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# Finite element analysis of planar 4:1 contraction flow with the tensor-logarithmic formulation of differential constitutive equations

**Youngdon Kwon***
*School of Applied Chemistry and Chemical Engineering, Sungkyunkwan University, Suwon, Kyunggi-do 440-746, Korea*

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## Abstract

High Deborah or Weissenberg number problems in viscoelastic flow modeling have been known formidably difficult even in the inertialess limit. There exists almost no result that shows satisfactory accuracy and proper mesh convergence at the same time. However recently, quite a breakthrough seems to have been made in this field of computational rheology. So called matrix-logarithm (here we name it tensor-logarithm) formulation of the viscoelastic constitutive equations originally written in terms of the conformation tensor has been suggested by Fattal and Kupferman (2004) and its finite element implementation has been first presented by Hulsen (2004). Both the works have reported almost unbounded convergence limit in solving two benchmark problems. This new formulation incorporates proper polynomial interpolations of the logarithm for the variables that exhibit steep exponential dependence near stagnation points, and it also strictly preserves the positive definiteness of the conformation tensor. In this study, we present an alternative procedure for deriving the tensor-logarithmic representation of the differential constitutive equations and provide a numerical example with the Leonov model in 4:1 planar contraction flows. Dramatic improvement of the computational algorithm with stable convergence has been demonstrated and it seems that there exists appropriate mesh convergence even though this conclusion requires further study. It is thought that this new formalism will work only for a few differential constitutive equations proven globally stable. Thus the mathematical stability criteria perhaps play an important role on the choice and development of the suitable constitutive equations. In this respect, the Leonov viscoelastic model is quite feasible and becomes more essential since it has been proven globally stable and it offers the simplest form in the tensor-logarithmic formulation.

***Keywords*** : high Deborah number, tensor-logarithm, constitutive equation, stability, Leonov model, contraction flow

## 1. Introduction

Numerical modeling of viscoelastic flow around a sharp corner has posed great challenge in computational non-Newtonian fluid dynamics, because it is extremely difficult to obtain solutions in the case of high Deborah (or Weissenberg) number flows. For viscoelastic fluid, the Deborah number defined as the ratio of liquid relaxation time to characteristic time of the flow expresses strength of elasticity accumulated in the flow. There are several reasons conjectured for the failure of the numerical convergence at high Deborah number in the planar 4:1 contraction flow modeling, the representative benchmark flow problem with singular geometry. It has been recognized that computational algorithm certainly plays a significant role in determining the stability of the numerical scheme. However the applied viscoelastic constitutive equation is thought to be also responsible for the numerical degradation. Nowadays one has come to a conclusion that selection of an appropriate constitutive equation constitutes a very crucial step although implementing a suitable numerical technique is still important for successful discrete modeling of non-Newtonian flows (Leonov, 1995).

Irrespective of extensive stability analysis performed for the constitutive equations as well as astonishing development of computational algorithm, it is indeed frustrating that even the viscoelastic model proven globally stable shows quite unsatisfactory limitation of computational convergence whatever numerical algorithm may be applied. Recently a breakthrough in this field seems to have been made by Fattal and Kupferman (2004). They have suggested simple tensor-logarithmic transform of the conformation tensor in the differential viscoelastic constitutive

*Corresponding author: kwon@skku.edu

equations and proved existence of such representation for differential constitutive models. Their idea is based on the following. The conformation tensor shows exponential dependence in regions of high strain rate for high Deborah number flows, and the polynomial interpolation of this behavior is inappropriate. If one employs its logarithmic function instead of the conformation tensor, the multiplication is substituted by the addition operation, and thus the polynomial interpolation of this logarithm function is thought to be proper and more effective in the spatial resolution of steep stress gradients.

In addition, this new formulation may grant another important characteristic. It is well known that the positive-definiteness of the conformation tensor is crucial for well-posedness of its evolution equation (Dupret and Marchal, 1986; Kwon and Leonov, 1995). In reality, even for the constitutive equations proven Hadamard stable (Hadamard stability means the well-posedness of constitutive equations under short and high frequency wave disturbance), violation of this positive-definiteness is frequently observed (Dupret *et al.*, 1985; Lee *et al.*, 2004) probably due to the spatial discretization error. However if we introduce this tensor-logarithm for the conformation tensor, the positive-definiteness is strictly preserved in any computational scheme and at any value of the Deborah number. Seemingly limitless convergence of the approximation scheme has already been reported in numerical computation of benchmark viscoelastic flow problems such as lid-driven cavity flow (Fattal and Kupferman, 2004) and flow past a cylinder in a straight pipe (Hulsen, 2004).

At this point, it is not certain that this new formalism based on tensor-logarithm transform can successfully work for every differential constitutive equation that can be written in the conformation tensor notation. Even if the existence of the tensor-logarithm representation for differential viscoelastic models has been proven (Fattal and Kupferman, 2004), it is not at all obvious that this sole reformulation stabilizes the computational scheme for any set of equations. In the current author's opinion, mathematical stability analysis of constitutive equations may provide quite feasible insight into optimal choice of viscoelastic models. Especially for Maxwell-type differential and time-strain separable single integral constitutive equations, one can find extensive and detailed results on mathematical stability (Joseph 1990; Kwon 2002; Kwon and Leonov 1995).

In this study we first present an alternative procedure obtaining the tensor-logarithmic formulation of the viscoelastic equations originally suggested by Fattal and Kupferman (2004). Then this procedure is applied to the 2D description of the Leonov model, which becomes more important and also the simplest especially in this formalism. We consider the isothermal incompressible inertialess 4:1 contraction flow problem to test this new representation in high Deborah number flow modeling.

