Multi-scale modelling of short fibre suspensions

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1 Introduction

In this manuscript we present the derivation of a micro-macro rheological model for a system of short non-Brownian, non sedimenting short fibres in the dilute regime. A micro-macro or multi-scale model is a model that explicitly accounts for two (at least) different time and/or length scales: First a macroscopic scale (here the level of continuum mechanics) which is e.g. the level of interest for the engineer and second a microscopic scale where phenomena responsible of the macroscopic properties occur. The model is derived using a few scale separation assumptions and a very simple micro mechanical model. A cornerstone of this approach is the link between the two different levels of description: How are the variables belonging to different levels of description coupled with each other.

2 Fibre model

Let us consider a Newtonian fluid with a viscosity η containing a small amount of short fibres with a density identical to that of the fluid. Furthermore, we will consider the fibres to be large enough that they are not affected by Brownian motion. At the macroscopic level we will consider that a representative element of fluid may potentially contain many fibres but that these would still be diluted enough not to influence each other's motion. At each material point we therefore have an ensemble of independent fibres. Then we choose to model the fibres using two beads connected by a rigid rod. These different levels are depicted in Fig. 1. The fibres interact with the surrounding fluid only through the beads which are friction points between the fluid and the fibre. Let us call $2L$ the fibre length and $\mathbf{p}$ the unit vector along the fibre axis.

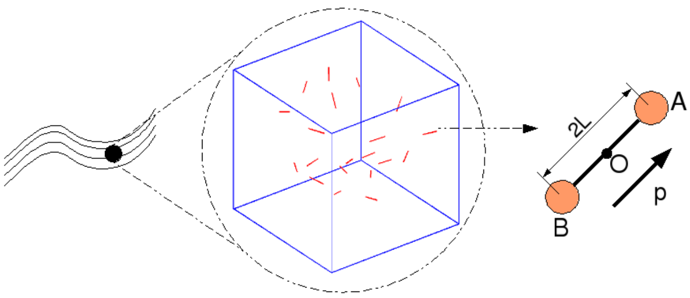

Figure 1: Illustration of the three different scales involved. From left to right: the continuum scale, the representative volume element containing many fibres, and a single fibre.

Defining $\mathbf{v}_{fO}$ as the fluid velocity at the fibre midpoint and $(\nabla\mathbf{v})_{loc}$ as the local velocity gradient of the fibre, we can write the fluid velocity at the beads as:

$$\mathbf{v}_{fA} = \mathbf{v}_{fO} + L(\nabla\mathbf{v})_{\text{loc}} \cdot \mathbf{p} \,, \quad (1)$$

$$\mathbf{v}_{fB} = \mathbf{v}_{fO} - L(\nabla\mathbf{v})_{\text{loc}} \cdot \mathbf{p} \,. \quad (2)$$

The beads velocity simply reads:

$$\mathbf{v}_A = \mathbf{v}_O + L\dot{\mathbf{p}} \, , \quad (3)$$
$$\mathbf{v}_B = \mathbf{v}_O - L\dot{\mathbf{p}} \, , \quad (4)$$

where $\mathbf{v}_O$ is the velocity of the fibre midpoint.

We make the additional assumption that the local (microscopic) velocity gradient $(\nabla\mathbf{v})_{loc}$ is equal to the macroscopic velocity gradient $\nabla\mathbf{v}$. This hypothesis which might seem reasonable is actually not obvious at all since it explicitly couples the two different levels of description. The macroscopic velocity is defined from the average over the representative volume of fluid which is much larger than the fibre. The macroscopic velocity gradient is in turn defined from the spatial variation of the macroscopic velocity. This hypothesis also implies that the movement of a single fibre does not perturb its local velocity field. Some more advanced microscopic model can actually take into account the hydrodynamic interactions between beads A and B or between fibres.

Finally, as $\mathbf{p}$ is a unit vector ($1 = \|\mathbf{p}\|^2 = \mathbf{p}\cdot\mathbf{p}$), we have $\frac{\partial \mathbf{p}\cdot\mathbf{p}}{\partial t} = \dot{\mathbf{p}}\cdot\mathbf{p} + \mathbf{p}\cdot\dot{\mathbf{p}} = \mathbf{p}\cdot\dot{\mathbf{p}} = 0$. This very simple property will be used later.

In order to compute the evolution of the fibre configuration (its $\mathbf{p}$ vector) we make the assumption that the fibres are non inertial objects (their mass is negligible). For such objects the sum of the external forces as well as the sum of their moments should be zero. The only forces we will consider here are viscous forces between the beads and the fluid.

