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[short communication]

Vector decomposition of the evolution equations of the conformation tensor of Maxwellian fluids

Kwang Soo Cho*
Department of Polymer Science and Engineering, Kyungpook National University, Deagu, 702-701, Korea
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Abstract

Breakthrough of high Weisenberg number problem is related with keeping the positive definiteness of the conformation tensor in numerical procedures. In this paper, we suggest a simple method to preserve the positive definiteness by use of vector decomposition of the conformation tensor which does not require eigenvalue problem. We also derive the constitutive equation of tensor-logarithmic transform in simpler way than that of Fattal and Kupferman and discuss the comparison between the vector decomposition and tensor-logarithmic transformation.

Keywords **:** high Weisenberg number, vector decomposition, conformation tensor, nonlinear viscoelasticity, Maxwellian fluid

1. Introduction

Numerical calculation with nonlinear viscoelastic models suffers from convergence problem when Weisenberg number is considerably high (Keunings, 1986). The high Weisenberg number problem is thought to be originated from singular geometry in case of 4:1 contraction flow modeling, instability of numerical algorithm and nonlinear viscoelastic constitutive equations. The instability of constitutive equation can be removed by adopting stable constitutive equations such as the Leonov model, the Phan-Thien and Tanner model and so on (Kwon and Leonov, 1995). However, some numerical errors which may be due to spatial discretization, result in the break of positive definiteness of the conformation tensor of the stable constitutive equations. The breakthrough of this problem seems to have been developed by Fattal and Kupferman (2004). The method is called tensor-logarithmic transformation of the conformation tensor.

The tensor-logarithmic transformation is known to preserve positive definiteness of the conformation tensors in any computational steps. It is also known that the positive definiteness of conformation tensor is very important for the well-posedness of its evolution equation (Kwon, 2004). Preserving the positive definiteness can be done by vector decomposition of the conformation tensor which is simpler than the tensor-logarithmic transformation in mathematics. In this paper, an alternative of the tensor-logarithmic transform is suggested which is called vector decomposition of the conformation tensor. We derived the evolution equation of the logarithmic conformation tensor developed by Fattal and Kupferman in a simpler way, too.

*Corresponding author: polphy@knu.ac.kr

2. Vector Decomposition

2.1. Positive Definiteness

It is easily understood that a symmetric tensor made of the dyadic of a vector $\mathbf{A}=\mathbf{aa}$ is positive definite, because $\mathbf{x}\cdot\mathbf{A}\cdot\mathbf{x}=(\mathbf{a}\cdot\mathbf{x})^2$. It is also straightforward that a tensor made of the product of a tensor with its transpose $\mathbf{C}=\mathbf{F}_e\cdot\mathbf{F}_e^T$ is symmetric and positive definite. Here we consider $\mathbf{C}$ as the conformation tensor. We define conformation vector as $\mathbf{C}=\mathbf{f}_i\mathbf{f}_i$. We adopt $\{\mathbf{e}_i\}$ as the orthonormal base vectors and use summation convention. Then $\mathbf{f}_i=\mathbf{F}_e\cdot\mathbf{e}_i$ is an example of the conformation vector, because there are so many ways possible to construct the conformation tensor by the summation of the dyadics of vectors. Since the conformation tensor is the identity tensor at initial time $t=0$, it is clear that the conformation vectors are initially the orthonormal base vectors, say $\mathbf{f}_i(0)=\mathbf{e}_i$.

2.2. Evolution Equation of the Conformation Tensor

It is well known that most Maxwellian fluid models can be converted into the canonical form such that

$$\frac{d\boldsymbol{C}}{dt}-\mathbf{L}\cdot\mathbf{C}-\mathbf{C}\cdot\mathbf{L}^T+\frac{1}{\lambda}\mathbf{H}(\mathbf{C})=\mathbf{0} \tag{1}$$

where the tensor valued function $\mathbf{H}$ is called dissipation tensor. The extra stress tensor is given by $\mathbf{T}=G(\mathbf{C}-\mathbf{I})$ in the simplest case, where G is the shear modulus, λ is the relaxation time and $\mathbf{I}$ is the identity tensor (Kwon and Leonov 1995). In case of the Leonov model we know that