## 2. Tensor-logarithmic formulation of the constitutive equation

Most of differential viscoelastic constitutive equations can be written into the following quite general form:

$$\dot{\boldsymbol{c}} - \nabla \boldsymbol{v}^T \cdot \boldsymbol{c} - \boldsymbol{c} \cdot \nabla \boldsymbol{v} + \frac{1}{\theta}\boldsymbol{\psi} = 0 \tag{1}$$

Here $\boldsymbol{c}$ is the conformation tensor that describes the macromolecular conformation under flow for the constitutive models based on molecular kinetic theory, $\boldsymbol{v}$ is the velocity, $\dot{\boldsymbol{c}} = \frac{d\boldsymbol{c}}{dt} = \frac{\partial \boldsymbol{c}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{c}$ is the material time derivative of $\boldsymbol{c}$, $\nabla$ is the usual gradient operator in tensor calculus, $\dot{\boldsymbol{c}} - \nabla \boldsymbol{v}^T \cdot \boldsymbol{c} - \boldsymbol{c} \cdot \nabla \boldsymbol{v}$ is the upper convected time derivative, and $\theta$ is the relaxation time. $\psi$ is usually represented as the polynomial of $\boldsymbol{c}$ with coefficients possibly dependent on the invariants of $\boldsymbol{c}$ or $\boldsymbol{e} = (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T)/2$, whose specific form has to be given by the constitutive equation employed. For example, the upper convected Maxwell model can be rewritten as Eq.(1) with $\boldsymbol{\psi} = \boldsymbol{c} - \boldsymbol{\delta}$ and its extra-stress takes the form of $\boldsymbol{\tau} = G(\boldsymbol{c} - \boldsymbol{\delta})$ with $G$ as the modulus. More examples can be found in Kwon and Leonov (1995) and Lee *et al.* (2004). The conformation tensor $\boldsymbol{c}$ reduces to the unit tensor $\boldsymbol{\delta}$ in the rest state and this condition also serves as the initial condition in the start-up flow situation. In contrast, for the Leonov model that has been derived from the irreversible thermodynamics and thus is not endowed with molecular concept, the $\boldsymbol{c}$-tensor explains the accumulated elastic strain in the Finger measure during flow. In the asymptotic limit of $\theta \to \infty$ where the material exhibits purely elastic behavior, it becomes the total Finger strain tensor.

The essential idea presented by Fattal and Kupferman (2004) in reformulating the constitutive equations is the tensor-logarithmic transformation of $\boldsymbol{c}$ as follows:

$$\boldsymbol{h} = \log \boldsymbol{c}. \tag{2}$$

Here the logarithm operates as the isotropic tensor function, which implies the identical set of principal axes for both $\boldsymbol{c}$ and $\boldsymbol{h}$. In the case of the Leonov model, this $\boldsymbol{h}$ becomes another measure of elastic strain, that is, twice the Hencky elastic strain.

In this section, a simple alternative derivation of the tensor-logarithmic transform for Eq.(1) (formulation of the constitutive equation in terms of $\boldsymbol{h}$) originally given by Fattal and Kupferman (2004), is suggested. For this purpose we adopt following notations:
$c_i$: eigenvalues of $\mathbf{c}$, $h_i$: eigenvalues of $\boldsymbol{h}$, $\boldsymbol{n}_i$: corresponding unit eigenvectors.

Here due to the isotropic function relation, $\boldsymbol{c}$ and $\boldsymbol{h}$ have the same set of eigenvectors. The characteristic relation for $\boldsymbol{c}$ is written as

$$\boldsymbol{c} \cdot \boldsymbol{n}_i = c_i \boldsymbol{n}_i \text{ (no sum)}. \tag{3}$$

Differentiation and scalar product with another eigenvector yield

$$\boldsymbol{n}_j \cdot \dot{\boldsymbol{c}} \cdot \boldsymbol{n}_i = \dot{c}_i \delta_{ij} + (c_i - c_j)\dot{\boldsymbol{n}}_i \cdot \boldsymbol{n}_j \quad \text{(no sum)}. \tag{4}$$

We may rewrite it as

$$\left\{ \begin{array}{ll} i)\ \dot{c}_i = \boldsymbol{n}_i \cdot \dot{\boldsymbol{c}} \cdot \boldsymbol{n}_i & when\ i=j \\ ii)\ \dot{\boldsymbol{n}}_i \cdot \boldsymbol{n}_j = \dfrac{1}{c_i - c_j}\boldsymbol{n}_j \cdot \dot{\boldsymbol{c}} \cdot \boldsymbol{n}_i & when\ i \neq j \end{array} \right\} \text{(no sum)}. \tag{5}$$

For $\boldsymbol{h}$-tensor, an equivalent relation is readily obtained as

$$\boldsymbol{n}_j \cdot \dot{\boldsymbol{h}} \cdot \boldsymbol{n}_i = \dot{h}_i \delta_{ij} + (h_i - h_j)\dot{\boldsymbol{n}}_i \cdot \boldsymbol{n}_j \quad \text{(no sum)}. \tag{6}$$

Due to Eq.(2), one has $c_i = e^{h_i}$ and thus $\dot{h}_i = \frac{1}{c_i}\dot{c}_i$ (no sum) holds. With this and Eqs.(5), Eq.(6) represents the following resultant relation for the time variation of $\boldsymbol{h}$-tensor:

$$\left\{ \begin{array}{ll} i)\ \boldsymbol{n}_i \cdot \dot{\boldsymbol{h}} \cdot \boldsymbol{n}_i = \dfrac{1}{c_i}\dot{c}_i = \dfrac{1}{c_i}\boldsymbol{n}_i \cdot \dot{\boldsymbol{c}} \cdot \boldsymbol{n}_i & when\ i=j \\ ii)\ \boldsymbol{n}_i \cdot \dot{\boldsymbol{h}} \cdot \boldsymbol{n}_j = (h_j - h_i)\dot{\boldsymbol{n}}_j \cdot \boldsymbol{n}_i = \dfrac{h_i - h_j}{c_i - c_j}\boldsymbol{n}_i \cdot \dot{\boldsymbol{c}} \cdot \boldsymbol{n}_j & when\ i \neq j \end{array} \right\}$$

$$\text{(no sum)}. \tag{7}$$

When one denotes $\boldsymbol{Q}$ as the orthogonal matrix that transforms $\boldsymbol{c}$ or $\boldsymbol{h}$ into the corresponding diagonal form $\tilde{\boldsymbol{c}}$ or $\tilde{\boldsymbol{h}}$ in principal axes, the following simple relations hold:

$$\boldsymbol{c} = \boldsymbol{Q} \cdot \exp(\tilde{\boldsymbol{h}}) \cdot \boldsymbol{Q}^T, \quad \exp(\tilde{\boldsymbol{h}}) = \tilde{\boldsymbol{c}} = \begin{bmatrix} e^{h_1} & 0 & 0 \\ 0 & e^{h_2} & 0 \\ 0 & 0 & e^{h_3} \end{bmatrix}. \tag{8}$$

