

This is an Open Access document downloaded from ORCA, Cardiff University's institutional repository:<https://orca.cardiff.ac.uk/id/eprint/114954/>

This is the author's version of a work that was submitted to / accepted for publication.

Citation for final published version:

Jafari, Azadeh, Chitsaz, Alizera, Nouri, Reza and Phillips, Timothy N. 2018. Property preserving reformulation of constitutive laws for the conformation tensor. *Theoretical and Computational Fluid Dynamics* 32 , pp. 789-803. 10.1007/s00162-018-0476-y

Publishers page: <https://doi.org/10.1007/s00162-018-0476-y>

Please note:

Changes made as a result of publishing processes such as copy-editing, formatting and page numbers may not be reflected in this version. For the definitive version of this publication, please refer to the published source. You are advised to consult the publisher's version if you wish to cite this paper.

This version is being made available in accordance with publisher policies. See <http://orca.cf.ac.uk/policies.html> for usage policies. Copyright and moral rights for publications made available in ORCA are retained by the copyright holders.



1 **Property Preserving Reformulation of Constitutive**
2 **Laws for the Conformation Tensor**

3 **Azadeh Jafari · Alireza Chitsaz · Reza**
4 **Nouri · Timothy N. Phillips**

5
6 Received: date / Accepted: date

7 **Abstract** The challenge for computational rheologists is to develop efficient
8 and stable numerical schemes in order to obtain accurate numerical solutions
9 for the governing equations at values of practical interest of the Weissenberg
10 numbers. This study presents a new approach to preserve the symmetric positive
11 definiteness of the conformation tensor and to bound the magnitude of
12 its eigenvalues. The idea behind this transformation is lies with the matrix
13 logarithm formulation. Under the logarithmic transformation, the eigenvalue
14 spectrum of the new conformation tensor varies from infinite positive to infinite
15 negative. But, reconstruction the classical formulation from unbounded
16 eigenvalues doesn't achieve meaningful results. This enhanced formulation,
17 hyperbolic tangent, prevails the previous numerical failure by bounding the
18 magnitude of eigenvalues in a manner that positive definite is always satisfied.
19 In order to evaluate the capability of the hyperbolic tangent formulation we
20 performed a numerical simulation of FENE-P fluids in a rectangular channel
21 in the context of the finite element method. Under this new transformation,
22 the maximum attainable Weissenberg number increases 21.4% and 112.5%
23 comparing the standard log-conformation and classical constitutive equation
24 respectively.

A. Jafari
School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran,
P.O. Box: 11155-4563, Iran
Tel.: +98-21-61114037
E-mail: azadeh.jafari@ut.ac.ir

R. Nouri
School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran,
P.O. Box: 11155-4563, Iran

A. Chitsaz
School of Mechanical Engineering, College of Engineering, University of Tehran, Tehran,
P.O. Box: 11155-4563, Iran

T.N. Phillips
School of Mathematics, Cardiff University, Cardiff, CF24 4AG, United Kingdom

25 **Keywords** Viscoelastic fluid flows · High Weissenberg number problem ·
26 Hyperbolic tangent

27 1 Introduction

28 It is well known that the conformation tensor should, in principle, remain sym-
29 metric positive definite (SPD) as it evolves in time [8]. In fact, this property is
30 crucial for the well-posedness of its evolution equation [12,4]. Although many
31 constitutive equations have been proven to be Hadamard stable, in practice
32 this property is violated in many numerical simulations. Most likely, this is
33 caused by the accumulation of spatial discretization error that arises from
34 numerical integration of the governing equations. This gives rise to spurious
35 negative eigenvalues, causing the conformation tensor to lose its SPD property
36 and Hadamard instabilities to grow. This was an obstacle to early attempts
37 to numerically simulate viscoelastic fluids [14].

38 Recently, a logarithm representation of the conformation tensor was proposed
39 by Fattal and Kupferman [5,6]. The essential idea is based on the conjecture
40 that the high Weissenberg number problem (HWNP) may be caused by the
41 failure of polynomial-based approximations to properly represent exponential
42 profiles developed by the conformation tensor in regions of high strain rate for
43 high Deborah number flows. The deformation term in the constitutive equation
44 is composed of extensional and rotational components. The extensional com-
45 ponent under the logarithmic transformation acts additively rather than mul-
46 tiplicatively in the standard formulation. So, the polynomial interpolation can
47 properly capture the steep stress gradient in the logarithmic transformation.
48 This proposed transformation preserves the symmetric positive definiteness of
49 the conformation tensor even at high Weissenberg number for any numerical
50 scheme.

51 Hulsen et al. [9] first implemented the log conformation formulation in a fi-
52 nite element context, using the DEVSS/DG formulation for the flow around a
53 cylinder for the Oldroyd-B and Giesekus models. Under the logarithm trans-
54 formation, the maximum attainable Weissenber number was around 100. How-
55 ever they reported a lack of convergence near the cylinder for the Oldroyd-B
56 model.

57 Kwon [11] presented an alternative derivation of the tensor logarithmic rep-
58 resentation of the differential constitutive equation and provided a numerical
59 example with the Leonov model for the flow through a 4:1 planar contrac-
60 tion using SUPG and SU stabilization techniques. Dramatic improvement
61 of the performance of the computational algorithm with stable convergence
62 was demonstrated. The author achieved converged numerical solutions for
63 $De = 132$ with a coarse mesh and $De = 193$ for a refined mesh. This new
64 formulation can be used only for the few differential constitutive equations
65 that have been proven to be globally stable [13].

66 Vaithianathan and Collins [17] recently presented two matrix decompositions
67 that guaranteed the construction of a conformation tensor in a manner that

68 ensures that positive definiteness is always satisfied. In parallel, they also pro-
69 posed a change of variable in the conformation tensor in order to also enforce
70 the boundness of its trace, as dictated by the constitutive model used (FENE-
71 P). The algorithms were implemented into isotropic turbulence simulations.

72 A simple alternative form of the log conformation formulation was proposed
73 by Coronado et al. [3]. The flows of Oldroyd-B and Larson-type fluids were
74 simulated for the benchmark problem of flow past a cylinder in a channel
75 using DEVSSS-TG/SUPG methods. The maximum attainable Weissenberg
76 numbers were 1.05 and 12.3, respectively.

77 Housiadas et al. [7] introduced a different implementation of the log-conformation
78 representation to allow for very accurate spectral approximations and efficient
79 time integration while smoothing the final result explicitly by applying a multi-
80 grid diffusion correction directly to the classical conformation tensor. In order
81 to eradicate numerical errors, they introduced a smoothing operation that re-
82 moved non-physical instabilities from the numerical approximation.

83 Jafari et al. [10] showed that although the use of the log conformation tensor
84 can be helpful in preserving the symmetric positive definiteness of the confor-
85 mation tensor, it is also mandatory for the FENE family of models to satisfy
86 the boundedness of the conformation tensor. In order to remove numerical
87 instabilities a new extended matrix logarithm formulation was developed.

88 Tomé et al. [16] applied the log formulation for time dependent extrudate swell
89 and jet buckling of UCM fluids. The momentum equation is solved using a fi-
90 nite difference marker-and-cell type method. Their numerical results showed a
91 significant increase in the maximum attainable Weissenberg number for both
92 case studies.

93 Afonso et al. [1] presented a generic formulation for many transformation rules
94 applicable to conformation tensor models. The kernel-conformation transfor-
95 mation function can include any continuous, invertible and differentiable ma-
96 trix transformation. In their paper, Afonso et al. [1] considered the linear
97 shifted, logarithmic and k th root functions of the conformation tensor \mathbf{C} and
98 applied the approach to the benchmark problem of flow of an Oldroyd B fluid
99 past a confined cylinder to assess the relative merits of these functions. At low
100 Weissenberg numbers they found that this approach generates results that are
101 consistent with the standard discretization of the conformation tensor. How-
102 ever, the numerical efficiency of this approach at high Weissenberg numbers is
103 highly dependent on the choice of kernel function and the singularities intro-
104 duced either by physical description of the flow or the choice of constitutive
105 equation.

