

Non-Symmetric Constitutive Equation Theory of co-Rotational Type for Liquid Crystalline Polymer of Biomedical Materials

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Abstract— Certain biomedical materials can be considered as liquid crystalline (LC) polymer the charateric of which is considerably different from the common polymer. In the present paper a continuum theory of the constitutive equation of co-rotational derivative type is developed for the anisotropic viscoelastic fluid — LC biopolymers.

Keywords - biomedical liquid crystalline polymer; constitutive equation; co-rotational derivative; anisotropic fluid, biopolymer.

I. INTRUCTION

Certain biomedical materials can be considered as liquid crystalline (LC) biopolymer the charateric of which is considerably different from the common polymer. A new concept of simple anisotropic fluid is introduced. On the basis of principles of anisotropic simple fluid stress behaviour is described by velocity gradient tensor F and spin tensor W instead of velocity gradient tensor D in the classic Leslie-Ericksen continuum theory. Analyzing rheological nature of the fluid and using tensor analysis a general form of the constitutive equation of co-rotational type is founded. The special term in equation is introduced to describe the special change of the normal stress differences which is considered as a result of director tumbling by Larson et al. The characteristic behaviour of non-symmetry of the shear stress is predicted by using the present model for LC polymer liquids

II. PRINCIPLES OF NON-SYMMETRIC CONSTITUTIVE EQUATION

In construction of continuum theory of constitutive equation for the LC biopolymer-anisotropic viscoelastic fluids following principles are proposed:

1. According new definition of anisotropic simple fluid the stress is dependent on hole history of deformation gradient and hole history of spin tensor measured with respect to co-rotational coordinates.
2. The constitutive equation contains the both contributions due to the orientational motion of director and hydrodynamic motions of fluid, to describe anisotropic effects of LC polymer [1]. The stress tensor is considered as a functional of the deformation tensors and tensors composed of the director vector and its derivative. According statistic physics the macroscopic magnitudes are considered as an average of the microscopic values.
3. As nematic LC polymer solution is also viscoelastic

fluid the constitutive equation of co-rotational Oldroyd fluid B is starting point in constructing constitutive equation for anisotropic viscoelastic fluid. Constitutive equation for anisotropic viscoelastic fluid can be constructed by generalizing co-rotational Oldroyd fluid B.

III. CONSTITUTIVE EQUATION FOR LC POLYMER

Extending the general principle in constructing constitutive equation by Truesdell and Ericksen and generalizing constitutive equation of co-rotational Oldroyd fluid B and the generalized Maxwell equation stress components and its co-rotational derivative terms are assumed to be of functional of n_i , N_i , A_{ij} and W_{ij} , a general form of the constitutive equation of the fluid is assumed to be of

$$S_{ij} + \lambda_{ijkl} \overset{\circ}{S}_{kl} = \mu \overset{\circ}{A}_{ij} + \mathcal{Q}_{ij}^1 [A_{ij}, \omega_{ij}, n_i, N_i, \beta_j] \quad (1)$$

where the λ_s, β_j are material constants, A_{ij} — components of the first Rivlin-Ericksen tensor, ω_{ij} — components of spin tensor W , $N_i = \dot{n}_i - \omega_{ik} n_k$.

For anisotropic viscoelastic fluid— LC polymer melt and solution the stress tensor is an un-symmetric one. The anisotropy in elasticity of LC polymers leads to un-symmetry of the stress tensor. The rotation of the director vector is a source of dissipation in the nematic liquid even in the absence of flow, the stress relashinship derived by the Osssen integral equation shows that for the nematic fluid the orientational motion of the director vector characterized by the director surface body stress and intrinsic director body force, leads to un-symmetry in stress tensor. The first Rivlin-Ericksen tensor A_{ij} express deformation history due to the normal-symmetric part of the deformation velocity gradient in the fluid, the spin tensor W_{ij} express deformation history due to the un-symmetric part of the deformation velocity gradient in the fluid. However it should be noted that the un-symmetry of the stress tensor is determined by the un-symmetry of the shear stress components. It has any principal influence on the normal stress differences which is of completely symmetric.

The stress tensor is split into two parts: symmetric and un-symmetric

$$S_{ij} = S_{ij}^n + S_{ij}^s$$

where “n” denotes normal-symmetric part, “s” denotes shear un-symmetric part. The functional Ω_{ij} in (1) is split.

