Effect of Mobility Tensor on the Residence Time Distribution for Viscoelastic Fluids in the Tubular Reactor

Mahyar Saleh, Mohamad Samipourgiry, Nasrollah Majidian, and AmirSahand Gooyavar

Abstract—**In this paper, the effect of mobility tensor on the residence time distribution (RTD) for viscoelastic fluids in the tubular reactor have been investigated using the conformational models. From industrial point of view, determination of the residence time distribution for viscoelastic fluids in tubular reactors is very important because it is used to achieving optimum performance conditions of tubular reactor. In order to determinate the residence time distribution function for viscoelastic fluids in the tubular reactor, the conformational rheological models and the motion equations have been considered together. The model predictions have been compared for the two families of mobility expressions. The Study of the model prediction sensitivity to its mobility term shows that model predictions can cover a wide range of exprimental results for residence time distribution generally observed for viscoelastic fluids in the tubular reactor.**

Index Terms—**Conformational models, mobility tensor, tubular reactor, viscoelastic fluid**

I. Introduction

Tubular reactors are very important pieces of equipment in any chemical industry facility. They are always used in a continuous flow mode with reagents flowing in and products being removed. They can be the simplest of all reactor designs which are used in a variety of industries such as petroleum, petrochemical, polymer, pharmaceutical, waste treatment and specialty chemical. In other to achieving optimum performance condition of tubular reactor, the residence time distribution (RTD) curves give the useful information. It is evident that elements of fluid taking different routes through the reactor may take different lengths of time to pass through the reactor. The distribution of these times for the stream of fluid leaving the reactor is called the residence time distribution of fluid which has the units of time^{-1}[1]-[2].

The residence time distribution analysis is a very efficient diagnosis tool that can be used to inspect the mixing performance of a tubular reactor, initial, average and final residence times, presence of stagnation zones and etc. It can also be very useful in the modeling of reactor behavior, in the estimation of effluent properties, scale-up and improving equipment design [1]-[3].

Study of the residence time distribution function for viscoelastic fluids with relatively long molecular chains is very complex because their behavior lies between the Newtonian fluids and the ideal elastic solids. A useful instrument to understand the behavior of these fluids, commonly used in industrial polymer processing, is the theoretical modeling of their behavior [1]-[5].

After the first goal in viscoelastic fluids,finding the residence time distribution.

RTD is calculated experimental and analytical methods for each type of fluids [1].

In this paper, the residence time distribution function for viscoelastic fluids in tubular reactor have been investigated using conformational rheological models.

There are many developed models which usually relate the stress tensor to the rate of the strain tensor or its derivatives, where conformational models relate the stress tensor to the molecular conformation tensor changes during flow. In these types of models a micro-structural state variable called conformation tensor *c* shows the state of deformations of polymer molecules during flow. In conformation tensor model, if the length of polymer chains during flow remains constant, this is called Fenp model in which *trc©=constant* must be satisfied.

And the volume of polymer chains during flow remains constant, this is called VPCR(volume permanency conformation rheological) or Leonov-like model in which *det c = constant* must be satisfied [6]-[9].

In this paper, Leonov-like model is used due to more attention.

II. Viscoelastic Fluid Modeling

For a non-compressible viscoelastic fluid with a microstructure represented by a second order symmetric tensor, *c*, the Poisson bracket formalism leads to the following equations for the time evolution of *c* and the stress tensor, σ:[6] -[12].

$$\frac{\partial c}{\partial t} = \frac{1}{2}(\dot{\gamma}\cdot c + c.\dot{\gamma}) - \frac{1}{2}(\omega c - c.\omega) - \Lambda\frac{\partial \Phi}{\partial c} \quad (1)$$

$$\sigma = -2\left(c.\frac{\partial \Phi}{\partial c}\right) \quad (2)$$

where Λ is a fourth-order tensor, called the mobility tensor which is essentially an inverse relaxation time to the viscoelastic fluids, $\dot{\gamma}$ is the strain tensor, *c* is conformation tensor, ω is the vorticity tensor, σ is the extra tensor, and Φ is the Helmholtz free energy function. The first term $(1/2(\dot{\gamma}\cdot c + c.\dot{\gamma}) - 1/2(\omega.c - c.\omega))$ is a convective term describing the conservative effects derived from the Poisson

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bracket which is only related to the conformation tensor in specific radius of die. The second term ($\Lambda : \partial\Phi/\partial c$) is dissipative term accounting for non-conservative phenomena derived from the dissipative bracket in the generalized Poisson bracket formalism.