106 Saramito [15] proposed a new log-conformation formulation for Johnson-Segalman
107 viscoelastic fluids. In contrast to the formulation of Fattal and Kupferman, this
108 new transformation is non-singular as the Weissenberg number tends to zero.
109 He applied this new formulation to the lid driven cavity in the context of the
110 finite element method using velocity-pressure approximation and discontinu-
111 ous Galerkin upwind treatment for stress. The numerical results are in good
112 agreement qualitatively with experimental measurements.

113 Comminal et al. [2] presented a new streamfunction/log-conformation formula-

tion for Oldroyd-B fluids. Regarding the pressureless formulation, the numerical results are free from pressure-velocity decoupling errors, which enhances the robustness and efficiency of the algorithm. Their numerical results at high Wessener number around 5 show quasi-periodic instability at the upstream corner of the moving wall.

The log transformation guarantees the positive eigenvalues of the conformation tensor during numerical simulations. While the action of the symmetric positive definite (SPD) property of the conformation tensor during the simulation is a necessary condition for stable simulations, it is definitely not a sufficient condition to reach meaningful results. Actually, solving the constitutive equation in the new scale, logarithmically, allows the eigenvalues of the new conformation tensor to range over the entire real line from infinite negative to infinite positive values while reconstructing the classical conformation tensor from either infinite positive or infinite negative eigenvalues does not have any physical meaning.

The aim of this paper is the development of a mathematical model to preserve both the SPD of the conformation tensor and also to bound the magnitude of the eigenvalues. The hyperbolic tangent formulation of the constitutive equation removes some of the stiffness associated with the standard form of the constitutive equation. We demonstrate that this has the effect of increasing the critical Weissenberg number, thereby delaying the so-called high Weissenberg number problem.

There are a number of alternative formulations proposed in the literature such as the new extended matrix logarithm formulation [13] and the sequence mapping of Housiadas et al. [12]. These two formulations are based on the log conformation representation for viscoelastic fluids which is designed to preserve symmetric positive definiteness. Both formulations use an additional mapping to ensure that the eigenvalues of the conformation tensor are bounded. In contrast, the hyperbolic tangent formulation proposed in the present article preserves the symmetric positive definiteness and bounds the eigenvalues of the conformation tensor simultaneously. This is a major advantage of the approach described in this paper.

This paper is organized as follows. A new state-of-the-art reformation of the constitutive equation using the hyperbolic tangent tensor is introduced in Section 2. The detailed differential constitutive equation for the hyperbolic tangent tensor in 2D is presented in Section 3. Some numerical results are presented in Section 4 that demonstrate the enhanced stability properties of the new reformulation of the constitutive equation.

2 The state-of-the-art of the hyperbolic tangent tensor

Most differential constitutive models can be written in the following general form:

$$\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} - (\nabla \mathbf{u})^T \cdot \mathbf{C} - \mathbf{C} \cdot \nabla \mathbf{u} = \frac{1}{We} \boldsymbol{\Psi} \quad (1)$$

155 where \mathbf{C} is the conformation tensor, \mathbf{u} is the velocity field and $\boldsymbol{\Psi}$ is a model-
 156 dependent tensor function of \mathbf{C} with coefficients that possibly depend on the
 157 invariants of \mathbf{C} or the rate of deformation tensor. For example, the Oldroyd-B
 158 model is characterized by $\boldsymbol{\Psi} = \mathbf{I} - \mathbf{C}$, the FENE-CR model by $\boldsymbol{\Psi} = \frac{\mathbf{I} - \mathbf{C}}{1 - \frac{\text{tr}(\mathbf{C})}{b^2}}$
 159 where the parameter b measures the maximum extensibility of the dumbbells,
 160 and the FENE-P model by $\boldsymbol{\Psi} = \mathbf{I} - \frac{\mathbf{C}}{1 - \frac{\text{tr}(\mathbf{C})}{b^2}}$.

161 As explained in the introduction, Fattal and Kupferman [5] proposed a re-
 162 formulation of classical constitutive equations by introducing a new variable
 163 $\mathbf{H} = \ln(\mathbf{C})$ to derive the so-called logarithmic formulation. An important
 164 observation is that the logarithm is an isotropic tensor function and so \mathbf{C}
 165 and \mathbf{H} possess an identical set of principal axes. This transformation forces
 166 the eigenvalues of the conformation tensor to remain positive throughout the
 167 simulation. Solving the constitutive equation in the new formulation for the
 168 logarithm of the conformation tensor means that the eigenvalues of the new
 169 conformation tensor, \mathbf{H} , range over the whole real line $(-\infty, +\infty)$, which en-
 170 forces the eigenvalues of the classical conformation tensor, \mathbf{C} , to range over
 171 the positive semi-infinite interval $[0, +\infty)$ (Fig.1a).

172 Reconstructing the classical conformation and viscoelastic stress tensors
 173 from eigenvalues that are unbounded does not have any physical meaning. A
 174 possible remedy which would bound the magnitude of the eigenvalues of \mathbf{C} is
 175 to use the hyperbolic tangent of \mathbf{H} (Fig.1b). As is obvious from this figure,
 176 however, the variation of the eigenvalues of \mathbf{H} is in the interval $(-\infty, +\infty)$,
 177 while the eigenvalues of \mathbf{C} are totally bounded and contained in the interval
 178 $[-1, +1]$. To preserve the symmetric positive definiteness of the conformation
 179 tensor, it is mandatory to ensure that the eigenvalues of the conformation
 180 tensor, \mathbf{C} , are non-negative. To do so, we use the enhanced formulation of
 181 hyperbolic tangent of the conformation tensor. We transform the classical
 182 constitutive equation based on the conformation tensor, \mathbf{C} , to a new one based
 183 on the tensor \mathbf{H} , where \mathbf{C} and \mathbf{H} are related by:

$$\mathbf{C} = M(\tanh(\mathbf{H}) + \mathbf{I}) \quad (2)$$

184 or:

$$\mathbf{C} = 2M \frac{e^{\mathbf{H}}}{e^{\mathbf{H}} + e^{-\mathbf{H}}} \quad (3)$$

185 where M is a constant that is model-dependent. For example, for the FENE
 186 family, the square of the corresponding finite extensibility parameter of the
 187 polymer must be an upper limit for the trace of the conformation tensor. So
 188 M should be chosen in some way to satisfy this condition ($M \geq \frac{b^2}{2}$). This
 189 new formulation preserves both the SPD of the conformation tensor and also
 190 bounds the magnitude of the eigenvalues of \mathbf{C} . Any function of a positive
 191 definite matrix is by definition an isotropic function of the original tensor.
 192 Therefore \mathbf{C} and \mathbf{H} have a common set of eigenvectors.