$$\mathbf{H} = \frac{b(\mathrm{I_C},\mathrm{II_C})}{2}\left(\mathbf{C}^2-\mathbf{I}-\frac{\mathrm{I_C}-\mathrm{II_C}}{3}\mathbf{C}\right) \tag{2}$$

where $b(\mathrm{I_C}, \mathrm{II_C})$ is a positive function of the principal invariants of the conformation tensor. For the Phan-Thien and Tanner model, we know that

$$\mathbf{H} = \phi(\mathrm{I_C})(\mathbf{C}-\mathbf{I}) \tag{3}$$

where

$$\phi(\mathrm{I_C}) = \exp[\varepsilon(\mathrm{I_C}-3)] \tag{4}$$

and ε is the nonlinear parameter of the Phan-Thien and Tanner model. For the Giesekus model

$$\mathbf{H} = \alpha\mathbf{C}^2+(1-2\alpha)\mathbf{C}-(1-\alpha)\mathbf{I} \tag{5}$$

where a is the nonlinear parameter of the Giesekus model whose value is in the range $0<\alpha<1$.

We need evolution equations of the conformation vectors which must be coincide with that of the conformation tensor. We assume the evolution equations of the conformation vectors as

$$\frac{d\mathbf{f}_k}{dt} = \mathbf{L}\cdot\mathbf{f}_k-\frac{1}{\lambda}\mathbf{D}_\mathrm{P}\cdot\mathbf{f}_k \tag{6}$$

where the tensor $\mathbf{L}$ is the velocity gradient $\mathbf{L} = (\nabla\mathbf{v})^T$ and the symmetric tensor $\mathbf{D}_p$ will be determined by the comparison of Eq. (6) with Eq. (1). From Eq. (6) we know that the conformation vector increases as time due to velocity gradient and relaxes by the influence of the irreversible deformation rate tensor $\mathbf{D}_p$. The relaxation time λ controls the speed of the relaxation.

2.3. Determination of $\mathbf{D}_p$

Using the definition of the conformation vector, the material time derivative of the conformation tensor is given by

$$\frac{d\mathbf{C}}{dt} = \frac{d\mathbf{f}_k}{dt}\mathbf{f}_k+\mathbf{f}_k\frac{d\mathbf{f}_k}{dt} \tag{7}$$

Hence substitution of Eq. (7) into Eq. (1), we know that

$$\frac{d\mathbf{C}}{dt}-\mathbf{L}\cdot\mathbf{C}-\mathbf{C}\cdot\mathbf{L}^T+\frac{1}{\lambda}(\mathbf{C}\cdot\mathbf{D}_\mathrm{P}+\mathbf{D}_\mathrm{P}\cdot\mathbf{C}) = \mathbf{0} \tag{8}$$

Comparison of Eq. (8) with Eq. (1) yields

$$\mathbf{C}\cdot\mathbf{D}_\mathrm{P}+\mathbf{D}_\mathrm{P}\cdot\mathbf{C} = \mathbf{H} \tag{9}$$

In order to express $\mathbf{D}_p$ in terms of $\mathbf{H}$ and $\mathbf{C}$, we use the results of Rosati (2000):

$$\begin{aligned}2k\mathrm{III_C}\mathbf{D_P} &= 2(\mathrm{I_C^2}-\mathrm{III_C})\mathrm{III_C}\mathbf{H}-2\mathrm{III_C}(\mathbf{C}^2\cdot\mathbf{H}+\mathbf{H}\cdot\mathbf{C}^2)\\&+(\mathrm{I_C}\mathrm{II_C^2}+\mathrm{II_C}\mathrm{III_C}-\mathrm{I_C^2}\mathrm{III_C})\mathrm{tr}(\mathbf{H})\mathbf{I}-\mathrm{I_C^2}\mathrm{II}[\mathrm{tr}(\mathbf{H})\mathbf{C}-\mathrm{tr}(\mathbf{H}\cdot\mathbf{C})\mathbf{I}]\\&+(\mathrm{I_C}\mathrm{II_C}+\mathrm{III_C})[\mathrm{tr}(\mathbf{H})\mathbf{C}^2+\mathrm{tr}(\mathbf{H}\cdot\mathbf{C}^2)\mathbf{I}]+\mathrm{I_C^3}\mathrm{III_C}\mathrm{tr}(\mathbf{H}\cdot\mathbf{C})\mathbf{C}\\&\mathrm{I_C}\mathrm{tr}(\mathbf{H}\cdot\mathbf{C}^2)\mathbf{C}^2-\mathrm{I_C^2}[\mathrm{tr}(\mathbf{H}\cdot\mathbf{C})\mathbf{C}^2+\mathrm{tr}(\mathbf{H}\cdot\mathbf{C}^2)\mathbf{C}]\end{aligned} \tag{10}$$

