NEW ENTROPY ESTIMATES FOR OLDROYD-B AND RELATED MODELS∗

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Abstract. This short note presents the derivation of a new a priori estimate for the Oldroyd-B model. Such an estimate may provide useful information when investigating the long-time behaviour of macro-macro models, and the stability of numerical schemes. We show how this estimate can be used as a guideline to derive new estimates for other macroscopic models, like the FENE-P model.

Key words. a priori estimate, Oldroyd-B, FENE-P, entropy, conformation tensor.

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1. Introduction

We consider the Oldroyd-B model:

\[ \text{Re} \left( \frac{\partial u}{\partial t} + u \cdot \nabla u \right) = (1 - \varepsilon) \Delta u - \nabla p + \text{div} \ \tau, \]  \hspace{1cm} \text{(1.1)}

\[ \text{div} \ (u) = 0, \]  \hspace{1cm} \text{(1.2)}

\[ \frac{\partial \tau}{\partial t} + u \cdot \nabla \tau = \nabla u \tau + \tau (\nabla u)^T - \frac{1}{\text{We}} \tau + \frac{\varepsilon}{\text{We}} (\nabla u + (\nabla u)^T), \]  \hspace{1cm} \text{(1.3)}

where the Reynolds number \( \text{Re} > 0 \), the Weissenberg number \( \text{We} > 0 \) and \( \varepsilon \in (0, 1) \) are some non-dimensional numbers. We recall that the Reynolds number expresses the ratio of inertial forces to viscous forces in the fluid. The Weissenberg number is the ratio of the characteristic time of the microstructure in the complex fluid (typically the polymer chains for dilute polymer solutions) to the characteristic time of the fluid. The non-dimensional number \( \varepsilon \) is the ratio of the viscosity due to the microstructures to the total viscosity. We suppose that the space variable \( x \) lives in a bounded domain \( D \) of \( \mathbb{R}^d \). This system is supplied with initial conditions on the velocity \( u \) and on the stress tensor \( \tau \). For simplicity, we assume no-slip boundary conditions on the velocity \( u \):

\[ u = 0 \text{ on } \partial D. \]  \hspace{1cm} \text{(1.4)}

We suppose that the initial data and the geometry are such that there exists a unique regular solution to (1.1)–(1.3) and our aim is to derive some a priori estimates on this solution.

Let us introduce the so-called conformation tensor \( A = \frac{\text{We}}{\varepsilon} \tau + \text{Id} \). The partial differential equation (PDE) on \( \tau \) translates into the following PDE on \( A \):

\[ \frac{\partial A}{\partial t} + u \cdot \nabla A = \nabla u A + A (\nabla u)^T - \frac{1}{\text{We}} A + \frac{1}{\text{We}} \text{Id}. \]  \hspace{1cm} \text{(1.5)}

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One can check that if
\[ A(t=0) = \frac{We}{\varepsilon} \tau(t=0) + \text{Id} \]
is a positive definite symmetric matrix, then this property is propagated forward in time by (1.5) (and, in particular, \( \tau \) is symmetric). Assuming uniqueness of solution, this can be proven for example by using the probabilistic interpretation of \( A \) as a covariance matrix, as explained in Section 3. We will assume throughout this note that (1.6) is satisfied. Concerning the importance of positive-definiteness of \( A \), we refer for example to [13, Section 9.8.10] and also to the recent work [6, 7]. In [18], a formulation based on the deformation tensor is used to study the Oldroyd-B model, and in [19], a derivation of micro-macro models based on a least action principle (formal minimization of an appropriate energy) is proposed, and a global existence result near equilibrium is proved. For other existence results for the Oldroyd-B model and related models, we refer to [1, 2, 8, 9, 10, 16, 20, 21, 22, 26, 27, 29, 30]. For a review of the mathematical issues related to complex fluids, we refer to [14, 17].

In Section 2, we recall how the classical a priori estimate for the Oldroyd-B model is derived. Next we show how it can be used to derive some bounds on the stress tensor, provided the initial condition satisfies \( \det A(t=0) > 1 \). In Section 3, we establish a new estimate, which comes from an entropy estimate on the micro-macro model associated with the Oldroyd-B model (see [11]). This estimate provides bounds on \((u, \tau)\) without any assumption on \( \tau(t=0) \) (apart from (1.6)). This new estimate could be useful to study the longtime behavior of some macro-macro models, or to analyze the stability of some numerical schemes. Current research is directed towards clarifying this [5].