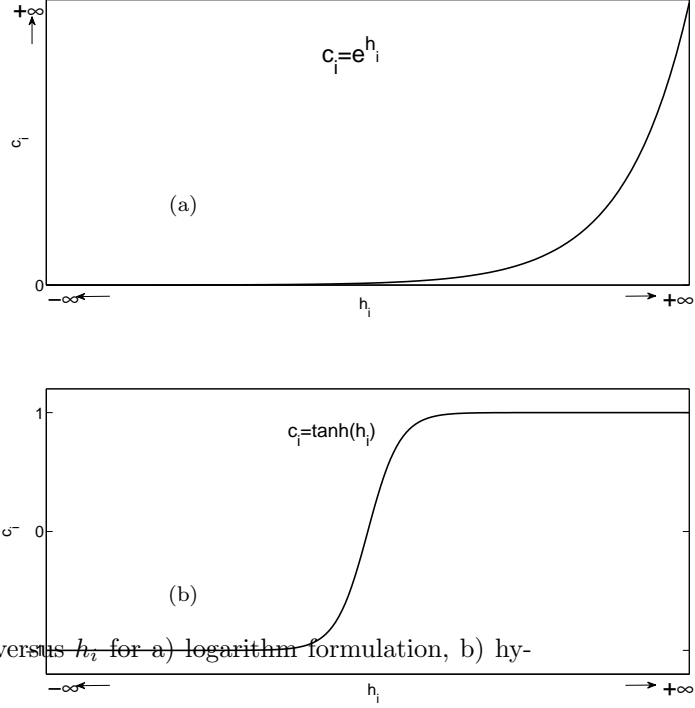


Fig. 1: Typical variation of c_i versus h_i for a) logarithm formulation, b) hyperbolic tangent formulation.

193 3 Hyperbolic Tangent Formulation of the Constitutive Equation

194 In this study, we follow the approach adopted by Kwon [11] for deriving the
 195 evolution equations. In the case of 2D planar flow, and adopting the same
 196 notation as Kwon, the eigenvalue problem for the conformation tensor \mathbf{H} in
 197 the continuous domain yields the eigenvalues:

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

$$h_2 = \frac{1}{2} \left[h_{11} + h_{22} - \sqrt{(h_{11} - h_{22})^2 + 4h_{12}^2} \right] \quad (5)$$

198 The eigenvectors of \mathbf{H} are written in the form:

$$\mathbf{n}_1 = \begin{bmatrix} n_1 \\ n_2 \end{bmatrix} \quad \text{and} \quad \mathbf{n}_2 = \begin{bmatrix} -n_2 \\ n_1 \end{bmatrix} \quad (6)$$

199 with $n_1^2 + n_2^2 = 1$. The components of the eigenvectors can be determined by
 200 solving the characteristic equation for \mathbf{H} :

$$n_1^2 = \frac{h_{12}^2}{(h_1 - h_{11})^2 + h_{12}^2} \quad (7)$$

$$n_2^2 = \frac{(h_1 - h_{11})^2}{(h_1 - h_{11})^2 + h_{12}^2} \quad (8)$$

$$n_1 n_2 = \frac{h_{12}(h_1 - h_{11})}{(h_1 - h_{11})^2 + h_{12}^2} \quad (9)$$

201 The characteristic equation for \mathbf{C} is written as:

$$\mathbf{C} \cdot \mathbf{n}_i = c_i \mathbf{n}_i \quad (10)$$

202 Differentiation of the above equation with respect to time yields:

$$\dot{\mathbf{C}} \cdot \mathbf{n}_i + \mathbf{C} \cdot \dot{\mathbf{n}}_i = \dot{c}_i \mathbf{n}_i + c_i \dot{\mathbf{n}}_i \quad (11)$$

203 Then taking the scalar product with another eigenvector yields the following
204 result:

$$\begin{aligned} \mathbf{n}_j \cdot \dot{\mathbf{C}} \cdot \mathbf{n}_i &= \mathbf{n}_j \cdot (\dot{c}_i \mathbf{n}_i) + \mathbf{n}_j \cdot (c_i \dot{\mathbf{n}}_i) - \mathbf{n}_j \cdot (\mathbf{C} \cdot \dot{\mathbf{n}}_i) \\ &= \dot{c}_i \delta_{ij} + (c_i - c_j) \dot{\mathbf{n}}_i \cdot \mathbf{n}_j \end{aligned} \quad (12)$$

205 from which we deduce:

$$\begin{aligned} i) \quad \dot{c}_i &= \mathbf{n}_i \cdot \dot{\mathbf{C}} \cdot \mathbf{n}_i && \text{when } i = j \\ ii) \quad \dot{\mathbf{n}}_i \cdot \mathbf{n}_j &= \frac{1}{c_i - c_j} \mathbf{n}_j \cdot \dot{\mathbf{C}} \cdot \mathbf{n}_i && \text{when } i \neq j \end{aligned} \quad (13)$$

206 Due to the isotropic function relation, \mathbf{C} and \mathbf{H} have the same set of eigen-
207 vectors. For the \mathbf{H} -tensor, an equivalent relation is readily obtained as:

$$\mathbf{n}_j \cdot \dot{\mathbf{H}} \cdot \mathbf{n}_i = \dot{h}_i \delta_{ij} + (h_i - h_j) \dot{\mathbf{n}}_i \cdot \mathbf{n}_j \quad (14)$$

208 Introducing $h_i = \frac{1}{2} \ln\left(\frac{c_i}{2M - c_i}\right)$ so that $\dot{h}_i = M \frac{\dot{c}_i}{c_i(2M - c_i)}$, and combining Eqs.
209 (13) and (14), one obtains:

$$\begin{aligned} i) \quad \mathbf{n}_i \cdot \dot{\mathbf{H}} \cdot \mathbf{n}_i &= M \frac{\dot{c}_i}{c_i(2M - c_i)} = \frac{M}{c_i(2M - c_i)} \mathbf{n}_i \cdot \dot{\mathbf{C}} \cdot \mathbf{n}_i && \text{when } i = j \\ ii) \quad \mathbf{n}_i \cdot \dot{\mathbf{H}} \cdot \mathbf{n}_j &= (h_j - h_i) \dot{\mathbf{n}}_j \cdot \mathbf{n}_i = \frac{h_i - h_j}{c_i - c_j} \mathbf{n}_i \cdot \dot{\mathbf{C}} \cdot \mathbf{n}_j && \text{when } i \neq j \end{aligned} \quad (15)$$

210 In the 2D case Eq. (15) yields:

$$A \begin{pmatrix} \dot{H}_{11} \\ \dot{H}_{12} \\ \dot{H}_{22} \end{pmatrix} = B \quad (16)$$

211 where A is defined by:

$$A = \begin{pmatrix} n_1^2 & 2n_1n_2 & n_2^2 \\ n_2^2 & -2n_1n_2 & n_1^2 \\ -n_1n_2 & (n_1^2 - n_2^2) & n_1n_2 \end{pmatrix} \quad (17)$$

212 and B by:

$$B = \begin{pmatrix} \frac{M}{c_1(2M-c_1)}(n_1^2\dot{C}_{11} + 2n_1n_2\dot{C}_{12} + n_2^2\dot{C}_{22}) \\ \frac{M}{c_2(2M-c_2)}(n_2^2\dot{C}_{11} - 2n_1n_2\dot{C}_{12} + n_1^2\dot{C}_{22}) \\ \frac{h_1-h_2}{c_1-c_2}(-n_1n_2\dot{C}_{11} + (n_1^2 - n_2^2)\dot{C}_{12} + n_1n_2\dot{C}_{22}) \end{pmatrix} \quad (18)$$