where $k=\mathrm{I_C}\mathrm{II_C}-\mathrm{III_C}$ and $\mathrm{III_C}=\det\mathbf{C}$. At the first look, Eq. (10) seems too complex to be used in numerical calculation. Because $\mathbf{H}$ is a polynomial of $\mathbf{C}$, Eq. (10) implies that $\mathbf{D}_\mathrm{P}$ has the form of

$$\mathbf{D}_\mathrm{P} = d_0\mathbf{I}+d_1\mathbf{C}+d_2\mathbf{C}^2 \tag{11}$$

where $\{d_i\}$ are functions of the principal invariants of $\mathbf{C}$. Eq. (11) implies that $\mathbf{D}_\mathrm{P}$ is coaxial with $\mathbf{C}$, $\mathbf{D}_\mathrm{P}\cdot\mathbf{C} = \mathbf{C}\cdot\mathbf{D}_\mathrm{P}$. Hence Eq. (9) becomes simpler:

$$\mathbf{D}_\mathrm{P} = \frac{1}{2}\mathbf{C}^{-1}\cdot\mathbf{H} \tag{12}$$

Eq. (12) allows us to calculate the tensor $\mathbf{D}_\mathrm{P}$ for the three viscoelastic models as follows:

$$\text{Leonov model}\quad \mathbf{D}_\mathrm{P} = \frac{b(\mathrm{I_C},\mathrm{II_C})}{4}\left(\mathbf{C}-\mathbf{C}^{-1}-\frac{\mathrm{I_C}-\mathrm{II_C}}{3}\mathbf{I}\right) \tag{13}$$

$$\text{PTT model}\quad \mathbf{D}_\mathrm{P} = \frac{\phi(\mathrm{I_C})}{2}(\mathbf{I}-\mathbf{C}^{-1}) \tag{14}$$

$$\text{Giesekus model}\quad \mathbf{D}_\mathrm{P} = \frac{\alpha}{2}\mathbf{C}+\frac{1-2\alpha}{2}\mathbf{I}-\frac{1-\alpha}{2}\mathbf{C}^{-1} \tag{15}$$

Instead of Eq. (1), the use of Eq. (6) with $\mathbf{C}=\mathbf{f}_k\mathbf{f}_k$ guarantees the positive definiteness of the conformation tensors irrespective of computational schemes and the value of the Weisenberg number.

By use of the Hamilton-Cayley theorem, we know that

$$\mathbf{C}^{-1} = \frac{1}{\mathrm{III_C}}\mathbf{C}^2-\frac{\mathrm{I_C}}{\mathrm{III_C}}\mathbf{C}+\frac{\mathrm{II_C}}{\mathrm{III_C}}\mathbf{I} \tag{16}$$

and

$$\mathrm{I}_{\mathrm{C}^{-1}} = \frac{\mathrm{II_C}}{\mathrm{III_C}},\ \mathrm{II}_{\mathrm{C}^{-1}} = \frac{\mathrm{I_C}}{\mathrm{III_C}},\ \mathrm{III}_{\mathrm{C}^{-1}} = \frac{1}{\mathrm{III_C}} \tag{17}$$

In case of the Leonov model, the determinant of the conformation tensor is unity and from Eqs. (13), (16) and (17), we know that

$$\mathrm{tr}(\mathbf{D}_\mathrm{P}) = 0 \tag{18}$$

Furthermore the tensor $\mathbf{D}_\mathrm{P}$ of Eq. (13) is equivalent to the irreversible deformation rate tensor defined from the original Leonov model (Leonov 1976).