2. The classical estimate

Let us first introduce the kinetic energy:

\[ E(t) = \frac{1}{2} \int_D |u|^2. \quad (2.1) \]

We easily obtain from (1.1)–(1.2):

\[ \text{Re} \frac{dE}{dt} = -(1 - \varepsilon) \int_D |\nabla u|^2 - \int_D \tau : \nabla u, \quad (2.2) \]

where for two matrices \( A \) and \( B \), we denote \( A : B = A_{i,j}B_{i,j} = \text{tr}(A^T B) \). On the other hand, taking the trace of the PDE (1.3) on \( \tau \) and integrating over \( D \), we get:

\[ \frac{d}{dt} \int_D \text{tr} \tau = 2 \int_D \nabla u : \tau - \frac{1}{We} \int_D \text{tr} \tau. \]

We thus obtain the following estimate:

\[ \frac{d}{dt} \left( \text{Re} \frac{1}{2} \int_D |u|^2 + \frac{1}{2} \int_D \text{tr} \tau \right) + (1 - \varepsilon) \int_D |\nabla u|^2 + \frac{1}{2We} \int_D \text{tr} \tau = 0. \quad (2.3) \]

**Remark 2.1.** In terms of \( A \), the energy estimate (2.3) writes:

\[ \frac{d}{dt} \left( \text{Re} \frac{1}{2} \int_D |u|^2 + \frac{\varepsilon}{2We} \int_D \text{tr} A \right) + (1 - \varepsilon) \int_D |\nabla u|^2 + \frac{\varepsilon}{2We} \int_D \text{tr}(A - \text{Id}) = 0. \quad (2.4) \]
Lemma 2.1. Let us assume that \( \det A(t=0) > 1 \). This result combined with the estimate (2.3) thus yields some a priori bounds on \( (u, \tau) \) provided \( \det(A)(t=0) > 1 \). In particular, it shows that \( u \) and \( \tau \) go exponentially fast to 0 in the long time limit, using (2.3) and the Poincaré inequality: \( \int_D |u|^2 \leq C \int_D |\nabla u|^2 \).

**Lemma 2.1.** Let us assume that \( \det A(t=0) > 1 \). Then, we have \( \forall t \geq 0, \det A(t) > 1 \) and this implies that \( \text{tr} \tau(t) > 0 \).

**Proof.** Using (1.5) and the Jacobi identity (which states that for any invertible matrix \( M \) of size \( d \times d \),
\[
\det(M) \geq (1/d) \text{tr}(M)
\]
we obtain
\[
\frac{\partial \ln(\det A)}{\partial t} + u \cdot \nabla \ln(\det A) \geq \frac{d}{\text{We}} \left( (\det A)^{-1/d} - 1 \right),
\]
which we can rewrite in terms of \( y = (\det A)^{1/d} \):
\[
\text{We} \left( \frac{\partial y}{\partial t} + u \cdot \nabla y \right) \geq (1 - y).
\]
This shows that \( y > 1 \) if \( y(t=0) > 1 \), and thus that \( \det A > 1 \) if \( \det A(t=0) > 1 \).

Indeed, using the characteristic method (by integrating the vector field \( u(t,x) \)), one can rewrite (2.7) as
\[
\text{We} \frac{Dy}{Dt} \geq (1 - y).
\]
This implies \( \frac{D}{Dt} ((y - 1) \exp(t/\text{We})) \geq 0 \), which shows that \( y > 1 \) if \( y(t=0) > 1 \).

We thus have \( \det A > 1 \) and therefore, using again (2.6), \( \text{tr} A > d \). Since \( \tau = \text{We}(A - \text{Id}) \), this is equivalent to \( \text{tr} \tau > 0 \).

**Remark 2.2.** If \( \det A(t=0) < 1 \) (which is the case if \( \text{tr} \tau(t=0) < 0 \)), Equation (2.7) shows that \( \det A \) grows along the characteristics as long as \( \det A < 1 \).

### 3. Entropy estimate

We now consider a micro-macro (or multiscale) formulation of the Oldroyd-B model and some estimates based on entropy, inspired from [11].