Using a viscous friction model, we write the forces acting at A and B as:

$$\mathbf{F}_A = \xi \left((\mathbf{v}_{fO} - \mathbf{v}_O) + L(\nabla\mathbf{v}\cdot\mathbf{p} - \dot{\mathbf{p}}) \right) \, , \quad (5)$$
$$\mathbf{F}_B = \xi \left((\mathbf{v}_{fO} - \mathbf{v}_O) - L(\nabla\mathbf{v}\cdot\mathbf{p} - \dot{\mathbf{p}}) \right) \, . \quad (6)$$

From the equilibrium of forces $\mathbf{F}_A + \mathbf{F}_B = 0$ we deduce that

$$\mathbf{v}_O = \mathbf{v}_{fO} \, . \quad (7)$$

The fibres flow with the same velocity as the fluid, in other words fibres associated with a material point of the fluid will remain associated with the same material point. This would not be the case if external forces like gravity of electromagnetic forces were present.

The sum of the force moments with respect to O writes

$$L\mathbf{p}\times\mathbf{F}_A - L\mathbf{p}\times\mathbf{F}_B = 2L\mathbf{p}\times\xi L(\nabla\mathbf{v}\cdot\mathbf{p} - \dot{\mathbf{p}}) = 0 \, .$$

Which simply states that the forces $\mathbf{F}_A$ and $\mathbf{F}_B$ are aligned along the fibre. We can rewrite Eq. (5) as:

$$\mathbf{F}_A = \alpha\mathbf{p} = \xi L(\nabla\mathbf{v}\cdot\mathbf{p} - \dot{\mathbf{p}}) \, . \quad (8)$$

For a given fibre orientation $\mathbf{p}$ and a given velocity gradient $\nabla\mathbf{v}$ Eq.(8) is a linear system of three equations where the unknowns are α and $\dot{\mathbf{p}}$. Indeed, since $\mathbf{p}$ is a unit vector $\dot{\mathbf{p}}$ is a vector orthogonal to $\mathbf{p}$ and only two of its components are independent. We first obtain α by taking the scalar product of Eq.(8) with $\mathbf{p}$ (remember that $\mathbf{p}\cdot\dot{\mathbf{p}} = 0$):

$$\alpha = \xi L(\mathbf{p}\cdot\nabla\mathbf{v}\cdot\mathbf{p}) \, , \quad (9)$$

which is half the tension inside the rod connecting A and B. Substituting the value of α into Eq.(8), yields the following equation for the evolution of $\mathbf{p}$:

$$\dot{\mathbf{p}} = \nabla\mathbf{v}\cdot\mathbf{p} - (\mathbf{p}\cdot\nabla\mathbf{v}\cdot\mathbf{p})\mathbf{p} \, . \quad (10)$$

For a given set of fibres with known initial positions and orientations and a given flow field, we can now compute the evolution of these positions and orientations as well as the tension inside each fibre. The only missing block is the answer to the following question: do the fibres generate additional stresses inside the fluid. These additional stresses would of course modify the flow field through the macroscopic balance equations.

3 Extra stress tensor

In this section we provide a heuristic derivation of the fibres contribution to the Cauchy stress tensor. For the sake of simplicity, we will use both the indicial and vectorial notations The elements of the Cauchy stress tensor σ_{ij} represent the force in the direction j that would be be exerted on a unit surface with a normal vector oriented along direction i. We can write σ as:

$$\sigma_{ij} = -p\delta_{ij} + 2\eta D_{ij} + \tau_{ij} \, , \tag{11}$$

where p is the pressure, η is the fluid viscosity, $\mathbf{D} = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^{\mathrm{T}}\right)$ and τ_{ij} an additional contribution from the fibres. Since the fibres do not interact with each other, τ_{ij} can be obtained from the sum of individual contributions from each fibre.

Let us consider a single fibre in the representative volume element, a cube with edges of length l. In this elementary volume let us consider a plane with its normal oriented along i. On average, the force per unit area on the plane is equal to:

$$\tau_{ij} = \frac{1}{l^2} 2\alpha p_j P_i(\text{intersection}) \, ,$$

where $2\alpha p_j$ is the force inside the rod and $P_i(\text{intersection})$ is the probability of the plane with orientation i to cut the fibre. It is straightforward to notice that $P_i(\text{intersection}) = \frac{Lp_i}{l}$, yielding:

$$\tau_{ij} = \frac{L}{l^3} 2\alpha p_i p_j \, .$$

Accounting for all the fibres and substituting the value of α gives the final expression for the stress tensor:

$$\tau_{ij} = \nu(2\xi L^2) \left\langle p_i p_j p_k p_l \right\rangle \nabla_k v_l \, . \tag{12}$$

In the previous expression, ν is the fibre number density and $\langle\cdot\rangle$ represents the average over all fibres in the representative volume element. Because the velocity gradient is the same for all fibres in a given representative volume element, it has been factorised out of the $\langle\cdot\rangle$ average. The somewhat arbitrary length l that was introduced in order to compute the stress tensor has disappeared in the averaging process.