For the normal-symmetric part of the stress tensor the general form of the constitutive equation is proposed as

$$S_{ij}^n + \lambda_{ijkl} \overset{o}{S}_{ij}^n = \Psi_{ij} \left[\overset{o}{A}_{ij}, \overset{o}{A}_{ij}, n_i, N_i, \beta_j \right] + \mu_1 \omega_{jk} \overset{o}{A}_{ki} + \mu_2 \omega_{ik} \overset{o}{A}_{kj} \quad (2)$$

The special term $\mu_1 \omega_{jk} \overset{o}{A}_{ki} + \mu_2 \omega_{ik} \overset{o}{A}_{kj}$ of high order in equation (1) is introduced by author to describe the special change of the normal stress differences which is considered as a result of director tumbling by Larson et al.

For the shear un-symmetric part of the stress tensor the general form of the constitutive equation is proposed as

$$S_{ij}^n + \lambda_k \overset{o}{S}_{ijk}^s = \Phi_{ij} [\omega_{ij}, n_i, N_i, \gamma_j], \quad i \neq j, \quad k=1,2,3 \quad (3)$$

In Eqs. the relaxation time tensor λ_{ijkl} and relaxation time λ_k are introduced for normal-symmetric and shear un-symmetric parts respectively.

IV NORMAL STRESS DIFFERENCES FOR SHEAR FLOW

A special case of the LCP-H model is considered, the rheological behaviour of the normal stress differences are studied for anisotropic biopolymer fluid..

The flow of the LC biopolymer fluid in circular tube with radius of R is studied, the Poiseuille flow is such a typical shear flow of the fluid. The flow of the LC polymer fluid in circular tube with radius of R is studied, such a typical shear flow is the Poiseuille flow for the fluid. For the flow the components of velocity and director vector are expressed by

$$v_z = w(r), v_r = v_\phi = 0 \quad (4)$$

$$n_r = \sin \theta(r), n_z = \cos \theta(r), n_\phi = 0 \quad (5)$$

The first and second normal stress differences are given as

$$\sigma_1 = \frac{\dot{\gamma}^2}{2 + [(\lambda_1 - \lambda_2)\lambda_6 + (\lambda_5 - \lambda_4)\lambda_3]\dot{\gamma} + (2\lambda_3 - \lambda_4 + \lambda_5)\dot{\gamma}}$$

$$\times \left[(\lambda_1 - \lambda_2)\mu^* \dot{\gamma}^2 - 2\lambda_3\mu_0 \dot{\gamma} + (\lambda_1 - \lambda_2)(\eta + \beta_3) - 2\mu_0 \right] \quad (6)$$

$$\sigma_2 = \frac{\dot{\gamma}^2}{2 + [(\lambda_1 - \lambda_2)\lambda_6 + (\lambda_5 - \lambda_4)\lambda_3]\dot{\gamma} + (2\lambda_3 - \lambda_4 + \lambda_5)\dot{\gamma}} \times \left\{ -2[\mu_0 - (\eta + \beta_3)\lambda_1] + [(2\lambda_3 + \lambda_4 + \lambda_5)\mu_0 + (\lambda_1\lambda_5 - \lambda_2\lambda_4)(\eta + \beta_3)]\dot{\gamma} - \langle 2\lambda_1\mu^* + [(\lambda_1 + \lambda_2)\lambda_6 - (\lambda_4 + \lambda_5)\lambda_3]\mu_0 \rangle \dot{\gamma}^2 - (\lambda_1\lambda_5 - \lambda_2\lambda_4)\mu^* \dot{\gamma}^3 \right\} \quad (7)$$

It can be seen from the analytical expression of the first normal stress, there are four zero points the first normal stress which are given as

$$\dot{\gamma}_1 = \dot{\gamma}_2 = 0$$

And other two points are determined by following equation

$$(\lambda_1 - \lambda_2)\mu^* \dot{\gamma}^2 - 2\lambda_3\mu_0 \dot{\gamma} + (\lambda_1 - \lambda_2)(\eta + \beta_3) - 2\mu_0 = 0 \quad (8)$$

Solving the equation two points are obtained for which the first normal stress difference are zero

$$\dot{\gamma}_{3,4} = \frac{2\lambda_3\mu_0 \pm \sqrt{2\lambda_3^2\mu_0^2 - 4[(\lambda_1 - \lambda_2)^2(\eta + \beta_3) - 2\mu_0\mu^*(\lambda_1 - \lambda_2)]\mu^*}}{2(\lambda_1 - \lambda_2)\mu^*} \quad (9)$$

For the principles of non-symmetric constitutive equation proposed by author it is theoretically proved that the plot of normal stress σ_1 changes sign two times at shear rate $\dot{\gamma}_3$ and $\dot{\gamma}_4$ which is in agreement with experiments by Baek, Magda, Larson and Hudson (1993,1994).