213 Multiplying both sides of Eq. (16) by A^{-1} one obtains the evolution equation
214 for the components of \mathbf{H} :

$$\begin{aligned} \dot{H}_{11} &= \left(\frac{M}{c_1(2M-c_1)}n_1^4 + \frac{M}{c_2(2M-c_2)}n_2^4 + 2n_1^2n_2^2\frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{11} \\ &+ \left(\frac{M}{c_1(2M-c_1)}2n_1^3n_2 - \frac{M}{c_2(2M-c_2)}2n_1n_2^3 - 2n_1n_2(n_1^2 - n_2^2)\frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{12} \\ &+ \left(\frac{M}{c_1(2M-c_1)}n_1^2n_2^2 + \frac{M}{c_2(2M-c_2)}n_1^2n_2^2 - 2n_1^2n_2^2\frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{22} \\ &= G_{11}\dot{C}_{11} + G_{12}\dot{C}_{12} + G_{13}\dot{C}_{22} \end{aligned} \quad (19)$$

$$\begin{aligned} \dot{H}_{12} &= \left(\frac{M}{c_1(2M-c_1)}n_1^3n_2 - \frac{M}{c_2(2M-c_2)}n_1n_2^3 - n_1n_2(n_1^2 - n_2^2)\frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{11} \\ &+ \left(\frac{M}{c_1(2M-c_1)}2n_1^2n_2^2 + \frac{M}{c_2(2M-c_2)}2n_1^2n_2^2 + (n_1^2 - n_2^2)^2\frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{12} \\ &+ \left(\frac{M}{c_1(2M-c_1)}n_1n_2^3 - \frac{M}{c_2(2M-c_2)}n_1^3n_2 + n_1n_2(n_1^2 - n_2^2)\frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{22} \\ &= G_{21}\dot{C}_{11} + G_{22}\dot{C}_{12} + G_{23}\dot{C}_{22} \end{aligned} \quad (20)$$

$$\begin{aligned}
\dot{H}_{22} &= \left(\frac{M}{c_1(2M-c_1)} n_1^2 n_2^2 + \frac{M}{c_2(2M-c_2)} n_1^2 n_2^2 - 2n_1^2 n_2^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{11} \\
&+ \left(\frac{M}{c_1(2M-c_1)} 2n_1 n_2^3 - \frac{M}{c_2(2M-c_2)} 2n_1^3 n_2 + 2n_1 n_2 (n_1^2 - n_2^2) \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{12} \\
&+ \left(\frac{M}{c_1(2M-c_1)} n_1^4 + \frac{M}{c_2(2M-c_2)} n_1^4 + 2n_1^2 n_2^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{22} \\
&= G_{31} \dot{C}_{11} + G_{32} \dot{C}_{12} + G_{33} \dot{C}_{22}
\end{aligned} \tag{21}$$

215 where \dot{H}_{ij} and \dot{C}_{ij} are the components of the material time derivative of the
216 corresponding matrices which can be expressed by:

$$\dot{\mathbf{H}} = \frac{\partial \mathbf{H}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{H} \tag{22}$$

$$\dot{\mathbf{C}} = \frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} \tag{23}$$

217 The above system of equations (19)-(21) can be summarized as:

$$\begin{pmatrix} \dot{H}_{11} \\ \dot{H}_{12} \\ \dot{H}_{22} \end{pmatrix} = \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix} \begin{pmatrix} \dot{C}_{11} \\ \dot{C}_{12} \\ \dot{C}_{22} \end{pmatrix} \tag{24}$$

218 If we substitute Eq. (22) and (23) in Eq. (24), we get the following equation:

$$\frac{\partial \mathbf{H}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{H} = \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix} \left(\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} \right) \tag{25}$$

219 4 Numerical Validation

220 In order to validate the proposed formulation, we compared the hyperbolic
221 tangent conformation formulation for FENE-P fluids with the classical and
222 logarithmic conformation formulations. To achieve this purpose, numerical
223 simulations in a 2D rectangular channel were performed. The computational
224 domain is shown in Fig. 2.

225 In this section, we use the centerline velocity, U_{max} , as the characteristic flow
226 speed, the channel width, D , as the length scale, the time scale $\frac{D}{U_{max}}$, the
227 reference pressure ρU_{max}^2 and $\frac{\mu_t U_{max}}{D}$ as the characteristic polymeric stress
228 tensor. The total viscosity of the flow can be defined as $\mu_t = \mu_s + \mu_p$ where μ_s
229 is the solvent viscosity and μ_p is the additional viscosity due to the polymer.

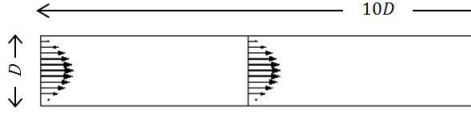


Fig. 2: Computational domain

230 Subsequently, R_n is introduced as the ratio between solvent viscosity and total
 231 viscosity. The Reynolds number is defined as $Re = \rho DU_{max}/\mu_t$.
 232 The governing equations in dimensionless form are as follows:

$$\nabla \cdot \mathbf{u} = 0 \quad (26)$$

$$\frac{D\mathbf{u}}{Dt} = -\nabla p + \frac{R_n}{Re} \nabla^2 \mathbf{u} + \frac{1-R_n}{Re} \nabla \cdot \frac{\boldsymbol{\tau}_p}{We} \quad (27)$$

$$\boldsymbol{\tau}_p = \frac{\mathbf{C}}{1 - \frac{\text{tr}(\mathbf{C})}{b^2}} - \mathbf{I} \quad (28)$$

$$\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} - (\nabla \mathbf{u})^T \cdot \mathbf{C} - \mathbf{C} \cdot (\nabla \mathbf{u}) = - \frac{\boldsymbol{\tau}_p}{We} \quad (29)$$

236 Eq.(28) states the relationship between the polymeric stress and conformation
 237 (\mathbf{C}) tensors for the FENE-P model. In the kernel conformation framework the
 238 evolution equation for the hyperbolic tangent tensor H is

$$\begin{aligned} \frac{D\mathbf{H}}{Dt} - \boldsymbol{\Omega} \mathbf{H} - \mathbf{H} \boldsymbol{\Omega} + 2B(\tanh(\mathbf{H}) - \mathbf{I})^{-1} &= \frac{1}{We} \left[\frac{\cosh^2(H)}{M} \right. \\ &\left. - \frac{1}{1 - \frac{\text{tr}(M(\tanh(\mathbf{H}) + \mathbf{I}))}{b^2}} \frac{(I + e^{2H})}{2} \right] \end{aligned} \quad (30)$$

239 where $\boldsymbol{\Omega}$ is an anti-symmetric pure rotation component of velocity gradient,
 240 and B is a symmetric traceless pure extension component of velocity gradient.
 241 We consider $Re = 1$ and $R_n = 0.1$ and $b = \sqrt{60}$.

242 Since constitutive equations are hyperbolic partial differential equations, we
 243 merely need to impose the stress at inlet for Eq. (29). Dirichlet Boundary
 244 conditions from semi-analytical solution of governing equation are imposed for
 245 velocity and viscoelastic stress at inlet (the semi-analytical solution is derived
 246 in Appendix A). Open boundary conditions for velocity and viscoelastic stress
 247 with zero pressure field are applied at outflow. Initial conditions can affect the
 248 numerical results significantly. Consequently, we implement identical initial
 249 conditions for each method. For velocity, pressure and conformation tensor
 250 (\mathbf{C}), we implement zero initial conditions.

251 Finally, we implement the finite element method to compute an approximation
 252 to the governing equations. All numerical simulations in this section are based
 253 on $\Delta t = 10^{-3}$. In order to demonstrate the strength of each formulation,
 254 numerical simulations were performed under analogous conditions. In order
 255 to use an optimal number of elements, we investigate the dependence of the

256 outlet velocity on the number of finite elements used in the discretization.
 257 Several meshes were considered with 110, 230, 720, 1380, 5600, and 67200
 258 quadrilateral elements and the results from the mesh convergence study are
 259 shown in Fig. 3. On more refined meshes, the computation time is increased,
 260 while the variations of outlet velocity are less than 1%. Therefore, all remaining
 261 computations were performed with 1380 elements, using linear interpolation
 262 for the pressure and quadratic interpolation for the velocity and conformation
 263 tensor.