The orthogonal matrix $\boldsymbol{Q}$ contains the eigenvectors $\boldsymbol{n}_i$ as its column vectors. In principle, all the components of $\boldsymbol{n}_i$ and eigenvalues $h_i$ can be obtained by solving the characteristic equation for $\boldsymbol{h}$, even though obtaining its analytic expression may become a formidable task in 3D flow domain. If we substitute the constitutive equation (1) for $\dot{\boldsymbol{c}}$ in Eqs.(7) that does not contain the derivative of $\boldsymbol{c}$ any more and utilize the solution of the characteristic equation for $\boldsymbol{h}$, then Eqs.(7) eventually represent the desired constitutive relation written in terms of $\boldsymbol{h}$. For $(i,j)$ such as (1,1), (2,2), (3,3), (1,2), (2,3) and (1,3), Eqs.(7) yield exactly 6 differential equations for $h_{ij}$.

Above derivation holds in every flow situation except when there locally exists 2D or 3D isotropy. However in this case, the relation yields simpler equation. Without loss of generality, we assume that $\boldsymbol{n}_i$ and $\boldsymbol{n}_j$ $(i \neq j)$ are the vectors perpendicular to the cylindrical symmetry axis (i.e. $\boldsymbol{n}_i$ and $\boldsymbol{n}_j$ are contained in the plane of isotropy). Then $c_i = c_j$, $h_i = h_j$, and $\boldsymbol{n}_i$ and $\boldsymbol{n}_j$ are indeterminate except the fact that they consist in the isotropic plane. Since the asymptotic relation $\lim_{h_j \to h_i} \frac{h_i - h_j}{c_i - c_j} = \frac{1}{c_i}$ is valid, Eqs.(7) combine to $\boldsymbol{n}_i \cdot \dot{\boldsymbol{h}} \cdot \boldsymbol{n}_j = \frac{1}{c_i}\boldsymbol{n}_i \cdot \dot{\boldsymbol{c}} \cdot \boldsymbol{n}_j$. Using the representation for $\boldsymbol{n}_i$ in terms of $h_i$ and $h_{ij}$ and applying appropriate asymptotic relations, we possibly obtain corresponding constitutive equations in $\boldsymbol{h}$-tensor form. Since the original constitutive model (1) in the $\boldsymbol{c}$ formulation is known to be regular for $c_i = c_j$, such transformation into $\boldsymbol{h}$-form certainly exists. In the following sections we present illustrative example in simple planar 2D flow with numerical results for the Leonov constitutive equation.

## 3. Formulation in 2D flow

In the case of 2D planar flow, the direction orthogonal to the computation domain automatically constitutes one fixed eigenvector. Here we designate the axes of flow domain as $x_1$ and $x_2$. When we write the first eigenvector as the following, the second eigenvector is determined accordingly:

$$\boldsymbol{n}_1 = \begin{bmatrix} n_1 \\ n_2 \end{bmatrix}, \text{ and then } \boldsymbol{n}_2 = \begin{bmatrix} -n_2 \\ n_1 \end{bmatrix} \text{ with } n_1^2 + n_2^2 = 1. \tag{9}$$

Solving the characteristic equation of $\boldsymbol{h}$, one obtains

$$h_1 = \frac{1}{2}[h_{11} + h_{22} + \sqrt{(h_{11} - h_{22})^2 + 4h_{12}^2}],$$

$$h_2 = \frac{1}{2}[h_{11} + h_{22} - \sqrt{(h_{11} - h_{22})^2 + 4h_{12}^2}],$$

$$n_1^2 = \frac{h_{12}^2}{(h_1 - h_{11})^2 + h_{12}^2}, \quad n_2^2 = \frac{(h_1 - h_{11})^2}{(h_1 - h_{11})^2 + h_{12}^2},$$

$$n_1 n_2 = \frac{h_{12}(h_1 - h_{11})}{(h_1 - h_{11})^2 + h_{12}^2}. \tag{10}$$

In the rest state, all $h_{ij}$ and the eigenvalues vanish, and therefore the components of the eigenvector become indeterminate as can be seen from the equations. In Eqs.(10), the two characteristic values may be interchanged, however the resultant constitutive equations remain invariable.

In this simple 2D consideration, Eqs.(7) with (9) represent 3 equations as

$$n_1^2\dot{h}_{11} + 2n_1n_2\dot{h}_{12} + n_2^2\dot{h}_{22} = \frac{1}{c_1}(n_1^2\dot{c}_{11} + 2n_1n_2\dot{c}_{12} + n_2^2\dot{c}_{22}),$$

$$n_2^2\dot{h}_{11} - 2n_1n_2\dot{h}_{12} + n_1^2\dot{h}_{22} = \frac{1}{c_2}(n_2^2\dot{c}_{11} - 2n_1n_2\dot{c}_{12} + n_1^2\dot{c}_{22}),$$

$$-n_1n_2\dot{h}_{11} + (n_1^2 - n_2^2)\dot{h}_{12} + n_1n_2\dot{h}_{22}$$

$$= \frac{h_1 - h_2}{c_1 - c_2}[-n_1n_2\dot{c}_{11} + (n_1^2 - n_2^2)\dot{c}_{12} + n_1n_2\dot{c}_{22}]. \tag{11}$$

Substitution of the specific constitutive equations for $\dot{c}_{ij}$ with Eqs.(10) and transformation rule (8) eventually yields the desired set of viscoelastic field equations in 2D represented in $\boldsymbol{h}$-tensor form.

