Short Communication

A lower bound for the invariants of the configuration tensor for some well-known differential models

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Abstract

A method will be given to determine lower bounds for the invariants of a configuration tensor in 3D flows. For some well-known differential models these lower bounds will be given. Except for the Giesekus and the FENE-P model the lower bounds are the values in equilibrium.

Keywords: configuration tensor; differential models; lower bounds of invariants

1 Introduction

Hulsen [1] has shown that it is possible to identify a positive definite configuration tensor $\boldsymbol{b}$ for some well-known differential stress models. In numerical computations this tensor may become indefinite and lead to severe non-linear instabilities [2]. A remedy for these problems may be the development of numerical schemes that preserve the positiveness of $\boldsymbol{b}$, i.e. its invariants. If it would be possible to prove that the lower bounds of the invariants of $\boldsymbol{b}$ are positive, the numerical scheme could be improved further by preserving these lower bounds as well. A positive lower bound is still more important for the calculation of the mechanical dissipation in the temperature equation. For a number of models the dissipation contains a term that depends on the inverse of the determinant of $\boldsymbol{b}$, as will be demonstrated in section 2. Therefore we try to find a *positive* lower bound for the invariants of $\boldsymbol{b}$ for 3D flows of some well-known differential models.

2 Stress constitutive equations

Differential models for the extra-stress may be written as follows

$$\boldsymbol{\tau} = 2\eta_s \boldsymbol{d} + \boldsymbol{\tau}_p, \tag{1}$$

where $\boldsymbol{\tau}$ is the extra-stress tensor that consists of a Newtonian part with viscosity η_s and a polymer part $\boldsymbol{\tau}_p$. The Euler rate of deformation tensor is $\boldsymbol{d} = (\boldsymbol{L}+\boldsymbol{L}^T)/2$, with the velocity gradient $\boldsymbol{L}^T = \nabla \underline{v}$. The polymer part of the extra-stress $\boldsymbol{\tau}_p$ may be related to the configuration tensor $\boldsymbol{b}$ by the simple algebraic relation

$$\boldsymbol{\tau}_p = \frac{G}{1-\xi}\left(B\boldsymbol{b} - \boldsymbol{I}\right), \tag{2}$$

where G is the shear modulus. The parameter B equals $B = 1$ for neo-Hookean models. For the Larson, Chilcott–Rallison and FENE-P models B depends on the first invariant of $\boldsymbol{b}$. The parameter ξ appears in the Gordon–Schowalter derivative in the differential equation for $\boldsymbol{b}$:

$$\lambda \overset{\square}{\boldsymbol{b}} = g_1(\boldsymbol{b})\,\boldsymbol{I} + g_2(\boldsymbol{b})\,\boldsymbol{b} + g_3(\boldsymbol{b})\,\boldsymbol{b}^2, \tag{3}$$

where λ is the relaxation time and g_i are scalars which may be functions of the invariants of the configuration tensor. The Gordon–Schowalter derivative $\overset{\square}{\boldsymbol{b}}$, is given by

$$\begin{aligned} \overset{\square}{(\,)} &= \dot{(\,)} - \hat{\boldsymbol{L}}\cdot(\,) - (\,)\cdot\hat{\boldsymbol{L}}^T, \\ \hat{\boldsymbol{L}} &= \boldsymbol{L} - \xi \boldsymbol{d}, \end{aligned} \tag{4}$$

where the parameter ξ fulfils the condition $0 \leq \xi \leq 2$.

The polymer part of the stress, given by (2), can be derived from a potential, the free energy ψ, as follows

$$\boldsymbol{\tau}_p = 2\rho \boldsymbol{b}\cdot\frac{\partial \psi}{\partial \boldsymbol{b}}, \tag{5}$$

where ρ is the density of the fluid and we have assumed that $\xi = 0$. The mechanical dissipation $D_{m,p}$ of the polymeric part equals

$$D_{m,p} = \boldsymbol{\tau}_p : \boldsymbol{d} - \rho\dot{\psi} = \boldsymbol{\tau}_p : \boldsymbol{d} - \rho\frac{\partial \psi}{\partial \boldsymbol{b}} : \dot{\boldsymbol{b}} = -\frac{1}{2}\,\mathrm{tr}\left(\boldsymbol{\tau}_p\cdot\boldsymbol{b}^{-1}\cdot\overset{\triangledown}{\boldsymbol{b}}\right), \tag{6}$$

see for example [3] or [4]. Substitution of (3) into (6) shows that the dissipation contains a term $g_1(\boldsymbol{b})\,\mathrm{tr}\,\boldsymbol{b}^{-1} = g_1(\boldsymbol{b})I_2/I_3$. For all the models we will consider the scalar $g_1(\boldsymbol{b})$ is positive, which means that the dissipation contains a term with I_3^{-1}. Whenever $\boldsymbol{b}$ loses positive definiteness in computations,