It is noteworthy to express the principal invariants of the conformation tensor in terms of conformation vectors:

$$\mathrm{I_C} = \mathrm{tr}\mathbf{C} = |\mathbf{f}_1|^2+|\mathbf{f}_2|^2+|\mathbf{f}_3|^2 = \mathbf{f}_k\cdot\mathbf{f}_k \geq 0 \tag{19}$$

$$\begin{aligned}\mathrm{II_C} &= (\mathbf{f}_1\cdot\mathbf{f}_1)(\mathbf{f}_2\cdot\mathbf{f}_2)-(\mathbf{f}_1\cdot\mathbf{f}_2)^2+(\mathbf{f}_2\cdot\mathbf{f}_2)(\mathbf{f}_3\cdot\mathbf{f}_3)-(\mathbf{f}_2\cdot\mathbf{f}_3)^2\\&+(\mathbf{f}_3\cdot\mathbf{f}_3)(\mathbf{f}_1\cdot\mathbf{f}_1)-(\mathbf{f}_3\cdot\mathbf{f}_1)^2 \geq 0\end{aligned} \tag{20}$$

$$\mathrm{III_C} = [\mathbf{f}_1\cdot(\mathbf{f}_2\times\mathbf{f}_3)]^2 \geq 0 \tag{21}$$

3. Tensor-Logarithmic Transformation

Fattal and Kupferman (2004) suggested the tensor-logarithmic transformation of the conformation tensor. Their derivation of the transformation is not easy to be understood because they used a matrix decomposition theorem which is not widely known and decomposition of the evolution of the logarithmic conformation tensor into four special cases: advection, rotation, extension and sources. In this section, we derive the tensor-logarithmic transformation in a simpler way.

If we denote the eigenvectors of the conformation tensor as $\{\mathbf{n}_i\}$ and eigenvalues as $\{c_i\}$, we have

$$\mathbf{C}=c_1\mathbf{n}_1\mathbf{n}_1+c_2\mathbf{n}_2\mathbf{n}_2+c_3\mathbf{n}_3\mathbf{n}_3 \tag{22}$$

Since a symmetric and positive definite tensor has positive distinct eigenvalues and its eigenvectors are orthogonal, we can adopt the eigenvectors as the orthonormal vectors. Assume that $\mathbf{n}_i\cdot\mathbf{n}_k=\delta_{ik}$.

Since the unit eigenvectors $\mathbf{n}_i$ must keep orthonormal, it is reasonable assumption that

$$\frac{\mathrm{d}\mathbf{n}_i}{\mathrm{d}t}=\boldsymbol{\Omega}\cdot\mathbf{n}_i \tag{23}$$

where $\boldsymbol{\Omega}$ is a skew-symmetric tensor because the orthogonality of the eigenvectors should be preserved:

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{n}_i\cdot\mathbf{n}_k)=\mathbf{n}_i\cdot(\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}^T)\cdot\mathbf{n}_k=0 \tag{24}$$

From Eq. (22), we know that

$$\frac{\mathrm{d}\mathbf{C}}{\mathrm{d}t}=\sum_{k=1}^{3}\frac{\mathrm{d}c_k}{\mathrm{d}t}\mathbf{n}_k\mathbf{n}_k+\boldsymbol{\Omega}\cdot\mathbf{C}+\mathbf{C}\cdot\boldsymbol{\Omega}^T \tag{25}$$

Comparison of Eq. (25) with Eq. (1) yields

$$\mathbf{L}\cdot\mathbf{C}+\mathbf{C}\cdot\mathbf{L}^T-\frac{1}{\lambda}\mathbf{H}(\mathbf{C})=\boldsymbol{\Omega}\cdot\mathbf{C}+\mathbf{C}\cdot\boldsymbol{\Omega}^T+\sum_{k=1}^{3}\frac{\mathrm{d}c_k}{\mathrm{d}t}\mathbf{n}_k\mathbf{n}_k \tag{26}$$

Since the dissipation tensor $\mathbf{H}$ is coaxial with $\mathbf{C}$, we can write

$$\frac{1}{\lambda}\mathbf{H}(\mathbf{C})=\sum_{K=1}^{3}\frac{h_k(\mathrm{I_C},\mathrm{II_C},\mathrm{III_C})}{\lambda}\mathbf{n}_k\mathbf{n}_k \tag{27}$$