For the Hookean based model, the Helmholtz free energy function can be written as:[6]- [11].

$$\Phi = \frac{\lambda}{2}\left[\mathrm{tr}\left(\frac{\delta - c^{-1}}{2}\right)\right]^2 + M\left[\mathrm{tr}\left(\frac{\delta - c^{-1}}{2}\right)^2\right] \tag{3}$$

In the above equation, M and λ is the model parameters related to the molecular weight and relaxation time respectively, and δ is a unit tensor. To ensure that this model remains volume preserving for different mobility tensors, Ramazani et al. introduced the following form for the dissipative term of the time evolution of the conformation tensor [9].

$$\Lambda : \frac{\partial\Phi}{\partial c} = \Lambda^1 : \frac{\partial\Phi}{\partial c} - \frac{1}{3}\mathrm{tr}\left(c^{-1}\cdot\Lambda^1 : \frac{\partial\Phi}{\partial c}\right)c \tag{4}$$

where Λ^1 could be any combination of the generalized form of the fourth order mobility tensors presented by Beris and Edwards as follows [13].

$$\begin{aligned}
\Lambda_{\alpha\beta\varepsilon\gamma} &= a_1\delta_{\alpha\beta}\delta_{\gamma\varepsilon} + a_2(\delta_{\alpha\gamma}\delta_{\beta\varepsilon} + \delta_{\alpha\varepsilon}\delta_{\beta\gamma}) \\
&+ a_3(c_{\alpha\beta}\delta_{\gamma\varepsilon} + \delta_{\alpha\beta}c_{\gamma\varepsilon}) \\
&+ a_4(c_{\alpha\gamma}\delta_{\beta\varepsilon} + c_{\alpha\varepsilon}\delta_{\beta\gamma} + \delta_{\alpha\gamma}c_{\beta\varepsilon} + \delta_{\alpha\varepsilon}c_{\beta\gamma}) \\
&+ a_5 c_{\beta\alpha}c_{\gamma\varepsilon} + a_6(c_{\alpha\gamma}c_{\beta\varepsilon} + c_{\alpha\varepsilon}c_{\beta\gamma}) \\
&+ a_7(c_{\alpha\mu}c_{\mu\beta}\delta_{\gamma\varepsilon} + \delta_{\alpha\beta}c_{\gamma\mu}c_{\mu\varepsilon}) + a_8(c_{\alpha\mu}c_{\mu\gamma}\delta_{\beta\varepsilon} \\
&+ c_{\alpha\mu}c_{\mu\varepsilon}\delta_{\beta\gamma} + \delta_{\alpha\gamma}c_{\beta\mu}c_{\mu\varepsilon} + \delta_{\alpha\varepsilon}c_{\beta\mu}c_{\mu\gamma}) \\
&+ a_9(c_{\alpha\mu}c_{\mu\beta}c_{\gamma\varepsilon} + c_{\alpha\beta}c_{\gamma\mu}c_{\mu\varepsilon}) \\
&+ a_{10}(c_{\alpha\mu}c_{\mu\gamma}c_{\beta\varepsilon} + c_{\alpha\mu}c_{\mu\varepsilon}c_{\beta\gamma} + c_{\alpha\gamma}c_{\beta\mu}c_{\mu\varepsilon} + c_{\alpha\varepsilon}c_{\beta\mu}c_{\mu\gamma}) \\
&+ a_{11}c_{\alpha\eta}c_{\eta\beta}c_{\gamma\mu}c_{\mu\varepsilon} + a_{12}(c_{\alpha\eta}c_{\eta\gamma}c_{\beta\mu}c_{\mu\varepsilon} + c_{\alpha\eta}c_{\eta\varepsilon}c_{\beta\mu}c_{\mu\gamma})
\end{aligned} \tag{5}$$

where c_{ij} are components of the conformation tensor as well as a_1, a_2 ... and a_{12} can be constants or functions of the scalar invariants of c.

TABLE I: TWO FAMILIES OF THE MOBILITY TENSOR

	$\Lambda^1_{\alpha\beta\gamma\varepsilon}$
order 3	$\Lambda_0(c_{\alpha\mu}c_{\mu\gamma}c_{\beta\varepsilon} + c_{\alpha\mu}c_{\mu\varepsilon}c_{\beta\varepsilon} + c_{\alpha\gamma}c_{\beta\mu}c_{\mu\varepsilon} + c_{\alpha\varepsilon}c_{\beta\mu}c_{\mu\gamma})$
order 4	$\Lambda_0(c_{\alpha\eta}c_{\eta\gamma}c_{\beta\mu}c_{\mu\varepsilon} + c_{\alpha\eta}c_{\eta\varepsilon}c_{\beta\mu}c_{\mu\gamma})$

Λ_0 is a phenomenological parameter of model that is inversely related to the zero shear rate viscosity.