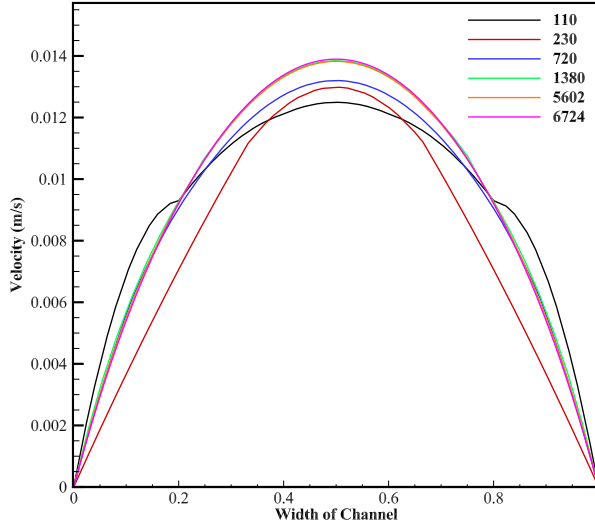


Fig. 3: Typical variation of outflow velocity with different number of elements

264 5 Results and discussion

265 In order to validate our numerical simulations, we compare the classical and
 266 hyperbolic tangent formulation results with the analytical solution of the
 267 Oldroyd-B model (the approach to derive the analytical solution is explained
 268 in Appendix B). The velocity and shear stress components at the outflow are
 269 selected as the criteria for the validation.

270 Fig. 4 illustrates agreement between numerical results and analytical solution,
 271 then validating our simulations.

272 As discussed in previous sections, instability of viscoelastic flow grows as the
 273 Weissenberg number is increased. In order to illustrate this fact we monitor
 274 the relative error for the first normal viscoelastic stress τ_{xx} , $\frac{\|\tau_{xx}^n - \tau_{xx}^{n-1}\|}{\|\tau_{xx}^{n-1}\|}$.

275 Fig.5 depicts the relative error of the first normal viscoelastic stress for the
 276 hyperbolic tangent, classical and logarithmic formulations. Instabilities in the

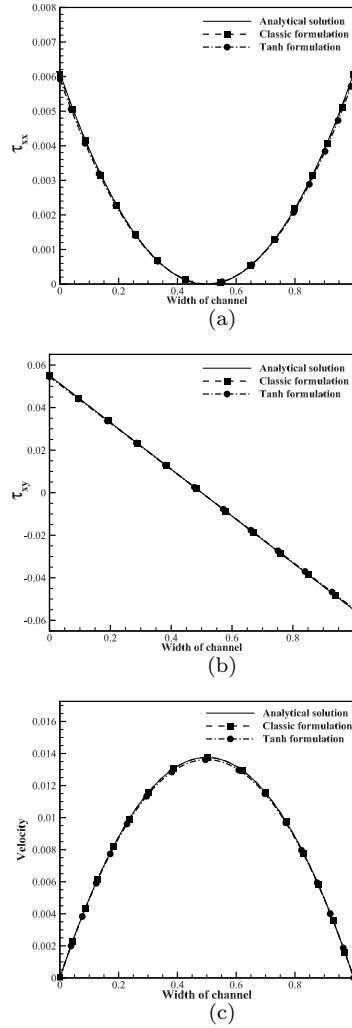


Fig. 4: Comparison for classical and hyperbolic tangent formulation simulations with the analytical solution of a) normal stress, τ_{xx} , b) shear stress, τ_{xy} and c) horizontal velocity for $We=1$, $Re=1$, and $\frac{\partial p}{\partial x} = -0.11$.

277 classical, logarithmic, and hyperbolic tangent formulations manifest exponential
 278 increase around Weissenberg number 39, 68 and 80, respectively. Hence,
 279 we are able to argue that, for planar channel flow, the hyperbolic tangent for-
 280 mulation can achieve higher Weissenberg numbers under analogous conditions.
 281 According to Eq. (28) when $\text{tr}(\mathbf{C})$ approaches b^2 , the polymeric stress tensor
 282 becomes unbounded and this causes instability in the computation. Therefore,
 283 $\text{tr}(\mathbf{C})$ plays an important role in the stability of the numerical simulation. Fig.6
 284 shows the time evolution of $\text{tr}(\mathbf{C})$ for the classical, logarithmic, and hyperbolic

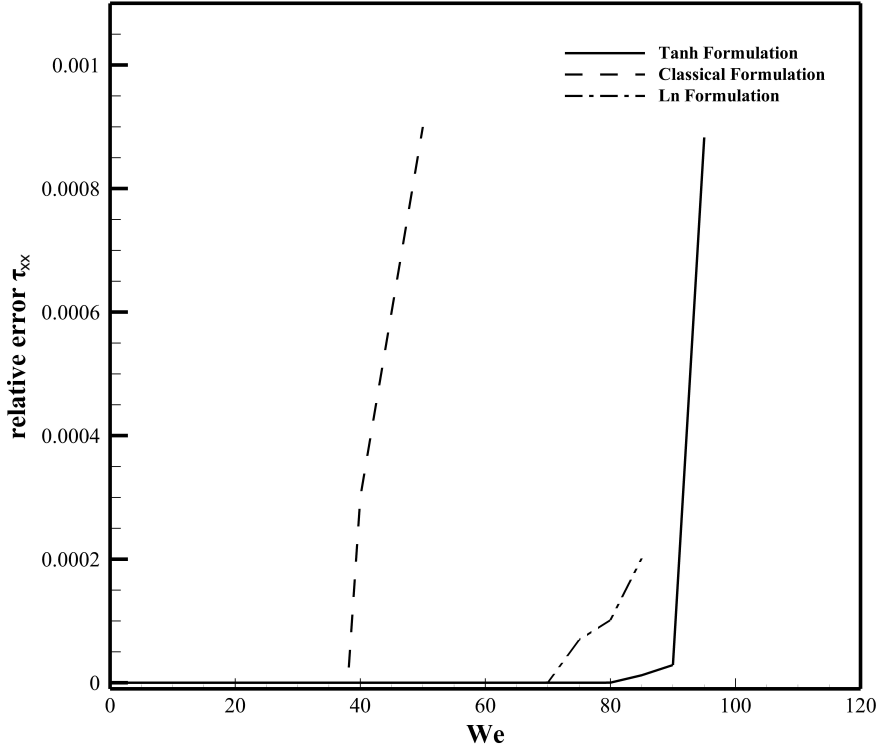


Fig. 5: Typical variation of the relative error for τ_{xx} versus the Weissenberg number

285 tangent formulations at Weissenberg number 39, 68 and 80, respectively (the
 286 critical Weissenberg numbers for each formulation, respectively). For the clas-
 287 sical and logarithmic formulations, $\text{tr}(\mathbf{C})$ manifests exponential increase and
 288 reaches its critical value of 60, the critical quantity of $\text{tr}(\mathbf{C})$, at time steps
 289 500 and 3000, respectively. After these time steps, the classical and logarith-
 290 mic formulations become unstable since the polymeric stress tensor becomes
 291 unbounded. However, the hyperbolic tangent formulation remains stable at
 292 the critical Weissenberg number of 80. Hence, we are able to claim that the
 293 instability of the hyperbolic tangent conformation is not due to $\text{tr}(\mathbf{C})$ and
 294 accumulation error may be the cause of instability in this formulation.