Using the eigenvectors as the base vector, we can write

$$\mathbf{L}=L_{ik}\mathbf{n}_i\mathbf{n}_k,\ \boldsymbol{\Omega}=\Omega_{ik}\mathbf{n}_i\mathbf{n}_k \tag{28}$$

$$\begin{aligned}\mathbf{L}\cdot\mathbf{C}+\mathbf{C}\cdot\mathbf{L}^T=\ &2L_{11}c_1\mathbf{n}_1\mathbf{n}_1\\ &2L_{22}c_2\mathbf{n}_2\mathbf{n}_2\\ &2L_{33}c_3\mathbf{n}_3\mathbf{n}_3\\ &+(L_{12}c_2+L_{21}c_1)(\mathbf{n}_1\mathbf{n}_2+\mathbf{n}_2\mathbf{n}_1)\\ &+(L_{23}c_3+L_{32}c_2)(\mathbf{n}_2\mathbf{n}_3+\mathbf{n}_3\mathbf{n}_2)\\ &+(L_{31}c_1+L_{13}c_3)(\mathbf{n}_3\mathbf{n}_1+\mathbf{n}_1\mathbf{n}_3)\end{aligned} \tag{29}$$

$$\begin{aligned}&\boldsymbol{\Omega}\cdot\mathbf{C}+\mathbf{C}\cdot\boldsymbol{\Omega}^T=\Omega_{12}(c_2-c_1)(\mathbf{n}_1\mathbf{n}_2+\mathbf{n}_2\mathbf{n}_1)\\ &+\Omega_{23}(c_3-c_2)(\mathbf{n}_2\mathbf{n}_3+\mathbf{n}_3\mathbf{n}_2)\\ &\Omega_{31}(c_1-c_3)(\mathbf{n}_3\mathbf{n}_1+\mathbf{n}_1\mathbf{n}_3)\end{aligned} \tag{30}$$

Hence Eq. (26) is equivalent to

$$\frac{\mathrm{d}c_k}{\mathrm{d}t}=2L_{kk}c_k-\frac{h_k}{\lambda}\ \text{(no sum on } k) \tag{31}$$

$$c_jL_{ij}+c_jL_{ji}=(c_j-c_i)\Omega_{ij},\ (i\neq j)\ \text{(no sum)} \tag{32}$$

Eq. (31) implies that

$$\sum_{k=1}^{3}\frac{\mathrm{d}c_k}{\mathrm{d}t}\mathrm{n}_k\mathrm{n}_k=2\mathbf{C}\cdot\mathbf{B}-\frac{1}{\lambda}\mathbf{H} \tag{33}$$

where the tensor $\mathbf{B}$ is symmetric because $\mathbf{B}$ is defined as

$$\mathbf{B}=\sum_{k=1}^{3}L_{kk}\mathbf{n}_k\mathbf{n}_k \tag{34}$$

Hence it is clear that for incompressible fluid

$$\mathrm{tr}(\mathbf{B})=\mathrm{tr}(\mathbf{L})=0 \tag{35}$$

Now we define $\mathrm{S}=\log\mathbf{C}$ such that

$$\mathbf{S}=\sum_{k=1}^{3}\log c_k\mathbf{n}_k\mathbf{n}_k \tag{36}$$

The material time derivative of $\mathbf{S}$ is given by

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}t}=\sum_{k=1}^{3}\frac{1}{\mathrm{c}_k}\frac{\mathrm{d}c_k}{\mathrm{d}t}\mathbf{n}_k\mathbf{n}_k+\boldsymbol{\Omega}\cdot\mathbf{S}+\mathbf{S}\cdot\boldsymbol{\Omega}^T \tag{37}$$

From Eq. (33), we know that

$$\sum_{K=1}^{3}\frac{1}{\mathrm{c}_k}\frac{\mathrm{d}c_k}{\mathrm{d}t}\mathbf{n}_k\mathbf{n}_k=2\mathbf{B}-\frac{1}{\lambda}\mathbf{C}^{-1}\cdot\mathbf{H} \tag{38}$$

Substitution of Eq. (38) into Eq. (37) yields

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}t}-\boldsymbol{\Omega}\cdot\mathbf{S}-\mathbf{S}\cdot\boldsymbol{\Omega}^T-2\mathbf{B}-\frac{1}{\lambda}e^{-\mathrm{S}}\cdot\mathbf{H}(e^{\mathrm{S}})=\mathbf{0} \tag{39}$$

which is the constitutive law derived by Fattal and Kupferman (2004). In Eq. (39) we used the notation such that $\mathbf{C}=\mathrm{e}^{\mathrm{S}}$ and $\mathbf{C}^{-1}=\mathrm{e}^{-\mathrm{S}}$. It is interesting that the last term of Eq. (39) is just the irreversible deformation rate tensor $\mathbf{D}_{\mathrm{P}}$ derived in Eq. (12).