From now on, only the Leonov constitutive equation (Leonov, 1976) is considered. Its one simple version has the following form for the evolution equation (1) and the stress relation:

$$\psi=\frac{1}{2}\left(\frac{I_1}{I_2}\right)^m\left(c^2+\frac{I_2-I_1}{3}c-\delta\right),\quad \tau=G\left(\frac{I_1}{3}\right)^n c,$$

$$W=\frac{3G}{2(n+1)}\left[\left(\frac{I_1}{3}\right)^{n+1}-1\right]. \tag{12}$$

Here $I_1=\mathrm{tr}\,c$ and $I_2=\mathrm{tr}\,c^{-1}$ are basic invariants of **c**, and they coincide in planar flows. In order to rigorously examine the computational robustness of the formulation we do not include any retardation (Newtonian viscous) term that bestows stabilizing effect on the numerical scheme by augmenting the elliptic character in equations of motion. The extra-stress tensor is obtained from the elastic potential $W$ based on the Murnaghan's relation. Since the extra-stress is invariant under the addition of arbitrary isotropic terms, when we present our numerical results we use $\tau=G\left(\frac{I_1}{3}\right)^n\times(c-\delta)$ instead in order to set 0 for the stress in the rest state. In addition to the linear viscoelastic parameters, it contains 2 nonlinear constants $m$ and $n$, which can be determined from simple shear and uniaxial extensional flow experiments. The value of the parameter $m$ does not have any effect on the flow characteristics in 2D situation, since two invariants are equal.

These Leonov equations contain one essential feature that becomes especially important and practically useful in current tensor-logarithmic formulation as follows:

$$\det c=1. \tag{13}$$

It can be seen as the first integral of the evolution equation (1), and it implies the liquid is incompressible (this relation is derived from the fact that volume change during the flow is completely recoverable). In 2D it reduces to $c_{11}c_{22}-c_{12}^2=1$. Since the logarithmic function transforms the multiplication into the operation of addition, this incompressibility relation (13) becomes

$$\mathrm{tr}\,h=0, \tag{14}$$

which dramatically simplifies all the relations derived above. In addition, it gives another advantage in computation. For example, in 3D due to $h_{11}+h_{22}+h_{33}=0$ one can eliminate one variable (and accordingly one equation) from the set of governing equations. In this 2D analysis, we remove $h_{22}$ from the set, and thus the viscoelastic model contains only 2 additional unknowns such as $h_{11}$ and $h_{12}$. Based on our numerical scheme explained afterwards, the computation time has diminished to a half.

Now employing Eq.(14), one can get simplified version of Eqs.(10) valid only for the Leonov model as

$$h_1\equiv h=\sqrt{h_{11}^2+h_{12}^2},\quad h_2=-h,$$

$$n_1^2=\frac{1}{2}\left(1+\frac{h_{11}}{h}\right),\quad n_2^2=\frac{1}{2}\left(1-\frac{h_{11}}{h}\right),\quad n_1n_2=\frac{h_{12}}{2h}. \tag{15}$$

Then the evolution relation (11) for $h_{ij}$ becomes

$$(n_1^2-n_2^2)\dot{h}_{11}+2n_1n_2\dot{h}_{12}=e^{-h}(n_1^2\dot{c}_{11}+2n_1n_2\dot{c}_{12}+n_2^2\dot{c}_{22}),$$

$$(n_1^2-n_2^2)\dot{h}_{11}+2n_1n_2\dot{h}_{12}=e^{h}(n_2^2\dot{c}_{11}-2n_1n_2\dot{c}_{12}+n_1^2\dot{c}_{22}),$$

$$2n_1n_2\dot{h}_{11}-(n_1^2-n_2^2)\dot{h}_{12}=\frac{2h}{e^h-e^{-h}}[n_1n_2\dot{c}_{11}-(n_1^2-n_2^2)\dot{c}_{12}-n_1n_2\dot{c}_{22}]. \tag{16}$$

Subtraction of the first two equations yields $0=c_{22}\dot{c}_{11}-2c_{12}\times\dot{c}_{12}+c_{11}\dot{c}_{22}=\frac{d}{dt}(\det c)$ that merely illustrates equivalence of these two equations (here we used $c_{11}=e^hn_1^2+e^{-h}n_2^2$, $c_{22}=e^{-h}n_1^2+e^hn_2^2$, and $c_{12}=(e^h+e^{-h})n_1n_2$). Thus we can safely remove one equation from further consideration.

When we insert all the necessary relations (15) and (1) with (12) and then solve for $\dot{h}_{11}$ and $\dot{h}_{12}$, following final form of viscoelastic equations in **h** form results:

$$\frac{\partial h_{11}}{\partial t}+v_1\frac{\partial h_{11}}{\partial x_1}+v_2\frac{\partial h_{11}}{\partial x_2}-\frac{2}{h^2}\left(h_{11}^2+h_{12}^2h\frac{e^h+e^{-h}}{e^h-e^{-h}}\right)\frac{\partial v_1}{\partial x_1}$$
$$-h_{12}\left[\frac{h_{11}}{h^2}\left(1-h\frac{e^h+e^{-h}}{e^h-e^{-h}}\right)+1\right]\frac{\partial v_1}{\partial x_2}-h_{12}\left[\frac{h_{11}}{h^2}\left(1-h\frac{e^h+e^{-h}}{e^h-e^{-h}}\right)-1\right]\frac{\partial v_2}{\partial x_1}$$
$$+\frac{1}{\theta}\frac{e^h-e^{-h}}{2h}h_{11}=0,$$

$$\frac{\partial h_{12}}{\partial t}+v_1\frac{\partial h_{12}}{\partial x_1}+v_2\frac{\partial h_{12}}{\partial x_2}-\frac{2h_{11}h_{12}}{h^2}\left(1-h\frac{e^h+e^{-h}}{e^h-e^{-h}}\right)\frac{\partial v_1}{\partial x_1}$$
$$-\left[\frac{1}{h^2}\left(h_{12}^2+h_{11}^2h\frac{e^h+e^{-h}}{e^h-e^{-h}}\right)-h_{11}\right]\frac{\partial v_1}{\partial x_2}$$
$$-\left[\frac{1}{h^2}\left(h_{12}^2+h_{11}^2h\frac{e^h+e^{-h}}{e^h-e^{-h}}\right)+h_{11}\right]\frac{\partial v_2}{\partial x_1}+\frac{1}{\theta}\frac{e^h-e^{-h}}{2h}h_{12}=0. \tag{17}$$