V CONCLUSION AND DISCUSSION

A report of advances is given for research on continuum theory of constitutive equation of liquid crystalline (LC) biopolymer fluids, Influence of un-symmetric stress tensor on material functions is given, vibrational shear flow of the fluid with small amplitudes is studied, for special case some results are give by Fig. 1 – Fig 4. A new concept of simple anisotropic fluid is introduced. On the basis of principle of anisotropic simple fluid stress behaviour is described by velocity gradient tensor F and spin tensor W instead of

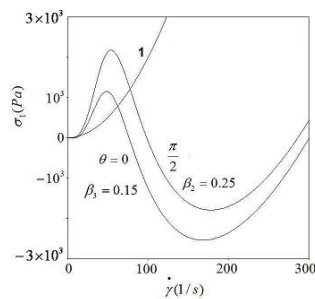
velocity gradient tensor D in the classic Leslie–Ericksen continuum theory. Six relaxation times are introduced. Analyzing rheological nature of the fluid and using tensor analysis a general form of the constitutive equation of co-rotational type is founded. The un-symmetry of the shear stress are predicted by the present continuum theory for anisotropic viscoelastic fluid – LC biopolymer liquids. The influence of the relaxation times on material functions is specially studied. It is important to study the unsteady vibrational rotating flow with small amplitudes , as it is a best way to obtain knowledge of elasticity of the LC polymer i.e. dynamic viscoelasticity. For the shear-unsymmetric stresses, two shear stresses are obtained thus two complex viscosities and two complex shear modulus (i.e. first and second one) are introduced by the constitutive equation which are defined by rotating shear rate introduced by author.

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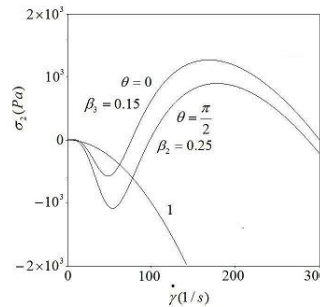
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REFERENCES