When we find a numerical solution of $\mathrm{d}x/\mathrm{d}t=ax$, any numerical method cannot give considerably accurate solution whenever $a>0$ is so large and we want a solution for long time $t>>1$. However, if we use $y=\log x$, the ordinary differential equation becomes simpler: $\mathrm{d}x/\mathrm{d}t=a$, which can be solved easily irrespective of the range of time and the magnitude of a. Hence, from this viewpoint, the transformation of Fattal and Kupferman seems to be effective for high Weisenberg problem. However, as seen in Eq. (39), the tensor-logarithmic transformation requires the determination of eigenvectors and eigenvalues of the conformation tensor at every calculation steps because we have to determine the tensors $\boldsymbol{\Omega}$, $\mathbf{B}$, and $\mathrm{C}=e^{\mathrm{S}}$ by use of the solution of eigenvalue problem.

Although tensor $\mathbf{S}$ may have some components whose magnitude is extraordinarily large, the formulation guarantees positive definiteness of the conformation tensor. Compared with tensor-logarithmic transformation, the vector decomposition keeps the positive definiteness at any calculation step irrespective of the magnitude of Weisenberg number, in principle. Furthermore, the vector decomposition does not require solving the eigenvalue problem at every calculation step.

The strong point of tensor-logarithmic transform, compared with vector decomposition, is the stability in numerical scheme as exampled by the ordinary differential equation $dx/dt = ax$ while its weak point is to use eigenvector. Although vector decomposition preserves the positive definiteness of the conformation tensor and does not require solution of eigenvalue problem, it does not seem to have the merit of the tensor-logarithmic transform in numerical stability. However, if the positive definiteness of the conformation tensor is the most important factor in high Weisenberg number problem, the vector decomposition will be very useful.

4. Diversity of the Conformation Vector

As mentioned in section 2, there may be several sets of conformation vectors which construct conformation tensor by $\mathbf{C} = \mathbf{f}_i\mathbf{f}_i$. For a laboratory coordinate system we can write $\mathbf{C} = C_{ik}\mathbf{e}_i\mathbf{e}_k$ and set $\mathbf{f}_a = f_i^a\mathbf{e}_i$ to satisfy $C_{ik} = f_i^a f_i^a$. However it is clear that two sets of conformation vectors that have the same initial conditions are identical during the whole deformation history if and only if their evolution equations are identical as Eq. (6). It is because the evolution equation Eq. (6) is deterministic.

In numerical procedure, it is one of the simplest initial conditions that $\mathbf{f}_i(0) = \mathbf{e}_i$. The initial conditions are expected to make the vector decomposition free from the diversity of the conformation vector.

5. Comparison of the Two Methods

Since tensor $\mathbf{S}$ of Eq. (39) is symmetric, the tensor-logarithmic transform deals with only six independent components. Although the conformation tensor has only six independent components, the vector decomposition, in general requires nine components to be calculated. Hence the vector decomposition seems not efficient in numerical calculation compared with the tensor-logarithmic transform.

However, in two-dimensional problem, both the vector decomposition and the tensor-logarithmic transform have the same number of independent components, four. In case of the Leonov model, the conformation tensor should satisfy $\mathrm{III}_C = 1$, which implies

$$\mathbf{f}_3 = \frac{\mathbf{f}_1 \times \mathbf{f}_2}{|\mathbf{f}_1 \times \mathbf{f}_2|^2} \tag{40}$$

Thus, the vector decomposition for the Leonov model deals with six independent components.

6. Conclusions

We suggest a simple method to preserve the positive definiteness of the conformation tensor at any step of numerical schemes by considering the conformation vector as the sum of the dyadics of the conformation vectors and by showing the evolution equation (6) of the conformation vectors is equivalent to that of the conformation tensor. The simple idea must be checked by the applications to a number of nonlinear viscoelastic flows.

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