Here again $h=\sqrt{h_{11}^2+h_{12}^2}$, and the initial condition is $\boldsymbol{h}=\mathbf{0}$. Together with the equations of continuity and motion, they constitute a complete set to describe isothermal incompressible viscoelastic flow in 2D. However due to the form presented in Eqs.(17), artificial numerical difficulty may arise. Except for the case of rest state, during flow vanishing of the eigenvalue $h$ (it means $\boldsymbol{h}=\mathbf{0}$) may occur locally, e.g. along the centerline in the fully developed Poiseuille flow through a straight pipe. Then the coefficients of $\frac{\partial v_i}{\partial x_j}$ and $h_{ij}$ become apparently indeterminate. However proper introduction of asymptotic relation for vanishing $h$ results in

$$\frac{\partial h_{11}}{\partial t}+v_1\frac{\partial h_{11}}{\partial x_1}+v_2\frac{\partial h_{11}}{\partial x_2}-2\frac{\partial v_1}{\partial x_1}-h_{12}\frac{\partial v_1}{\partial x_2}+h_{12}\frac{\partial v_2}{\partial x_1}+\frac{1}{\theta}h_{11}\approx 0,$$

$$\frac{\partial h_{12}}{\partial t}+v_1\frac{\partial h_{12}}{\partial x_1}+v_2\frac{\partial h_{12}}{\partial x_2}-(1-h_{11})\frac{\partial v_1}{\partial x_2}-(1+h_{11})\frac{\partial v_2}{\partial x_1}+\frac{1}{\theta}h_{12}\approx 0,$$

$$\text{when } h\approx 0. \tag{18}$$

When one employs a Newton's method in solving the nonlinear equations, partial derivatives of the coefficients are to be specified. For example, denoting the coefficient of

$\frac{\partial v_1}{\partial x_1}$ in the first of Eqs.(17) as $\phi(h_{11}, h_{12})$ we have

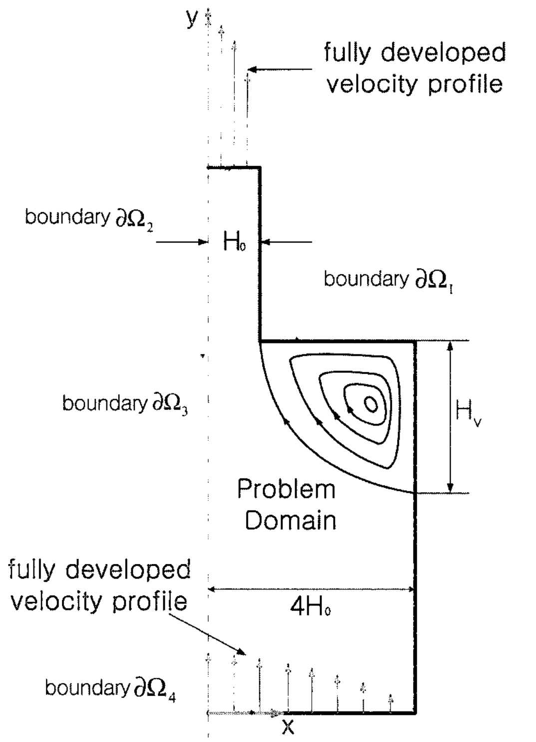
$$\frac{\partial \phi}{\partial h_{11}} = 2\frac{h_{11}h_{12}^2}{h^4}\left[2-h\frac{e^h+e^{-h}}{e^h-e^h}-\left(\frac{2h}{e^h-e^{-h}}\right)^2\right],$$

and its limit behavior becomes $\frac{\partial \phi}{\partial h_{11}} \approx 0$ when $h \approx 0$.

We want to make a last additional remark on the $\boldsymbol{h}$-tensor formulation of the Leonov model. Even in the simplified 2D case, the constitutive relation appears to be quite awkward in its tensor-logarithmic form (17), however the Leonov equation suggests the simplest of all nonlinear viscoelastic differential equations (and thus possibly the simplest of all viscoelastic constitutive models) due to the existence of the first integral, Eq.(13) or (14). Hence in the current author's opinion, this viscoelastic model forms the most efficient and practical equations in modeling especially 3D viscoelastic flows, where we may have to apply for the eigenvalues the cubic formula, the analytical expression of the roots for a cubic polynomial.

## 4. Numerical scheme

We investigate planar 4:1 abrupt contraction flow with centerline symmetry. The flow geometry and boundary conditions are illustrated in Fig. 1. We apply no-slip boundary condition at the wall and specify symmetric natural boundary on the centerline. To remove indeterminacy of pressure, we also set the pressure variable at the exit wall. Fully developed flow conditions are applied for the velocity and $\boldsymbol{h}$ tensor at the inlet but only for the velocity at the outlet. When we denote the half width of the downstream channel as $H_0$, we set the length of the downstream channel as $15H_0$ and the length of the reservoir as $20H_0$. Even though the downstream channel length is rather short to achieve fully developed flow, in order to alleviate computational burden we simply choose this flow geometry, and it seems that the length of the downstream channel does not have any effect on the stability of the compu-




$\partial\Omega_1$ : essential boundary condition for velocity ($\boldsymbol{v} = \boldsymbol{0}$)
$\partial\Omega_2$ : essential boundary condition for velocity
$\partial\Omega_3$ : symmetric boundary condition
$\partial\Omega_4$ : essential boundary condition for velocity and $\mathbf{h}$