- [1] Han Shifang(韩式方), Mechanics of anisotropic Non-Newtonian fluids — Rheology of liquid crystalline polymer, Science Press, Beijing 2008, in Chinese.
- [2] Onogi, S. and Asada T., Rheology and rheo-optics of polymer liquid crystal in Rheology ed. by G. Astria, G. Marrucci, and Nicolai (Plenum, New York, pp 127 - 147 (1980)
- [3] Baek S.-G., Magda J. J. and Larson R.G., Rheological differences among liquid-crystalline polymers I. The first and second normal stress differences of PBG solutions J. of Rheology 1993,
- [4] Baek S.-G., Magda J. J., Larson R.G. and Hudson S. D, Rheological differences among liquid- crystalline polymers II. T Disappearance of negative N_1 in densely packed lyotropic and thermotropes J. of Rheology ,1994, 38 (5) 1473 - 1503
- [5] Green A.E., Anisotropic simple fluid, Proc. Roy. Soc. Londonser, A 279 , p 437- 445 (1964)
- [6] Green A.E., A continuum theory of anisotropic fluids, Proc. Camb. Phil. Soc., 60 p 123 – 128 (1964)
- [7] Volkov V.S. and Kulichikhin V.G., Anisotropic Viscoelasticity of Liquid Crystalline Polymers , J. Rheol., 1990, 34(3) 281-293
- [8] Volkov V.S. and Kulichikhin V.G., Non-symmetric viscoelasticity of anisotropic polymer liquids, J. Rheol., 2000, 39(3) 360-370
- [9] R.G. Larson, 1993, Roll-cell instability in shearing flows of nematic polymers, **J. of Rheology**, 39, 2, Mar/Apr., 175---197.
- [10] Han Shifang, Constitutive equation of liquid crystalline polymer – anisotropic viscoelastic fluid **Acta Mechanica Sinica**, 2001, No 5, p 588-600, Beijing, China, in Chinese
- [11] Han Shifang, Constitutive equation of co-rotational derivative type for anisotropic viscoelastic fluid **Acta Mechanica** ,in English , No: 2 p 46-53 (2004)
- [12] Han Shifang, An unsymmetric constitutive equation for anisotropic viscoelastic fluid Beijing: **Acta Mechanica Sinica** , vol 23, No: 2 , p149-158 (2007) Springer
- [13] Han Shifang, A Constitutive Equation of Co-Rotational Type for Liquid Crystalline Polymer and Influence of Orientation on Material Functions, J. of central South Univ. Technol. v.14 Suppl. 1, p14-18, 2007, Springer
- [14] Han Shifang, Computational Analytical Approach to Shear -Extensional Flow in Fiber spinning of Liquid Crystalline Polymer Melt, J. of central South Univ. of Technol. , v. 14 Suppl. 1. p61-67, 2007, Springer
- [15] Han Shifang , Research advances in research on non-symmetric constitutive theory of anisotropic viscoelastic liquids and its hydrodynamic Behavior, J. of central South Univ. Technol. v. 15 Suppl. 1. p1-4 2008, Springer
- [16] Han Shifang , Vibrational shear flow of anisotropic viscoelastic fluid with small amplitudes, J. of central South Univ. Technol. v. 15 Suppl. 1. p29-32 , 2008, Springer
- [17] Han Shifang , Stability of shear-extensional flow in film extrusion of liquid crystalline polymer-anisotropic viscoelastic fluid , **AIP Conf. Proc.** -- July 7, 2008 -- Volume 1027, pp. 126-128 The XV Int.Congress on Rheology, The Society of Rheology USA, 80th Annual Meeting, 2008



(a)



(b)

Fig.1 First normal stress difference σ_1 (a) and second normal stress difference σ_2 (b) vs shear rate $\dot{\gamma}$,

LCP – Qs model , 1 — co-rotational Maxwell model (with director parallel and vertical to flow direction)

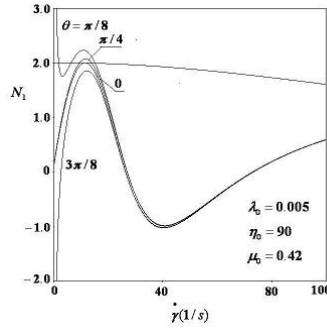
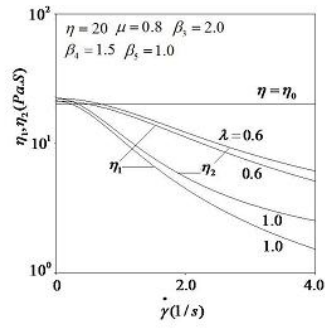
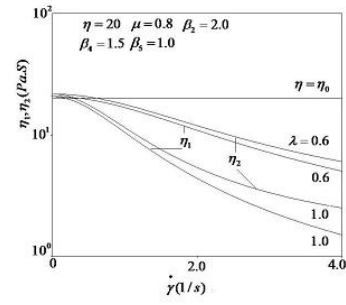


Fig.2 First and second normal stress difference functions N_1 (a) vs shear rate $\dot{\gamma}$
LCP-Qs model (with director angle $\theta = 0, \pi/8, 3\pi/8, \pi/4$)

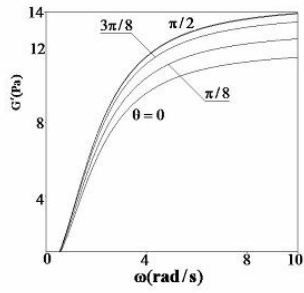


(a)

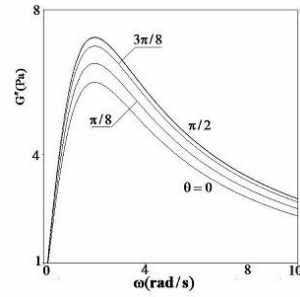


(b)

Fig.3 First and second apparent viscosity vs shear rate , director is parallel (a) and vertical (b) to flow direction
(with variation of relaxation time)



(a)



(b)

Fig.4 Storage modulus G' (a) and loss modulus G'' (b) vs oscillation amplitude with action of normal-symmetric stress