I_3 becomes zero while I_2 is still positive in most cases. This will cause great difficulties in computing the dissipation in numerical calculations. A positive lower bound for I_3 will be of great help here.

Combining equation (3) with the identity

$$\dot{I}_3 = \frac{\partial I_3}{\partial \boldsymbol{b}} : \dot{\boldsymbol{b}} = I_3 \boldsymbol{b}^{-1} : \dot{\boldsymbol{b}}, \tag{7}$$

the following expression for the material derivative of the third invariant is obtained:

$$\lambda \dot{I}_3 = 2\lambda(1-\xi) I_3 \nabla \cdot \underset{\sim}{v} + g_1 I_2 + (3g_2 + g_3 I_1)\, I_3, \tag{8}$$

where $I_2 = I_3 \operatorname{tr} \boldsymbol{b}^{-1}$ has been used. In the following we will assume an incompressible flow. Then the first term on the right-hand side of (8) vanishes. Equation (8) will be used in section 4 to track the value of I_3 along a particle path and possibly show that it remains positive.

3 A lower bound for I_1 and I_2 on a surface of constant I_3

In this section we will calculate the positive lower bounds for the invariants I_1 and I_2 for a given value of the determinant I_3.

For a surface with constant determinant $I_3 = C > 0$ the second invariant I_2 equals

$$I_2(b_1, b_2) = b_1 b_2 + \frac{C}{b_1} + \frac{C}{b_2}, \tag{9}$$

where b_1 and b_2 are two principal values of $\boldsymbol{b}$. The third principle value b_3 has been eliminated with $I_3 = b_1 b_2 b_3 = C$. The local extrema can be found from:

$$\frac{\partial I_2}{\partial b_1} = b_2 - \frac{C}{b_1^2} = 0,$$
$$\frac{\partial I_2}{\partial b_2} = b_1 - \frac{C}{b_2^2} = 0,$$

which gives one real extremum at $b_1 = b_2 = b_3 = \sqrt[3]{C}$. The second derivatives of I_2 in this extremum are

$$\frac{\partial^2 I_2}{\partial b_1^2} = 2, \qquad \frac{\partial^2 I_2}{\partial b_2^2} = 2, \qquad \frac{\partial^2 I_2}{\partial b_1 \partial b_2} = 1.$$

The conditions for a minimum are

$$\frac{\partial^2 I_2}{\partial b_1^2} > 0, \qquad \frac{\partial^2 I_2}{\partial b_1^2}\frac{\partial^2 I_2}{\partial b_2^2} > \left(\frac{\partial^2 I_2}{\partial b_1 \partial b_2}\right)^2,$$

which are fulfilled in the local extremum.

Substitution of $b_1 = b_2 = \sqrt[3]{C}$ in (9) gives the value for the second invariant in the local minimum: $I_2^{\min} = 3C^{2/3}$.

For a surface with constant determinant $I_3 = C$ the first invariant equals

$$I_1(b_1, b_2) = b_1 + b_2 + \frac{C}{b_1 b_2}. \tag{10}$$

The local extrema can be found from:

$$\begin{aligned} \frac{\partial I_1}{\partial b_1} &= 1 - \frac{C}{b_1^2 b_2} = 0, \\ \frac{\partial I_1}{\partial b_2} &= 1 - \frac{C}{b_2^2 b_1} = 0, \end{aligned}$$

which gives $b_1 = b_2 = b_3 = \sqrt[3]{C}$, identical to the extremum for the second invariant. Substitution of $b_1 = b_2 = \sqrt[3]{C}$ in (10) then gives the value for the first invariant in the local minimum: $I_1^{\min} = 3\sqrt[3]{C}$.

4 Lower bounds of the invariants for viscoelastic models

With equation (8) and the results of section 3 we will try to find a lower bound for the determinant I_3, and thus for I_1 and I_2, of some well-known differential models. For a more detailed description of most of these models refer to [5]. The models that have not been described in [5] the references will be given later on. We will show that with our method it is possible to obtain a positive lower bound for the invariants for most of the models, except the 3D Giesekus and the FENE-P model.