**Fig. 1.** Boundary conditions of the 4:1 contraction flow problem.

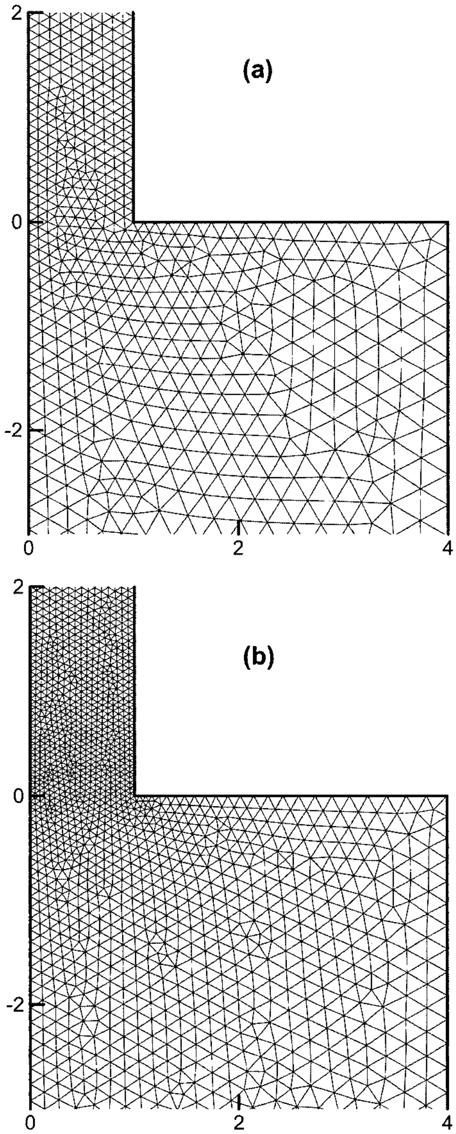



**Fig. 2.** Partial view of the (a) coarse and (b) fine meshes employed in this study.

tational procedure.

With the standard Galerkin formulation adopted as basic computational framework, either streamline-upwinding (SU) or streamline-upwind/Petrov-Galerkin (SUPG) method as well as discrete elastic viscous stress splitting (DEVSS) algorithm is implemented in order to build relatively robust numerical scheme at high Deborah number flows. The upwinding algorithm developed by Gupta (1997) has been applied. The SU method additionally adds to the original Galerkin formulation an inconsistent upwind term that gives only the first order accuracy in spatial discretization. However the SUPG scheme is consistent and endows a second order accuracy. Even though we report in this paper results based on both upwinding algorithms, we are mainly concerned with results under the SUPG method. Two types of meshes are employed for the computation, and they are illustrated in Fig. 2. The coarse mesh (Fig. 2a) has the smallest corner element with the side length of $0.1H_0$, while the fine mesh (Fig. 2b) contains the smallest one with the side length of $0.05H_0$. Corresponding mesh details are given in Table 1. As has been mentioned beforehand, in the $\boldsymbol{h}$-formulation we have fewer unknowns.

Linear for pressure and strain rate and quadratic interpolation for velocity and $\boldsymbol{h}$-tensor are applied for spatial continuation of the variables. In this work, we only consider steady inertialess flow of the isothermal incompressible liquid. In order to mimic dimensionless formulation, we simply assign unit values for $G$ and $\theta$ and adjust the Deborah number by the variation of the average flow rate. The Deborah number in this contraction flow is usually defined as

$$De \equiv \frac{U\theta}{H_0}, \tag{19}$$

where $U$ is the average downstream velocity. Also $n = 0.1$ is set to guarantee the mathematical stability even in stress predefined flow history (Kwon and Leonov, 1995) (e.g. in the situation where one assigns traction boundary conditions at the inlet and outlet), whereas $n = 0$ corresponds to the case of neo-Hookean potential in finite elasticity.

In order to solve the large nonlinear system of equations introduced, the Newton iteration is used in linearizing the system and the frontal elimination method is implemented for solution update. As an estimation measure to determine the solution convergence, the $L_\infty$ norm scaled with the maximum value in the computational domain is employed. Hence when the variation of each nodal variable in the Newton iteration does not exceed $10^{-4}$ of its value in the previous iteration, the algorithm concludes that the converged solution is attained. For the viscoelastic variables, we examine the relative error in terms of the eigenvalue of the $\boldsymbol{c}$-tensor. We have found that this convergence criterion imposes less stringent computational procedure, and it seems quite practical and appropriate since we mainly observe the results in terms of physically meaningful $\boldsymbol{c}$-tensor or stress rather than $\boldsymbol{h}$.

## 5. Results and discussion

The convergence limit in the scale of the Deborah number is listed in Table 2 for the original $\boldsymbol{c}$-formulation and the logarithm-transformed $\boldsymbol{h}$-formulation. With the SUPG method, in the conventional $\boldsymbol{c}$-tensor representation the convergence limits are 3.2 for the coarse mesh and as low as 0.3 for the fine mesh. In addition to this severe limitation of flow rate in computation, one can observe steep decrease of the limit Deborah number with the mesh refinement. On the contrary, when we switch to the $\boldsymbol{h}$-tensor equations, we can examine huge increase of the limit Deborah number to 132 and even higher value of 193 in finer discretization. Even though the results under the SU scheme are not major concern in this work due to its lower order accuracy, they deserve a brief summary. Even though the limit value is relatively high, it decreases as the mesh becomes finer under the $\boldsymbol{c}$-formulation. However with the logarithmic tensor formulation the limit values exceed 200 for both meshes and we simply have stopped further computation due to no further interest.