295 Fig.7 shows the onset of instability for the hyperbolic tangent conformation
 296 at the critical Weissenberg number, $We = 80$, at different time steps. The
 297 computation at this Weissenberg number becomes unstable and terminates at
 298 the 4523th time step. In Fig.7a, which depicts the flow at 10th time step, we
 299 do not observe any instability in the simulation. However, as time proceeds,
 300 the instability grows in the flow which can be perceived at 3500th time step

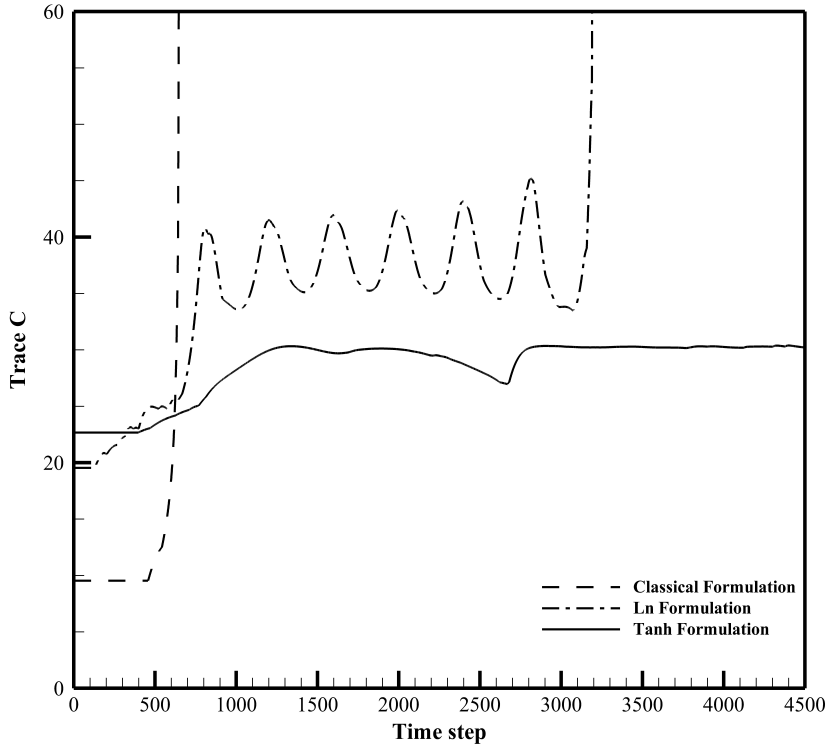


Fig. 6: Evolution of $\text{tr}(\mathbf{C})$ at the critical Weissenberg number

Table 1: Weissenberg limitation values at distinct polynomial orders

Velocity polynomial order	pressure polynomial order	conformation tensor polynomial order	Relative error at $We = 1$	Relative error at $We = 10$
quadratic	linear	quadratic	3.422e-12	1.224e-10
quadratic	linear	cubic	6.423e-13	9.107e-11
quadratic	linear	quartic	5.561e-09	6.543e-07
quadratic	linear	quintic	∞	∞
cubic	quadratic	cubic	9.423e-13	1.102e-11
cubic	quadratic	quartic	5.322e-13	8.651e-12
cubic	quadratic	quintic	6.423e-11	9.330e-08
cubic	quadratic	sextic	2.530e-07	∞
cubic	quadratic	septic	∞	∞

301 in Fig.7b. Finally, we observe the most instability in the flow at 4523th time
 302 step (last time step), which has been caused by accumulation errors, in Fig.7c.
 303 In order to investigate the effect of polynomial orders on the numerical sim-
 304 ulation, we consider the efficiency of the numerical method with respect to
 305 relative error of the first normal viscoelastic stress τ_{xx} . We investigate the
 306 performance of two choices of mixed finite element spaces: linear interpolation

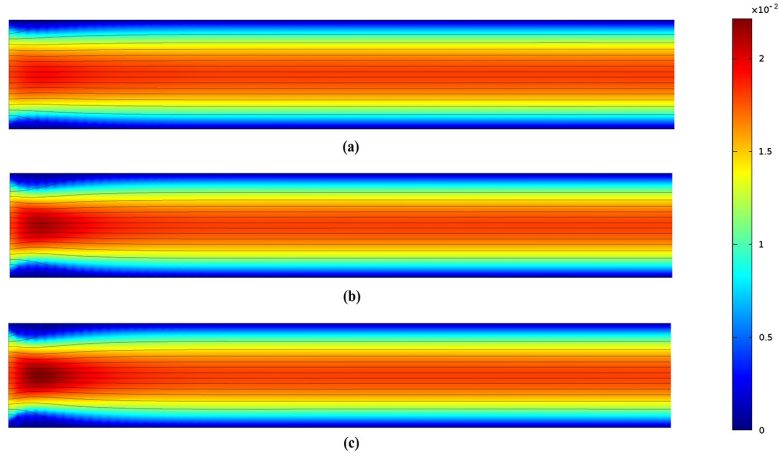


Fig. 7: Velocity fields at $We=80$ at $t = n\Delta t$. a) $n = 10$ b) $n = 3500$ c) $n = 4523$ (Last time step)

307 for the pressure and quadratic interpolation for the velocity with various inter-
 308 interpolations for the conformation tensor (quadratic, cubic, quartic and quintic
 309 interpolations); quadratic interpolation for the pressure and cubic interpola-
 310 tion for the velocity with different interpolations for the conformation tensor
 311 (cubic, quartic, quintic, sextic and septic interpolations). For the first choice,
 312 as can be seen from first 4 rows of Table 1, the capability of hyperbolic tangent
 313 formulations to tackle higher Weissenberg numbers initially improves by in-
 314 creasing the order of interpolation for the conformation tensor from quadratic
 315 to cubic. However, increasing the order of interpolation for the conformation
 316 tensor larger than cubic causes instabilities and the method is not able to
 317 reach high Weissenberg numbers. The last five rows of Table 1 illustrates the
 318 second choice. Analogous to the first category, initially, enhancing the order
 319 of interpolation results in higher accuracy. However, precision declines when
 320 the order of interpolation for the conformation tensor is increased to be more
 321 than quartic. Increasing the order of interpolation for velocity and pressure
 322 from quadratic and linear to cubic and quadratic results in greater accuracy,
 323 as lower relative errors are observed in the second category. Since the relative
 324 errors at $We = 1$ are lower than the errors at $We = 10$, we can claim that the
 325 Weissenberg number is an important factor in the accuracy of the simulation.
 326 For a given choice of velocity and pressure approximation spaces the optimum
 327 choice of conformation tensor approximation is one order greater than the
 328 velocity space.

329 6 Conclusions

330 In this study a new mathematical formulation of viscoelastic constitutive equa-
331 tions, the hyperbolic tangent formulation, which preserves both the symmetric
332 positive definiteness of the conformation tensor and bounds the magnitude of
333 its eigenvalues, is proposed. This new formulation has two important features.
334 First of all, it forces the eigenvalues of the conformation tensor to remain posi-
335 tive throughout the simulation. Secondly, reconstruction of the classical con-
336 formation tensor from the evolution equations does not encounter the problems
337 associated with the matrix logarithm formulation. In addition, we performed a
338 numerical simulation of viscoelastic flow in a 2D rectangular channel to investi-
339 gate the performance of the hyperbolic tangent formulation. Results illustrate
340 the advantage of the new formulation over the classical and logarithmic formu-
341 lations in 2D planar channel, since the hyperbolic tangent formulation attains
342 higher Weissenberg numbers under the same conditions.

343 Finally, the extension of the approach described in this paper to general 3D
344 flows is entirely possible. Although this is computationally demanding since
345 it requires the calculation of eigenvectors for 3D problems, the computational
346 overhead is not significantly different than for other formulations. The exten-
347 sion to 3D flows will form the basis of future research.

348 **Acknowledgements** This research was funded by a Swiss National Science Foundation
349 grant (No. 135676) whose support is gratefully acknowledged.