Helmholtz free energy functions can be used with the different mobility tensors; therefore a large family of volume preserving models can be defined. Effects of the mobility tensors on the shear rate distribution, the viscosity distribution, the first and the second normal stresses differences have been studies previously and it was concluded that the choice of mobility tensor type has a pronounced effect on the prediction results.[11]

Two types expression which have actually investigated in this paper are specified in table 1.

III. Constitutive Equations

Because of the shear rate dependency on the radius of reactor in the tubular reactor, the momentum relation has been used to solve the model. Consequently the model and the relevant motion equation have been solved simultaneously.

We considered a cylindrical coordinate system (r, θ, z) with the z axis in the axial direction.

For a steady state flow in the tubular reactor, velocity components are given by:

$$V_1 = V_z = V_z(r), \quad V_2 = V_r = 0, \quad V_3 = V_\theta = 0 \tag{6}$$

Therefore, the rate of strain tensor and the vorticity tensor have the following forms:[4]-[5]

$$\dot{\gamma}(r) = \nabla V + \nabla V^T \qquad \omega(r) = \nabla V - \nabla V^T \tag{7}$$

where $\dot{\gamma}(r)$ is the rate of strain tensor, ω(r) is the vorticity tensor and superscript T indicate to transpose matrix.

The relevant equation of motion in z-direction are given by:

$$\frac{\partial P}{\partial z} + \frac{1}{r}\frac{\partial}{\partial r}(r\tau_{rz}) = 0 \tag{8}$$

where $\frac{\partial P}{\partial z}$ is a constant, therefore,

$$\tau_{21} = \tau_{rz} = -\frac{r}{2}\frac{\partial P}{\partial z} \tag{9}$$

Therefore, tensor conformation calculated using of (2) equation.

Then, rate of strain calculated using of (1) equation.

The velocity in the z-direction calculated using of the following equation [1]-[3].

$$V_z(r) = -\int_o^R \dot{\gamma}(r)dr \tag{10}$$

Consequently, the residence time of fluid in the tubular reactor are given by:

$$t = \frac{l}{V_z(r)} \tag{11}$$

where l is length of tubular reactor.

In this paper,length of tubular reactor is assumed one *meter*.

Finally, the model that is in the form of a differential equations system with the motion equation as mentioned above are solved using MATHEMATICA software.

IV. RESULTS AND DISCUSSION

The shear rate distribution, the velocity distribution and the residence time distribution function have been predicted by the Leonov-like model in steady state flow and fully developed conditions. The closed reactor boundary condition is considered, so there should be no flow or diffusion or up-flow eddies at the entrance or at the reactor exit.

All predictions were obtained using the following set of parameters: Λ_0=1/19500(m.s)/kg, M=1000g/mol, λ=5000(1)/s, ∂p/∂z=5000 kPa , R=0.25m (R is radius of reactor), *l*=1m (*l* is length of reactor).

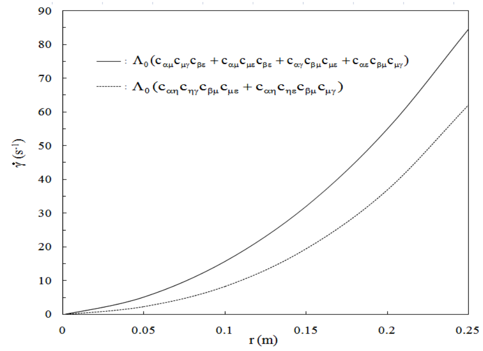

Fig. 1. The shear rate distribution versus the radius of tubular reactor.

Fig. 1. shows the effects of the mobility tensor on the shear rate distribution. The predictions indicate that the choice of mobility term has a pronounced effect on the shear rate distribution. The results presented in fig. 1. show that the shear rate increases with increasing the radius of reactor. The predictions of the shear rate are different for two mobility tensors across the tubular reactor and their differences becomes more significant as approaching to the center of reactor. It can be resulted that the flexibility in the choice of the mobility tensor permits a good fit of a whole class of experimental data presented in literature.

Fig. 2. shows the model prediction for the velocity distribution in z-direction in the tubular reactor. The results presented in fig. 2. shows that as the radius of reactor increases, the velocity reduces. It is observed that as expected, the maximum velocity of the fluid and the zero velocity of fluid will be in the center of reactor and in the wall of reactor respectively.

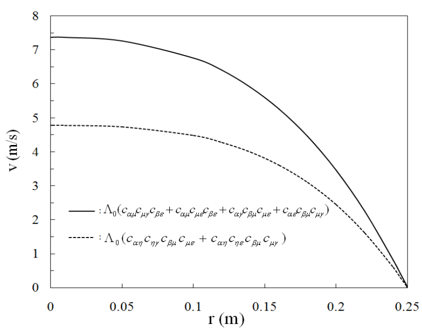

Fig. 2. The velocity distribution in z-direction versus the radius of tubular reactor.