In Fig. 3 the streamlines at the highest Deborah number

**Table 2.** Limit of Deborah numbers achievable for each mesh types under the SUPG method with each constitutive formulation indicated (the limit value for the SU scheme is given inside the parenthesis)

| | Coarse mesh (Fig. 2a) | Fine mesh (Fig. 2b) |
|---|---|---|
| $\boldsymbol{c}$-formulation | 3.2 (142) | 0.3 (65) |
| $\boldsymbol{h}$-formulation | 132 (> 200) | 193 (> 200) |

**Table 1.** Total numbers of elements, nodes and variables for two meshes

| | | No. of elements | No. of linear nodes | No. of quadratic nodes | No. of unknowns |
|---|---|---|---|---|---|
| Coarse mesh | $\boldsymbol{c}$-formulation | 3491 | 1920 | 7330 | 44330 |
| | $\boldsymbol{h}$-formulation | | | | 37000 |
| Fine mesh | $\boldsymbol{c}$-formulation | 7174 | 3835 | 14843 | 89555 |
| | $\boldsymbol{h}$-formulation | | | | 74712 |

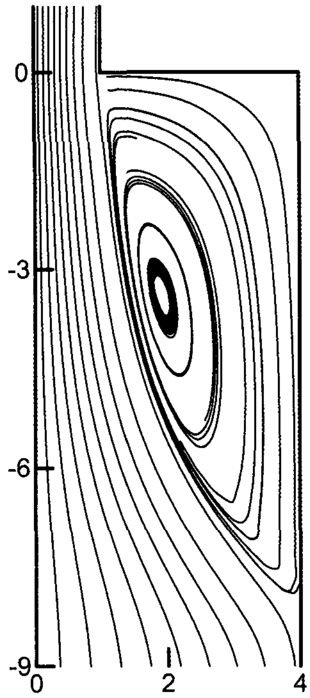



**Fig. 3.** Streamlines at $De = 193$ for the fine mesh (Fig. 2b) computed with the SUPG method.

of 193 for the fine mesh is depicted, where the size of the corner vortex reaches almost twice the half width of the reservoir channel. Fig. 4 illustrates highly inhomogeneous distribution of elastic potential and normal and shear stresses, respectively, all of which display extremely steep variation near the corner. Near the corner these three rheological variables achieve their maximum values such as $W_{max} = 93.9$, $\tau_{yy,max} = 189$ and $|\tau_{xy}|_{max} = 31$. In Fig. 5 the extra-stress profiles are shown as a function of $y$ (the flow direction) at $x = 1$ (scaled with $H_0$). Thus the region of $0 \le y \le 5$ means the location at the downstream wall. Here we do not observe fluctuation of stress variables along the wall, which have been frequently examined in many publications. At this point, we do not intend to explain this difference in results. This disappearance of numerical artifacts may be due either to this appropriate formulation or to the constitutive equations employed herein. At least, one may observe one proper tendency that the peaks of the stress variables become sharper as the mesh becomes finer.

The important advantage of this new formulation in computational rheology consists not only in the stabilizing effect of the whole numerical scheme demonstrated just now, but also in appropriate mesh convergence possibly achievable with this formalism since finer discretization seems to yield better convergence. Even though Hulsen (2004) and Fattal and Kupferman (2004) have reported almost unlimited convergence with this ***h***-formulation, in this current flow geometry one may not be able to expect such unconditional numerical stability since there exists

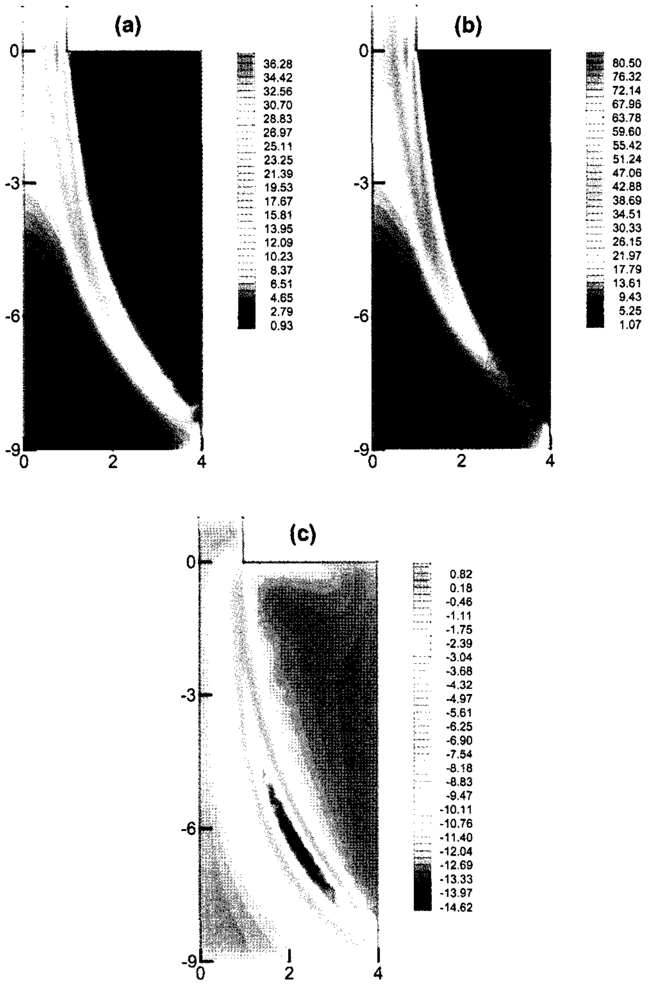



**Fig. 4.** Contour lines of (a) elastic potential $W$, (b) normal stress in the flow direction and (c) shear stress at $De = 193$ for the fine mesh (Fig. 2b) computed with the SUPG method.

corner singularity. In this type of computational domain, even the linear problem exhibits singular behavior, that is, the gradient of the solution function approaches infinity (actually integrable singularity) near the corner (e.g. Johnson, 1995). In this case, mesh refinement resolves such difficulty, in other words the solution becomes more accurate as the discretization refines. However until now, there has been no conclusive result in viscoelastic flow modeling, and most probably finer mesh in finite element analysis deteriorates the numerical scheme more severely (Crochet *et al.*, 1984; Baaijens, 1998).