Appendix A

For fully developed channel flow, Eq. (29) simplifies to:

$$(\nabla \mathbf{u})^T \cdot \mathbf{C} + \mathbf{C} \cdot (\nabla \mathbf{u}) = \frac{\boldsymbol{\tau}_p}{We} \quad (\text{A.1})$$

Hence

$$\tau_{xx} = 2We C_{xy} \frac{\partial u}{\partial y} \quad (\text{A.2})$$

$$\tau_{xy} = We C_{yy} \frac{\partial u}{\partial y} \quad (\text{A.3})$$

$$\tau_{yy} = 0 \quad (\text{A.4})$$

Furthermore, under these conditions Eq. (27) becomes:

$$\nabla p = \frac{R_n}{Re} \nabla^2 \mathbf{u} + \frac{1-R_n}{Re} \nabla \cdot \frac{\boldsymbol{\tau}_p}{We} \quad (\text{A.5})$$

so we obtain

$$\frac{\partial p}{\partial x} = \frac{R_n}{Re} \frac{\partial^2 u}{\partial y^2} + \frac{1-R_n}{We Re} \frac{\partial \tau_{xy}}{\partial y} = Const \quad (\text{A.6})$$

$$\frac{\partial p}{\partial y} = 0 \quad (\text{A.7})$$

By integrating Eq. (A.6) and applying boundary condition at centerline of the channel, we obtain:

$$\frac{\partial u}{\partial y} = -\frac{1-R_n}{We R_n} \tau_{xy} + \frac{Re \frac{\partial p}{\partial x}}{R_n} y - \frac{Re \frac{\partial p}{\partial x}}{2R_n} \quad (\text{A.8})$$

Hence, considering Eq. (A.3), we conclude:

$$\frac{\partial u}{\partial y} = \left(\frac{R_n}{R_n + C_{yy} - R_n C_{yy}} \right) \left(\frac{Re \frac{\partial p}{\partial x}}{R_n} y - \frac{Re \frac{\partial p}{\partial x}}{2R_n} \right) \quad (\text{A.9})$$

According to FENE-P model, Eq (28) and Eq. (A.2) to Eq. (A.4), following linear system of equations is obtained:

$$C_{yy} = \frac{b^2 - C_{xx}}{1 + b^2} \quad (\text{A.10})$$

$$C_{xy} = We C_{yy}^2 \frac{\partial u}{\partial y} \quad (\text{A.11})$$

$$C_{xx} = 2We^2 C_{yy}^3 \left(\frac{\partial u}{\partial y} \right)^2 + C_{yy} \quad (\text{A.12})$$

Employing Eq. (A.9), we solve this linear system to find the stress components under fully developed conditions. Furthermore, by integrating Eq. (A.8), the velocity of the flow is given by:

$$u = -\frac{1-R_n}{R_n} \int \frac{\tau_{xy}}{We} dy + \frac{Re \frac{\partial p}{\partial x}}{R_n} y^2 - \frac{Re \frac{\partial p}{\partial x}}{2R_n} y \quad (\text{A.13})$$

368 Appendix B

369 In order to find analytical solution of Oldroyd-B model, we consider fully
 370 developed condition. Hence, we employed the conformation and momentum
 371 equations in fully developed condition from appendix A. According to the
 372 Oldroyd-B model, stress components can be written as:

$$\tau_{xx} = \frac{C_{xx} - 1}{We} \quad (\text{B.1})$$

$$\tau_{xy} = \frac{C_{xy}}{We} \quad (\text{B.2})$$

$$\tau_{yy} = \frac{C_{yy} - 1}{We} \quad (\text{B.3})$$

375 Considering Eqs. (A.2) to (A.4), components of conformation tensor are given
 376 by:

$$C_{xx} = 1 + 2We^4 \left(\frac{\partial u}{\partial y} \right)^2 \quad (\text{B.4})$$

$$C_{xy} = We^2 \left(\frac{\partial u}{\partial y} \right) \quad (\text{B.5})$$

$$C_{yy} = 1 \quad (\text{B.6})$$

379 By inserting the value of C_{yy} to Eq. (A.9), we obtain:

$$\frac{\partial u}{\partial y} = Re \frac{\partial p}{\partial x} \left(y - \frac{1}{2} \right) \quad (\text{B.7})$$

380 By integrating from Eq. (B.7), the velocity profile can be defined as:

$$u = Re \frac{\partial p}{\partial x} \left(\frac{y^2}{2} - \frac{y}{2} \right) \quad (\text{B.8})$$

381 Finally, the stress tensor components can be obtained by combining Eqs. (B.1),
 382 (B.2) and (B.7)

$$\tau_{xx} = 2We^3 Re^2 \left(\frac{\partial p}{\partial x} \right)^2 \left(y - \frac{1}{2} \right)^2 \quad (\text{B.9})$$

$$\tau_{xy} = We Re \frac{\partial p}{\partial x} \left(y - \frac{1}{2} \right) \quad (\text{B.10})$$

384 Appendix C

385 In order to calculate the components (H_{11} , H_{12} and H_{22}) of the tensor \mathbf{H} , we
 386 determine the eigenvalues (h_1 and h_2) and the components of eigenvectors (n_1
 387 and n_2) of \mathbf{H} by solving equations (C.1) to (C.5)

$$388 \quad h_1 = \frac{1}{2} \left[h_{11} + h_{22} + \sqrt{(h_{11} - h_{22})^2 + 4h_{12}^2} \right] \quad (\text{C.1})$$

$$h_2 = \frac{1}{2} \left[h_{11} + h_{22} - \sqrt{(h_{11} - h_{22})^2 + 4h_{12}^2} \right] \quad (\text{C.2})$$

$$n_1^2 = \frac{h_{12}^2}{(h_1 - h_{11})^2 + h_{12}^2} \quad (\text{C.3})$$

$$n_2^2 = \frac{(h_1 - h_{11})^2}{(h_1 - h_{11})^2 + h_{12}^2} \quad (\text{C.4})$$

$$n_1 n_2 = \frac{h_{12}(h_1 - h_{11})}{(h_1 - h_{11})^2 + h_{12}^2} \quad (\text{C.5})$$

389 Then, by solving the characteristic equations of \mathbf{C} and \mathbf{H} , the relation
 390 between eigenvalues of \mathbf{H} and \mathbf{C} is derived (the approach is explained in Ap-
 391 pendix A):

$$392 \quad c_i = \frac{2Me^{2h_i}}{1 + e^{2h_i}} \quad (\text{C.6})$$

393 According to the characteristic equation for \mathbf{C} , the components are written in
 394 the form:

$$395 \quad c_{11} = n_1^2 c_1 + n_2^2 c_2 \quad (\text{C.7})$$

$$396 \quad c_{12} = n_1 n_2 (c_1 - c_2) \quad (\text{C.8})$$

$$397 \quad c_{22} = n_2^2 c_1 + n_1^2 c_2 \quad (\text{C.9})$$

398 Using equation (C.6), the components of \mathbf{C} are defined by:

$$399 \quad c_{11} = n_1^2 \frac{2Me^{2h_1}}{1 + e^{2h_1}} + n_2^2 \frac{2Me^{2h_2}}{1 + e^{2h_2}} \quad (\text{C.10})$$

$$400 \quad c_{12} = n_1 n_2 \left(\frac{2Me^{2h_1}}{1 + e^{2h_1}} - \frac{2Me^{2h_2}}{1 + e^{2h_2}} \right) \quad (\text{C.11})$$

$$401 \quad c_{22} = n_2^2 \frac{2Me^{2h_1}}{1 + e^{2h_1}} + n_1^2 \frac{2Me^{2h_2}}{1 + e^{2h_2}} \quad (\text{C.12})$$

402 According to the equations (C.1)-(C.5), the components of \mathbf{C} are derived from
 403 the components of \mathbf{H} . Due to Eqs. (19)-(21) the material derivative of \mathbf{H} is

404 determined as follows:

405

$$\begin{aligned}
\dot{H}_{11} &= \left(\frac{M}{c_1(2M-c_1)} n_1^4 + \frac{M}{c_2(2M-c_2)} n_2^4 + 2n_1^2 n_2^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{11} \\
&+ \left(\frac{M}{c_1(2M-c_1)} 2n_1^3 n_2 - \frac{M}{c_2(2M-c_2)} 2n_1 n_2^3 - 2n_1 n_2 (n_1^2 - n_2^2) \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{12} \\
&+ \left(\frac{M}{c_1(2M-c_1)} n_1^2 n_2^2 + \frac{M}{c_2(2M-c_2)} n_1^2 n_2^2 - 2n_1^2 n_2^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{22} \\
&= G_{11} \dot{C}_{11} + G_{12} \dot{C}_{12} + G_{13} \dot{C}_{22}
\end{aligned} \tag{C.13}$$

406

$$\begin{aligned}
\dot{H}_{12} &= \left(\frac{M}{c_1(2M-c_1)} n_1^3 n_2 - \frac{M}{c_2(2M-c_2)} n_1 n_2^3 - n_1 n_2 (n_1^2 - n_2^2) \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{11} \\
&+ \left(\frac{M}{c_1(2M-c_1)} 2n_1^2 n_2^2 + \frac{M}{c_2(2M-c_2)} 2n_1^2 n_2^2 + (n_1^2 - n_2^2)^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{12} \\
&+ \left(\frac{M}{c_1(2M-c_1)} n_1 n_2^3 - \frac{M}{c_2(2M-c_2)} n_1^3 n_2 + n_1 n_2 (n_1^2 - n_2^2) \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{22} \\
&= G_{21} \dot{C}_{11} + G_{22} \dot{C}_{12} + G_{23} \dot{C}_{22}
\end{aligned} \tag{C.14}$$

$$\begin{aligned}
\dot{H}_{22} &= \left(\frac{M}{c_1(2M-c_1)} n_1^2 n_2^2 + \frac{M}{c_2(2M-c_2)} n_1^2 n_2^2 - 2n_1^2 n_2^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{11} \\
&+ \left(\frac{M}{c_1(2M-c_1)} 2n_1 n_2^3 - \frac{M}{c_2(2M-c_2)} 2n_1^3 n_2 + 2n_1 n_2 (n_1^2 - n_2^2) \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{12} \\
&+ \left(\frac{M}{c_1(2M-c_1)} n_2^4 + \frac{M}{c_2(2M-c_2)} n_1^4 + 2n_1^2 n_2^2 \frac{h_1-h_2}{c_1-c_2} \right) \dot{C}_{22} \\
&= G_{31} \dot{C}_{11} + G_{32} \dot{C}_{12} + G_{33} \dot{C}_{22}
\end{aligned} \tag{C.15}$$

407 where \dot{C}_{ij} , are the components of the material time derivatives of \mathbf{C} . The dif-
408 ferential constitutive equation representing the FENE-P model is:

409

$$\dot{\mathbf{C}} = \mathbf{C} \cdot (\nabla \mathbf{u})^T + \nabla \mathbf{u} \cdot \mathbf{C} - \frac{1}{We} \left(\mathbf{I} - \frac{\mathbf{C}}{1 - \frac{\text{tr}(\mathbf{C})}{b^2}} \right) \tag{C.16}$$

410 Using Eq. (C.16) for the components of the material time derivative of \mathbf{C} and
411 Eqs. (C.10)-(C.12) for the components of \mathbf{C} , the components of the material

time derivative of \mathbf{H} , \dot{H}_{ij} , defined by Eqs. (C.13)-(C.15) we derive

$$\dot{\mathbf{H}} = \frac{\partial \mathbf{H}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{H} = \begin{pmatrix} G_{11} & G_{12} & G_{13} \\ G_{21} & G_{22} & G_{23} \\ G_{31} & G_{32} & G_{33} \end{pmatrix} \left(\frac{\partial \mathbf{C}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{C} \right) \quad (\text{C.17})$$

which is used as the basis of the numerical algorithm for calculating the components of \mathbf{H} .

References

1. Afonso, A., Pinho, F., Alves, M.: The kernel-conformation constitutive laws. *Journal of Non-Newtonian Fluid Mechanics* **167-168**, 30 – 37 (2012)
2. Comminal, R., Spangenberg, J., Hattel, J.H.: Robust simulations of viscoelastic flows at high weissenberg numbers with the streamfunction/log-conformation formulation. *Journal of Non-Newtonian Fluid Mechanics* **223**, 37 – 61 (2015)
3. Coronado, O.M., Arora, D., Behr, M., Pasquali, M.: A simple method for simulating general viscoelastic fluid flow with an alternate log conformation formulation. *J. Non-Newtonian Fluid Mech.* **147**, 189–199 (2007)
4. Dupret, F., Marchal, J.M.: Loss of evolution in the flow of viscoelastic fluids. *J. Non-Newtonian Fluid Mech.* **20(C)**, 143–171 (1986)
5. Fattal, R., Kupferman, R.: Constitutive laws for the matrix-logarithm of the conformation tensor. *J. Non-Newtonian Fluid Mech.* **123**, 281–285 (2004)
6. Fattal, R., Kupferman, R.: Time-dependent simulation of viscoelastic flow at high Weissenberg number using the log-conformation representation. *J. Non-Newtonian Fluid Mech.* **126**, 23–37 (2005)
7. Housiadas, K.D., Wang, L., Beris, A.N.: A new method preserving the positive definiteness of a second order tensor variable in flow simulations with application to viscoelastic turbulence. *Comput. Fluids* **39(2)**, 225–241 (2010)
8. Hulsen, M.A.: A sufficient condition for a positive definite configuration tensor in differential models. *J. Non-Newtonian Fluid Mech.* **38(1)**, 93–100 (1990)
9. Hulsen, M.A., Fattal, R., Kupferman, R.: Flow of viscoelastic fluid past a cylinder at high Weissenberg number: stabilized simulation using matrix logarithms. *J. Comput. Phys.* **127**, 27–39 (2005)
10. Jafari, A., Fiétier, N., Deville, M.O.: A new extended matrix logarithm formulation for the simulation of viscoelastic fluids by spectral elements. *Comput. Fluids* **39(9)**, 1425–1438 (2010)
11. Kwon, Y.: Finite element analysis of planar 4:1 contraction flow with the tensor-logarithmic formulation of differential constitutive equations. *Korea-Australia Rheology J.* **4**, 183–191 (2004)
12. Kwon, Y., Leonov, A.I.: Stability constraints in the formulation of viscoelastic constitutive equations. *J. Non-Newtonian Fluid Mech.* **58(1)**, 25–46 (1995)
13. Leonov, A.I.: Viscoelastic constitutive equations and Rheology for high-speed polymer processing. *J. Polym. Int.* **36**, 187–193 (1995)
14. Owens, R.G., Phillips, T.N.: *Computational Rheology*. Imperial College Press, London (2002)
15. Saramito, P.: On a modified non-singular log-conformation formulation for johnson-segalman viscoelastic fluids. *Journal of Non-Newtonian Fluid Mechanics* **211**, 16 – 30 (2014)
16. Tomé, M., Castelo, A., Afonso, A., Alves, M., Pinho, F.: Application of the log-conformation tensor to three-dimensional time-dependent free surface flows. *Journal of Non-Newtonian Fluid Mechanics* **175176**, 44 – 54 (2012)
17. Vaithianathan, T., Robert, A., Brasseur, J.G., Collins, L.R.: An improved algorithm for simulating three-dimensional, viscoelastic turbulence. *J. Non-Newtonian Fluid Mech.* **140(1-3)**, 3–22 (2006)