The Johnson–Segalman model and the Phan-Thien–Tanner model

For the Johnson–Segalman model and the Phan-Thien–Tanner model the scalars g_i are given by $g_1 = Y$, $g_2 = -Y$ and $g_3 = 0$. The function Y equals $Y = 1$ for the Johnson–Segalman model, $Y = 1 + \epsilon(I_1 - 3)$ for the linear Phan-Thien–Tanner model and $Y = \exp[\epsilon(I_1 - 3)]$ for the exponential Phan-Thien–Tanner model. Furthermore the coefficients in (2) are $B = 1$ and $0 \leq \xi \leq 2$. Substitution of the scalars g_i in equation (8) gives

$$\dot{I}_3 = \frac{Y}{\lambda} I_2 - \frac{3Y}{\lambda} I_3. \tag{11}$$

With the result of section 3 for the minimum of the second invariant equation (11) leads to

$$\dot{I}_3 \geq \frac{3YC^{2/3}}{\lambda} \left(1 - C^{1/3}\right), \tag{12}$$

on the surface $I_3 = C$. For $C = 1$ it follows that $\dot{I}_3 \geq 0$. Thus the lower bound for the Johnson–Segalman model and the Phan-Thien–Tanner model is $I_3^{\min} = 1$, if it is assumed that any path starts from $\boldsymbol{b} = \boldsymbol{I}$. From the results in section 3 it also follows that the minima of the first and second invariant are $I_1^{\min} = \sqrt[3]{C} = 3$ and $I_2^{\min} = 3C^{2/3} = 3$, which corresponds to the values of the invariants in equilibrium.

From (12) it also follows that for $0 < C < 1$ the material derivative of the determinant is positive. So, if for some reason the determinant is smaller than 1 at the starting point of the path, the value of the determinant will increase.

The Larson model

The scalars g_i of the Larson model are $g_1 = 1/B$, $g_2 = -1/B$ and $g_3 = 0$. The coefficients in (2) are $B = (1 + \beta(I_1 - 3)/3)^{-1}$, where β is a positive parameter, and $\xi = 0$. The differential equation for the configuration tensor is equal to the linear Phan-Thien–Tanner model, when $\beta = 3\epsilon$. So $I_1^{\min} = 3$, $I_2^{\min} = 3$ and $I_3^{\min} = 1$, the values of the invariants in equilibrium, are also lower bounds for the Larson model.

The (modified) Leonov model

The scalars g_i of the modified Leonov model are given by $g_1 = \phi/2$, $g_2 = -\phi(I_1 - I_2)/6$ and $g_3 = -\phi/2$, where $\phi^{-1} = 1 + 2\alpha/\pi \;\arctan(\beta/4 \;(I_1 + I_2 - 6))$. The coefficients in (2) are $B = 1$ and $\xi = 0$. Refer to [6] for a more extensive description of the modified Leonov model. The modified Leonov model reduces to the Leonov model if $\phi = 1$ is taken. Substitution of the scalars g_i in equation (8) gives

$$\dot{I}_3 = \frac{\phi}{2\lambda} I_2 (1 - I_3) . \tag{13}$$

If $I_3 = 1$ initially, then it always equals $I_3 = 1$. From the results in section 3 it also follows that the minima of the first and second invariant are $I_1^{\min} = \sqrt[3]{C} = 3$ and $I_2^{\min} = 3C^{2/3} = 3$, which are equal to the values of the invariants in equilibrium.

Otherwise, if for some reason the determinant is positive but does not equal 1 at the starting point of the path, it will tend to $I_3 = 1$ for $t \to \infty$.

