{60} \sum_{k=1}^{60} p_k \otimes p_k$$
Statistical studies (1) - Evolution of $a_2$ -

- Effect of the concentration

- Effect of the aspect ratio

- Sensibility of simulations to the concentration and the aspect ratio
  - Interaction
  - Closure approximation
Statistical studies (2) - Closure approximation -

- Test of Closure approximation
  - \( a_{4\_model} = \text{function} (a_{2\_measured}) \)
  - Comparison \( a_{4\_measured} & a_{4\_model} \)
- 60 fibers in shear flow, \( \beta = 12 \)

Quadratic closure : correct evolution in shear flow
Orthotropic closure : more accurate
- **Evolution of the viscosity in shear flow**

\[
\eta_{\text{apparent}} = \frac{\sigma_{\text{imposed}}}{\dot{\gamma}_{\text{apparent REV}}}
\]

- **Evolution of the Cauchy stress tensor**

\[
\sigma = \sigma_{\text{fluid}} + \sigma_{\text{fibers}}
\]

For Newtonian fluids:

\[
\sigma_{\text{fibers}} = 2\eta_f N_p \varepsilon(u) : a_4
\]
Conclusions

- We have developed a micromechanical modelling approach
  - Simulate directly the motion of a dense population of fibers
  - Model the exact particle interaction by using a multi-domain approach

- Very encouraging results for the
  - Study of macroscopic parameters as :
    - interaction between particles
    - closure approximations
  - Study of the suspension’s rheology : η and stress tensor

- Next Step
  - Multiple populations of fibers
  - Flexibility
  - Viscoelasticity