With thorough examination of all the available results obtained until now (Hulsen, 2004; Fattal and Kupferman, 2004) including the one in this manuscript, there is relatively high possibility of eventual resolution of the high Deborah number flow problem, even though more extensive study of mesh convergence, etc. in various flow geometries is certainly required. At least, one may conclude that this formalism seems quite promising and deserves inten-

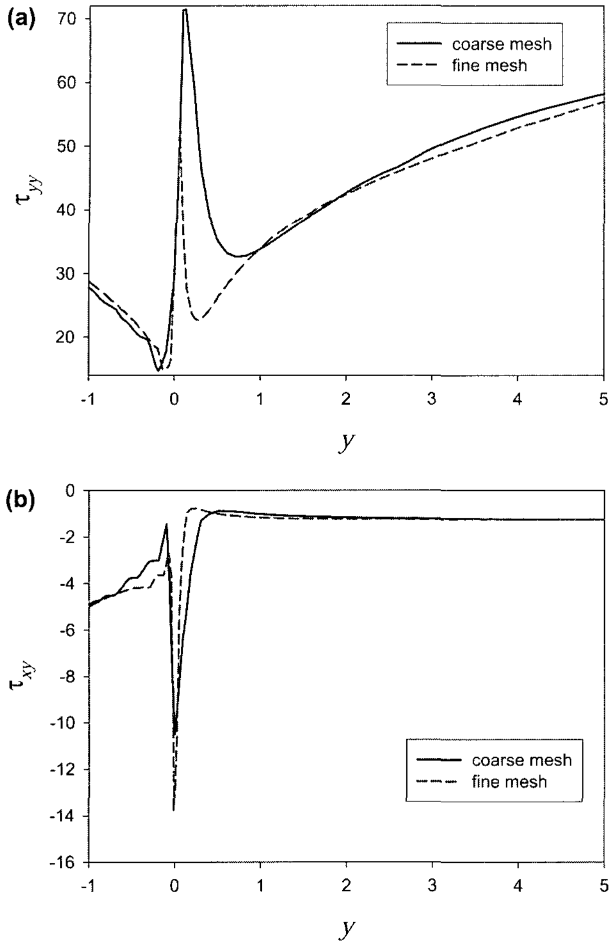



**Fig. 5.** Extra-stress profiles along the downstream wall ($x = 1$) at $De = 100$ for the coarse and fine meshes (Fig. 2) computed with the SUPG method: (a) the normal stress $\tau_{yy}$ in the flow direction, (b) shear stress $\tau_{xy}$.

sive further investigations.

In the author's opinion, understanding why this new formulation completely equivalent to the original model equations preserves better numerical characteristics and verifying whether it may work well for all other transformable differential constitutive equations, are extremely crucial. First, as mentioned by Fattal and Kupferman (2004), the polynomial interpolation of the logarithm of $\boldsymbol{c}$ seems quite appropriate and efficient, since inside the viscoelastic boundary layer or near the singular corner the solution of $\boldsymbol{c}$ exhibits steep exponential variation and this logarithmic formulation transforms exponential dependence into linear or polynomial one.

At this point, it is worthwhile to examine more carefully the result given by Hulsen (2004), where the benchmark problem of flow around a cylinder inside a straight pipe has been considered. When implementing this $\boldsymbol{h}$-formalism, he has observed almost limitless numerical convergence with the Giesekus model, whereas almost no improvement has been attained with the Oldroyd-B equation. The cause of this substantial difference is clearly evident if one is well aware of the mathematical stability characteristics of these two equations. There is one theorem on the positive definiteness of the conformation tensor $\boldsymbol{c}$ and its boundedness proven for the differential constitutive equations (Hulsen, 1990; Leonov, 1992; almost all available stability results are summarized in Kwon and Leonov, 1995). The upper-convected Maxwell and thus the Oldroyd-B models violate this theorem, and their unbounded stress behavior in uniaxial extensional flow in the strain rate exceeding the half of reciprocal relaxation time is this well-known example. However the Giesekus model with the numerical parameter (written as $\alpha$ in Kwon and Leonov, 1995) not exceeding 1/2 is always mathematically stable when we include the Newtonian term or consider only pre-defined strain history. Similar trend may be seen in finite element modeling of contraction flow in $\boldsymbol{c}$-formalism (Lee *et al.*, 2004).

It has been known for quite long time that the conformation tensor $\boldsymbol{c}$ has to remain strictly positive-definite in the whole flow domain at all time, the violation of which immediately invokes the Hadamard instability (Dupret and Marchal, 1986; Kwon and Leonov, 1995). Even for the constitutive equations proven Hadamard stable, numerical error seems to cause the violation of the positive-definiteness (Dupret *et al.*, 1985; Lee *et al.*, 2004). The tensor-logarithmic transformation by Fattal and Kupferman (2004) rigorously preserves this essential requirement, which seems to be the most important among all features in this formulation.

Note that for some differential constitutive equations even the positive-definiteness of the conformation tensor is not guaranteed (Kwon and Leonov, 1995; Kwon and Cho, 2001), for which the tensor-logarithmic transform itself is not valid at all. Therefore it is quite certain that this $\boldsymbol{h}$-tensor formulation will work in the high Deborah number flow modeling only for very limited versions of constitutive equations. As a conclusion, the stability criteria suggested in Kwon and Leonov (1995) may play an important role on the choice of viscoelastic equations in flow modeling and even on formulating new constitutive relations.

## 6. Conclusions

We present an alternative procedure obtaining the tensor-logarithm representation of the differential constitutive equations for the conformation tensor, which has been suggested originally by Fattal and Kupferman (2004). Concrete example of the procedure is also given in 2D case and numerical result for 4:1 planar contraction flow has been demonstrated with the Leonov constitutive equation. The result shows better convergence with mesh refinement as well as astonishing stabilization of the numerical scheme.

This new formalism exactly equivalent to the original constitutive model seems to work extremely well as long as proper viscoelastic field equations are employed. This tensor-logarithm formulation, if applied with careful consideration of mathematical stability of viscoelastic models, seems quite promising and possibly resolves the high Deborah number problems in computational rheology.

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