Fig. 3. shows the residence time distribution function in the tubular reactor for two mobility tensors. As it can be seen from the fig. 3, the trend of predicted results for the residence time distribution function for viscoelastic fluid in tubular reactor are similar to their experimental results presented in the literatures.

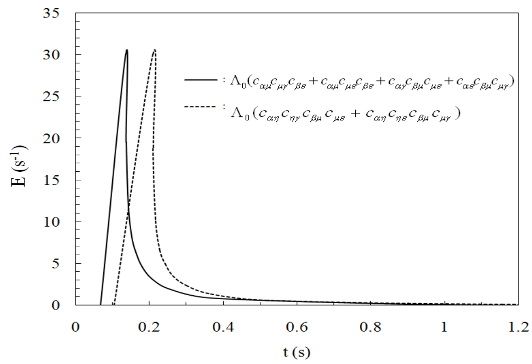

Fig. 3. The residence time distribution function in the tubular reactor and effect of mobility tensor.

V. CONCLUSION

The effect of mobility tensot on the residence time distribution (RTD) for viscoelastic fluids in the tubular reactor have been investigated using the conformational rheological models. It is observed that as expected, the maximum velocity of the fluid and the zero velocity of fluid will be in the center of reactor and in the wall of reactor respectively. Because of the flexibility in the choice of the various mobility tensors for the conformational rheological models, it is concluded that using from the conformational models can permit a good fit of a whole class of experimental data presented in literatures for residence time distribution of viscoelastic fluids. Moreover, it is concluded that, the trend of predicted results for the residence time distribution function is similar to their experimental results presented in the literatures.

Finally, we have calculated effect of reactor radius change on the residence time distribution,effect of reactor pressure drop on the residence time distribution,effect fluid molecular weight change on the residence time distribution,effect reactor temperature change on the residence time distribution ,..using tensor conformation.

In fact,here to help microscopic quantity get macroscopic quantity.

REFERENCES

[1] O. Levenspiel, *Chemical Reaction Engineering*, New York, pp. 300-312. 1999.

[2] E. Ludwig, *Applied Process Design for Chemical and Petrochemical Plants*, pp.49-52. 1999.

[3] W. Macosko and J. Wiley, *Rheology-Principles-Measurment and Application*, pp.78-83. 1994,

[4] R. Bird and R. Armstrong, *Dynamics Of Polymeric Liquids*,Vol. 1, pp.101-121. 1987.

[5] P. A. M. Dirac, The Principles of Quantum Mechanics, 4th ed, *Oxford University Press*, New York ,1967,pp.378-382

[6] J. B. Tatum, Classical Mechanics, 2004.

[7] H. Eslami, A. Ramezani, and H. A. Khonakdar. (2003). Volume-Preserving Conformational Rheological Models for Multi-Component Miscible Polymer Blends Using the GENERIC Formalism. *Macromolecular Science and Simulation*. [Online].12, pp.524-530.Available:http://www.wiley-vch.de/publish/en/journals/alphabeticIndex/2262

[8] M. Grmela and P. J. Carreau.(1987). Conformation Tensor Rheological Models. *Journal of Non-Newtonian Fluid Mech* . [Online]. 23, pp.271 Available:http://www.journals.elsevier.com/journal-of-non-newtonian-fluid-mechanics/

[9] R. Guenette , A. Zine, M. Grmela, and P. J. Carreau.(1992). Simulation of Viscoelastic Flows Using A Conformation Tensor Model. *Journal journal of Non-Newtonian Fluid Mech.* [Online]. 45, pp. 187 Available:http://www.journals.elsevier.com/journal-of-non-newtonian-fluid-mechanics/

[10] A. Ramezani, M. Grmela, and Ch. Zhou. Vol. preserving Rheological Model for Polymer Melts and Solutions Using, the Generic Formation. *Journal theology*. [Online]. 43, pp. 51. Available: http://www.journalofrheology.org/ 1999.

[11] H. Eslami, A. Ramezani, and H. A. Khonakdar.(2004). Predictions of Some Internal Microstructural Models for Polymer Melts and Solutions in Shear and Elongational Flows. *Macromolecular Science and Simulation*. [Online]. 13, pp. 664. Available: http://www.wiley-vch.de/publish/en/journals/alphabeticIndex/2262

[12] A. Ramazani , A. Kadi and M. Grmela.(1997).Rheological modeling of A short fiber thermoplastic composites. Journal of Non-Newtonian Fluid Mech. [Online].73, pp.241http://www.journals.elsevier.com/journal-of-non-newtonian-fluid-mechanics

[13] A. N. Beris and B. J. Edwards, T*hermodynamics of Flowing Systems with internal microstructure*, Oxford University Press, New York,USA,1994,pp.197-202.

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