#### 3.1. General derivation of the entropy estimate for micro-macro models.

We consider the following system:
\[
\left\{
\begin{array}{l}
\text{Re} \left( \frac{\partial \mathbf{u}(t,x)}{\partial t} + \mathbf{u}(t,x) \cdot \nabla \mathbf{u}(t,x) \right) = (1 - \varepsilon) \Delta \mathbf{u}(t,x) - \nabla p(t,x) + \text{div} \tau(t,x), \\
\text{div} \mathbf{u}(t,x) = 0, \\
\tau(t,x) = \frac{\varepsilon}{\text{We}} \left( \int_{\mathbb{R}^d} (X \otimes \nabla \mathbf{u}(x)) \psi(t,x,X) dX - \text{Id} \right), \\
\mathbf{v}(t,x,X) = \frac{\partial \psi}{\partial t}(t,x,X) + \mathbf{u}(t,x) \cdot \nabla_x \psi(t,x,X) \\
= -\text{div} \left( \left( \nabla_x \mathbf{u}(t,x) X - \frac{1}{2 \text{We}} \nabla \mathbf{u}(x) \right) \psi(t,x,X) \right) + \frac{1}{2 \text{We}} \Delta_x \psi(t,x,X).
\end{array}
\right.
\]
This system is supplied with initial conditions on the velocity \( u \) and on the distribution \( \psi \). We recall that we suppose no-slip boundary conditions (1.4) on the velocity \( u \). This system corresponds to a micro-macro model of polymeric fluids, the polymer being modelled by two beads linked by a spring with potential energy \( \Pi \). The configurational variable \( X \in \mathbb{R}^d \) models the end-to-end vector of the polymer. For more details on the modelling, we refer to [3, 23].

Notice that we could rewrite the former system as a system coupling a PDE and a stochastic differential equation (SDE), replacing the last two equations by:

\[
\begin{align*}
\tau(t, x) &= \frac{\varepsilon}{\text{We}} \left( \mathbf{E}(X_t(x)) \otimes \nabla \Pi(X_t(x)) \right) - \text{Id}, \\
\frac{dX_t(x)}{dt} + u(t, x) \cdot \nabla_x X_t(x) &= \left( \nabla_x u(t, x) X_t(x) - \frac{1}{2\text{We}} \nabla \Pi(X_t(x)) \right) dt + \frac{1}{\sqrt{\text{We}}} dW_t. 
\end{align*}
\]

There, \( \mathbf{E} \) denotes the expectation, \( W_t \) denotes a \( d \)-dimensional standard Brownian motion independent from the initial condition \( (X_0(x))_{x \in \mathcal{D}} \) which is such that, \( \forall x \in \mathcal{D}, X_0(x) \) is distributed with the probability density function \( \psi(0, x, X) dX \).

Let us introduce the kinetic energy:

\[
E(t) = \frac{1}{2} \int_{\mathcal{D}} |u|^2. \tag{3.4}
\]

We easily obtain:

\[
\text{Re} \frac{dE}{dt} = -(1 - \varepsilon) \int_{\mathcal{D}} |\nabla u|^2 - \frac{\varepsilon}{\text{We}} \int_{\mathcal{D}} \int_{\mathbb{R}^d} (X \otimes \nabla \Pi(X)) : \nabla u \psi. \tag{3.5}
\]

We now introduce the entropy of the system, namely:

\[
H(t) = \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi(t, x, X) \ln \left( \frac{\psi(t, x, X)}{\psi_{\infty}(X)} \right), \tag{3.6}
\]

\[
= \int_{\mathcal{D}} \int_{\mathbb{R}^d} \Pi(X) \psi(t, x, X) + \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi(t, x, X) \ln(\psi(t, x, X)) + C,
\]

with

\[
\psi_{\infty}(X) = \frac{\exp(-\Pi(X))}{\int_{\mathbb{R}^d} \exp(-\Pi(X))}, \tag{3.7}
\]

and \( C = \ln(\int_{\mathbb{R}^d} \exp(-\Pi(X)))|\mathcal{D}| \). The function \( H \) is actually the relative entropy of \( \psi \) with respect to the equilibrium distribution \( \psi_{\infty} \).

After some computations (see [11]), we obtain:

\[
\frac{dH}{dt} = -\frac{1}{2\text{We}} \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi \left| \nabla \ln \left( \frac{\psi}{\psi_{\infty}} \right) \right|^2 + \int_{\mathcal{D}} \int_{\mathbb{R}^d} (X \otimes \nabla \Pi(X)) : \nabla u \psi. \tag{3.8}
\]

Therefore, introducing the free energy \( F(t) = E(t) + \frac{\varepsilon}{\text{We}} H(t) \) of the system, we have:

\[
\begin{align*}
\frac{d}{dt} \left( \frac{\text{Re}}{2} \int_{\mathcal{D}} |u|^2 + \frac{\varepsilon}{\text{We}} \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi \ln \left( \frac{\psi}{\psi_{\infty}} \right) \right) \\
+ (1 - \varepsilon) \int_{\mathcal{D}} |\nabla u|^2 + \frac{\varepsilon}{2\text{We}^2} \int_{\mathcal{D}} \int_{\mathbb{R}^d} \psi \left| \nabla \ln \left( \frac{\psi}{\psi_{\infty}} \right) \right|^2 = 0. \tag{3.9}
\end{align*}
\]
Using a logarithmic Sobolev inequality with respect to $\psi_{\infty}$ and a Poincaré inequality for $u \in H^1_0(D)$, one can then obtain exponential convergence to equilibrium
$$\lim_{t \to \infty} (u(t), \psi_{\infty}) = (0, \psi_{\infty})$$
(see [11]). For some generalizations to the case $u \neq 0$ on $\partial D$, we refer to [11].