4 First steps towards a macroscopic model

We have shown that the macroscopic stress tensor is a function of $\langle\mathbf{pppp}\rangle$ which is a fourth order moment of the fibres orientational distribution $\Psi(t,\mathbf{p})$. Computing it as an average of the orientation of a representative ensemble of fibres corresponds to a Monte-Carlo like approach. This class of methods is known to be computationally expensive and to generate noisy results, unless many fibres are simulated. In order to circumvent these drawbacks, one might want to directly compute the evolution of the moments of the distribution $\Psi(t,\mathbf{p})$. Let us define the second order tensor $\mathbf{a}(t)$ as

$$\mathbf{a}(t) = \langle\mathbf{pp}\rangle = \int_{\mathbf{p}} \mathbf{pp}\Psi(t,\mathbf{p})\mathrm{d}\mathbf{p} \, . \tag{13}$$

Substituting (10) into (13) we get the following evolution equation for $\mathbf{a}$:

$$\begin{aligned} \frac{D}{Dt}\mathbf{a} &= \langle\dot{\mathbf{p}}\mathbf{p}\rangle + \langle\mathbf{p}\dot{\mathbf{p}}\rangle \\ &= \nabla\mathbf{v}\cdot\mathbf{a} + \mathbf{a}\cdot(\nabla\mathbf{v})^{\mathrm{T}} - 2\langle\mathbf{pppp}\rangle : \mathbf{D} \, . \end{aligned} \tag{14}$$

In the previous expression, we recognize the upper convected derivative of $\mathbf{a}$, followed by a term involving $\langle\mathbf{pppp}\rangle$. This term is needed to keep the trace of $\mathbf{a}$ at the constant value 1, but it cannot be expressed in terms of $\mathbf{a}$. We are facing what is called a closure problem, where the evolution equation of a second order moment of $\Psi(t,\mathbf{p})$ (i.e. $\mathbf{a}$) involves a fourth order moment $\langle\mathbf{pppp}\rangle$. It is left as an exercise to check that the evolution equation of $\langle\mathbf{pppp}\rangle$ will involve even higher moments. In order to break this vicious circle, one has to resort to closure approximations where e.g. $\langle \mathbf{pppp} \rangle$ is approximated as a function of $\langle \mathbf{pp} \rangle$. The other option would be to compute directly the evolution of $\Psi(t, \mathbf{p})$ at each point of the flow domain. This last approach which is by far the most elegant can nevertheless be computationally very expensive in the absence of efficient and optimized numerical methods.

Two simple closures are:

$$\begin{aligned}
&\text{linear closure} \\
&\langle p_i p_j p_k p_l \rangle \approx \frac{-1}{35}\left(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) \\
&\qquad + \frac{1}{7}\left(a_{ij}\delta_{kl} + a_{ik}\delta_{jl} + a_{il}\delta_{jk} + a_{kl}\delta_{ij} + a_{jl}\delta_{ik} + a_{jk}\delta_{il}\right) , \qquad (15)\\
&\text{quadratic closure} \\
&\langle p_i p_j p_k p_l \rangle \approx a_{ij}a_{kl} . \qquad (16)
\end{aligned}$$

The development of good closure approximation is a research theme by itself, and some advanced models may even interpolate between different closures.

5 Suggested exercises

1. Write a small program (e.g. using Matlab) that would, for a given velocity gradient, compute the time evolution of the orientation of a set fibres that have an initially isotropic distribution. You can use the `rand_sph` program provided below to generate the initial orientations.

2. Write a program that computes the extra stress tensor τ as a function of time from the velocity gradient and the fibre orientations computed previously.

3. Write a program to compute the time evolution of the second order orientation tensor $\mathbf{a}$ using Eq.(14) and a closure approximation of your choice.

4. Evaluate the quality of the chosen closure approximation when the fibres are isotropically distributed and when all the fibres are aligned in the same direction.

```
function result = rand_sph(N)
%generates N random unit vectors,
% uniformly distributed on the unit sphere
  NN = round(N*6/(pi)+20);
  pts = 2*rand([NN 3])-1;
  l = sqrt(pts(:,1).^2 +  pts(:,2).^2 +   pts(:,3).^2);
  p = pts(l<=1,:);
  clear pts
  l = l(l<=1);
  if(size(p,1)<N)
    p = p./(l*[1 1 1]);
    p = [p ;rand_sph(N-size(p,1))];
  else
    p = p(1:N,:)./(l(1:N)*[1 1 1]);
  end
  result = p;
end
```

6 Suggested references

- Bird RB, Curtiss CF, Armstrong RC, Hassager O. *Dynamics of polymeric liquids Vol. 2 Kinetic Theory*. NY Wiley, 1987.

- Advani SG, Tucker CL. The use of tensors to describe and predict fiber orientation in short fiber composites. *Journal of Rheology*,31(8):751-784, 1987.
- Dinh SM, Armstrong RC. A theological equation of state for semiconcentrated fiber suspensions, *Journal of Rheology*, 28(3):207-227, 1984.