The Giesekus model

For the Giesekus model the scalars g_i are $g_1 = (1 - \alpha)$, $g_2 = -(1 - 2\alpha)$ and $g_3 = -\alpha$, where $0 \leq \alpha < 1$. The coefficients in (2) are $B = 1$ and $\xi = 0$. Substitution of the scalars g_i in equation (8) gives

$$\dot{I}_3 = \frac{1-\alpha}{\lambda} I_2 - I_3 \left(\frac{3(1-2\alpha)}{\lambda} + \frac{\alpha}{\lambda} I_1 \right) . \tag{14}$$

Hulsen [2] has shown that a positive lower bound exists for a 2D flow. However, for a 3D flow of the Giesekus model it is not possible to find a positive lower bound for the determinant. This will be demonstrated with a counter example: a steady uniaxial elongation. The analytical solution for $0 < \alpha < 1$ has been given by [7]:

$$\begin{aligned} b_1 &= \frac{1}{2\alpha} \left[2\gamma - (1-2\alpha) + \sqrt{1 - 4(1-2\alpha)\gamma + 4\gamma^2} \right] , \\ b_2 = b_3 &= \frac{1}{2\alpha} \left[-\gamma - (1-2\alpha) + \sqrt{1 + 2(1-2\alpha)\gamma + \gamma^2} \right] , \\ \gamma &= \lambda \dot{\epsilon}, \end{aligned} \tag{15}$$

where b_1, b_2 and b_3 are the principal values of $\boldsymbol{b}$. The limit values of the principal values for $\gamma \to \infty$ can be found by a standard Taylor expansion of the square root:

$$
\begin{aligned}
b_1 &= \frac{1}{2\alpha}\left[2\gamma - (1-2\alpha) + 2\gamma\sqrt{1-(1-2\alpha)/\gamma + 1/\gamma^2}\right] = \frac{2\gamma}{\alpha}, \\
b_2 &= \frac{1}{2\alpha}\left[-\gamma - (1-2\alpha) + \gamma\sqrt{1+2(1-2\alpha)/\gamma + 1/\gamma^2}\right] = \frac{1-\alpha}{\gamma}.
\end{aligned}
$$

The limit solution of the determinant for large γ is then given by

$$
\lim_{\gamma\to\infty} I_3 = \lim_{\gamma\to\infty} \frac{2(1-\alpha)^2}{\alpha\gamma} = 0,
$$

which shows that no general positive lower bound can be given for the 3D Giesekus model. Together with the positive definiteness of the configuration tensor this gives that the lower bound for the determinant equals $I_3^{\min} = 0$.

Whether positive lower bounds for I_1 and I_2 exist remains inconclusive from our analysis in section 3 (only $I_1^{\min} = I_2^{\min} > 0$).

The Chilcott–Rallison model

The scalars g_i of the Chilcott–Rallison model are $g_1 = B$, $g_2 = -B$ and $g_3 = 0$. The coefficients in (2) are $\xi = 0$ and $B = (1 - I_1/L^2)^{-1}$, where L represents the ratio of the length of a fully extended dumbbell to its equilibrium length. Refer to [8] for a more extensive description of this model. The differential equation for the configuration tensor resembles the Phan-Thien–Tanner model. Only the factor Y has to be replaced by B. Due to the finite extensibility of a dumbbell, ($I_1 < L^2$), B is always positive. Therefore, the results discussed for equation (12) also holds for the Chilcott–Rallison model. So the lower bounds for the Chilcott–Rallison model $I_1^{\min} = 3$, $I_2^{\min} = 3$ and $I_3^{\min} = 1$ also correspond to the values of the invariants in equilibrium.

The FENE-P model

The scalars g_i of the FENE-P model are $g_1 = \alpha$, $g_2 = -B$ and $g_3 = 0$. The coefficients in (2) are $B = (1-\beta I_1)^{-1}$ and $\xi = 0$. Refer to [9] for a more extensive description of this model. In the notation of [9] the constants α and β correspond to $\alpha = 3(1-\epsilon b)X/b$ and $\beta = 1/X$, with $X = (1 - Z_{\text{eq}}^{-1})^{-1}$. For a steady uniaxial elongation it is easy to show that for large $\gamma = \lambda\dot{\epsilon}$

$$
\begin{aligned}
b_1 &= \frac{1}{\beta}, \\
b_2 &= \frac{\alpha}{3\gamma}.
\end{aligned}
$$

The limit solution of the determinant for large γ is then given by

$$
\lim_{\gamma\to\infty} I_3 = \lim_{\gamma\to\infty} \frac{\alpha^2}{9\beta\gamma^2} = 0,
$$

which shows that no general positive lower bound can be given for the FENE-P model. Together with the positive definiteness of the configuration tensor this gives that the lower bound for the determinant equals $I_3^{\min} = 0$.

Whether positive lower bounds for I_1 and I_2 exist remains inconclusive from our analysis in section 3 (only $I_1^{\min} = I_2^{\min} > 0$).

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