3.2. The Oldroyd-B case. Let us consider the Hookean dumbbell model, for which the potential $\Pi$ of the entropic force is:
$$\Pi(X) = \frac{1}{2} ||X||^2.$$  \tag{3.10}

By Itô’s calculus, it is easy to derive from (3.3) that $A = E(X_t \otimes X_t)$ satisfies the following PDE:
$$\frac{\partial A}{\partial t} + u \cdot \nabla A = \nabla u A + A(\nabla u)^T - \frac{1}{\text{We}} A + \frac{1}{\text{We}} \text{Id}. \tag{3.11}$$
This translates into the following PDE for $\tau = \frac{\varepsilon}{\text{We}} (A - \text{Id})$:
$$\frac{\partial \tau}{\partial t} + u \cdot \nabla \tau = \nabla u \tau + \tau (\nabla u)^T - \frac{1}{\text{We}} \tau + \frac{\varepsilon}{\text{We}} (\nabla u + (\nabla u)^T). \tag{3.12}$$
The Hookean dumbbell model is thus equivalent to the Oldroyd-B model (at least for regular enough solutions).

If $\psi(0, x, \cdot)$ is Gaussian (with zero mean), so is $\psi(t, x, \cdot)$:
$$\psi(t, x, X) = \frac{1}{(2\pi)^{d/2} \sqrt{\det(A)}} \exp\left(-\frac{X^T A^{-1} X}{2}\right)$$
where $A = E(X_t \otimes X_t) = \int_{\mathbb{R}^d} X \otimes X \psi(t, x, X) dX$ denotes as above the covariance matrix of $X_t$, which depends on time and also on the space variable $x$. The covariance matrix $A$ is symmetric and nonnegative. Moreover, since for almost all $t \geq 0$, $\int_D \int_{\mathbb{R}^d} \psi(t, x, X) \ln\left(\frac{\psi(t, x, X)}{\psi_{\infty}(X)}\right) < \infty$, then for almost all $t \geq 0$ and for almost all $x \in D$, $A$ is positive.

The following explicit expression of the relative entropy can then be derived:
$$\int_D \int_{\mathbb{R}^d} \psi(t, x, X) \ln\left(\frac{\psi(t, x, X)}{\psi_{\infty}(X)}\right) dX = \int_D \frac{1}{2} (-\ln(\det A) - d + \text{tr} A).$$

On the other hand,
$$\int_D \int_{\mathbb{R}^d} \psi(t, x, X) \left|\nabla \ln\left(\frac{\psi(t, x, X)}{\psi_{\infty}(X)}\right)\right|^2 dX = \int_D \text{tr}((\text{Id} - A^{-1})^2 A).$$

Rewriting (3.9), we thus obtain the following estimate, in terms of $A$:
$$\frac{d}{dt} \left(\frac{\text{Re}}{2} \int_D |u|^2 + \frac{\varepsilon}{\text{We}} \int_D (-\ln(\det A) - d + \text{tr} A)\right) + (1 - \varepsilon) \int_D |\nabla u|^2 + \frac{\varepsilon}{\text{We}} \int_D \text{tr}((\text{Id} - A^{-1})^2 A) = 0. \tag{3.13}$$
This is, in the specific case of Hookean dumbbells (that is, the Oldroyd-B model) the macroscopic version of (3.9).
Since \(-\ln(\det(A)) - d + \text{tr}(A) \geq 0\), this energy estimate yields some \emph{a priori} bounds on \((u, A)\), and thus on \((u, \tau)\). In sharp contrast to the classical estimate (2.3), it provides bounds on \((u, \tau)\) without any assumption on \(\tau(t=0)\) (apart from (1.6)).

Using a Poincaré inequality and the fact that, for any symmetric positive matrix \(M\) of size \(d \times d\),

\[-\ln(\det(M)) - d + \text{tr}(M) \leq \text{tr}((\text{Id} - M^{-1})^2 M),\]

exponential convergence to equilibrium (\(\lim_{t \to \infty} (u, A) = (0, \text{Id})\)) can be obtained from (3.13).

\textbf{Remark 3.1.} Notice that (3.13) can be schematically obtained as (2.4) - \(\frac{\varepsilon}{2 \text{We}} \int_D (2.5)\).

\textbf{Remark 3.2.} If \(\psi(0, x, \cdot)\) is not Gaussian, it is always possible to replace it by a Gaussian initial condition with the same mean and variance, so that the macroscopic quantities \((u, p, A)\) would be the same for the two initial conditions.

\textbf{3.3. Application to related macroscopic models.} The energy estimate (3.13) can be used as a guideline to derive energy estimates for other macroscopic models, even though they cannot be recast as a microscopic model of the form (3.1).

Let us consider the example of the FENE-P model [25, 4], for which

\(\tau = \text{We} \left( -\frac{A}{1 - \text{tr}(A)/b} - \text{Id} \right),\) (3.14)

\[\frac{\partial A}{\partial t} + u \cdot \nabla A = \nabla u A + A(\nabla u)^T - \frac{1}{\text{We}} \frac{A}{1 - \text{tr}(A)/b} + \frac{1}{\text{We}} \text{Id}.\] (3.15)

For this model, we assume (1.6), and also that \(\text{tr}(A)(t=0) < b\), and this property is propagated forward in time by (3.15) (see [12]).

Using the same ideas as for the Oldroyd-B model, we consider the “entropy” \(H(t) = -\ln(\det(A)) - b \ln(1 - \text{tr}(A)/b)\), and we compute its time-derivative:

\[\frac{d}{dt} \int_D -b \ln(1 - \text{tr}(A)/b)\] (3.16)

\[= 2 \int_D \frac{\nabla u : A}{1 - \text{tr}(A)/b} + \frac{1}{\text{We}} \int_D \left( - \frac{\text{tr}(A)}{(1 - \text{tr}(A)/b)^2} + \frac{d}{1 - \text{tr}(A)/b} \right),\] (3.17)

\[\frac{d}{dt} \int_D \ln(\det(A)) = \frac{1}{\text{We}} \int_D \left( - \frac{d}{1 - \text{tr}(A)/b} + \text{tr}(A^{-1}) \right).\] (3.18)

Combining these expressions with (2.2), we obtain

\[
\frac{d}{dt} \left( \frac{\text{Re}}{2} \int_D |u|^2 + \frac{\varepsilon}{2 \text{We}} \int_D \left( -\ln(\det(A)) - b \ln(1 - \text{tr}(A)/b) \right) \right) \\
+ (1 - \varepsilon) \int_D |\nabla u|^2 + \frac{\varepsilon}{2 \text{We}^2} \int_D \left( \frac{\text{tr}(A)}{(1 - \text{tr}(A)/b)^2} - \frac{2d}{1 - \text{tr}(A)/b} + \text{tr}(A^{-1}) \right) = 0.
\]

One can check that for any symmetric positive matrix \(M\) of size \(d \times d\):

\[-\ln(\det(M)) - b \ln(1 - \text{tr}(M)/b) \geq -(b + d) \ln \left( \frac{b}{b + d} \right) \geq d\] (3.19)

\footnote{which can be seen as the logarithmic Sobolev inequality for Gaussian random variables translated on their covariance matrices}
and that
\[ -\ln(\det(M)) - b\ln(1 - \text{tr}(M)/b) + (b + d)\ln\left(\frac{b}{b + d}\right) \leq \left(\frac{\text{tr}(M)}{(1 - \text{tr}(M)/b)^2} - \frac{2d}{1 - \text{tr}(M)/b}\right) + \text{tr}(M^{-1}). \]  

(3.20)\)

(3.21)

The proof of these inequalities is tedious and can be done by diagonalizing the matrix \( M \).

Equ. (3.19) shows that
\[ \text{Re} \int_{\mathcal{D}} |\mathbf{u}|^2 + \frac{\varepsilon}{2\text{We}} \int_{\mathcal{D}} \left( -\ln(\det\mathbf{A}) - b\ln(1 - \text{tr}(\mathbf{A})/b) + (b + d)\ln\left(\frac{b}{b + d}\right) \right) \]

is a non-negative quantity, and thus that (3.3) indeed yields some a priori bounds on \( (\mathbf{u}, \mathbf{A}) \).

Equ. (3.21) (which plays the role of the log-Sobolev inequality in the micro-macro models) shows that the estimate (3.3) can be used to prove exponential convergence to equilibrium.

**Addendum:** After completing this work, the authors’ attention was drawn to related works in the physics literature about thermodynamic theory for viscoelastic models with internal variables. See for example [15, 24, 28]

**REFERENCES**


