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Evaluation of a Modified Jeffreys Type Model for Viscoelastic Fluids

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Abstract

In this study using some existing constitutive equations, a modified Jeffreys type model with retardation time is developed which is successful with the experimental data for simple shear flow and shear free flow. Nonlinear regression analysis based on Marquardt Algorithm is used for determination of material parameters for simple shear flow. The general form of the modified model is reduced by using the simple shear flow conditions and Oldroyd derivative for cartesian coordinates. In the determination of material parameters of the modified model is used experimental data of Leider and Lilleleht(1973) for viscometric functions. When viscometric functions of the modified model is compared with viscometric functions of the existing constitutive equations which use the material parameters of Leider and Lilleleht(1973), viscometric functions of the modified model is found to be more successful.

Key Words: Viscoelastic fluids; Nonlinear regression; Numerical simulations; Constitutive equations

Değiştirilmiş Jeffreys Tipli Bir Modelin Viskoelastik Akışkanlar İçin Değerlendirilmesi

Özet

Bazı mevcut bünye denklemlerinin kullanıldığı bu çalışmada, basit kaymalı(simple shear) ve kaymasız(shear free) akımlar için deneysel verilere göre daha başarılı olan değiştirilmiş Jeffreys tipli bir model geliştirilmiştir. Basit kaymalı akımda malzeme parametrelerin belirlenmesi için, Marquardt Algoritmasının temel teşkil ettiği lineer olmayan regresyon analizi kullanılmıştır. Değiştirilen modelin genel formu, basit kaymalı akım şartları ve karteziyan koordinatlar için Oldroyd türev operatörü kullanılarak indirgenmiştir. Modelin malzeme parametrelerinin belirlenmesinde, Leider ve Lilleleht(1973)'ın viskometrik fonksiyonlarına ait deneysel veriler kullanılmıştır. Değiştirilen modele ait viskometrik fonksiyonlarının, Leider ve Lilleleht(1973)'ın malzeme parametrelerinin kullanıldığı mevcut bünye denklemlerinin viskometrik fonksiyonları ile karşılaştırıldığında, değişiklik yapılan modelin daha başarılı olduğu bulunmuştur.

Anahtar Sözcükler: Viskoelastik akışkanlar, lineer olmayan regresyon; Nümerik simulasyon; bünye denklemleri

Introduction

The formulation of a general rheological equation of state which completely describes a given material is the ultimate objective of the rheologist. This tensor equation is a completely general mathematical model for the rheological behavior of the material, and may be used to predict a variety of specific material functions. The test of validity of the model is the degree to which it can represent measured material functions. If agreement between the model and observed data is achieved, the constant parameters which appear in the model equation, which constitute the rheological properties of the material, may be evaluated.

By proper application of the basic principles, mathematical model or general rheological equations of state for viscoelastic fluids may be formulated which should be valid for any deformation, regardless of magnitude or time history. By employing these models to calculate the response(i.e., stress behavior) in various specific deformations such as steady simple shear, oscillatory shear, etc., analytical expressions for the corresponding material functions such as apparent viscosity, normal stress functions complex modulus, etc., may be determined.

Materials and their generalized models or rheological equations of state may be broadly classified as linear or nonlinear(Bird et al., 1987; Bird and Wiest, 1995). One consequence of nonlinearity is shear dependent apparent viscosity and normal stress coefficients. Essentially all real materials of complex structure are nonlinear except under conditions of very small deformation.

A comparison and evaluation of a number of viscoelastic models has been presented by Bogue and Doughty(1966). Leider and Lilleleht(1973) obtained the material parameters in the White-Metzner(White and Metzner, 1965) and Oldroyd 3-constant(Williams and Bird, 1962) models for steady shear flow.

Arıkol(1985) obtained the point velocity and first normal stress difference data via non-contact measurements techniques, namely laser Doppler anemometry(LDA) and stress birefringence for the periodic contractions and expansions channel. The non-newtonian fluid was a 5% polyisobutylene solution in mineral oil flowing through the channel shown in Fig. 1. This type of flow is interesting and challenging since it is considered as a reasonable simulation of flow through porous media(Arıkol, 1985) owing to its periodic contractions and expansions. Davidson et al.(1993) used both LDA and stress birefringence to determine velocity and stress data in the straight-walled portion of a periodically constricted channel.

Nonlinear hydrodynamic stability analysis has been done by Park and Lee(1995) for viscoelastic fluids heated from below for the cases of rigid-rigid and rigid-free boundary conditions that can be compared with experimental results(Schlüter et al., 1965). In that study a very general constitutive relation, which encompasses the Maxwell model, the Jeffreys model(or Oldroyd model) and the Phan-Thien-Tanner model(Sokolov and Tanner, 1972) has been adopted.

A comparative evaluation of existing rate-type constitutive equations have been provided by Kopaç et al.(1997) for a viscoelastic fluid undergoing accelerated flow. For each constitutive equations, the numerical values of material parameters which yield the best fit with experimental data are determined via non-linear regression analysis. Kopaç and Arıkol(1997) proposed a model which is more consistent with the experimental stress difference values using non linear regression analysis in the periodic contractions and expansions channel for shear free flow.

In this study, the model proposed by Kopaç and Arıkol(1997) and Kopaç et al.(1998) that's successful for shear free flow will be used for simple shear flow. For this reason the viscometric functions of the model has to be determined. Upon comparison of the viscometric functions determined with the experimental results(Leider and Lilleleht, 1973), the material parameters appearing in constitutive equations are determined via non linear regression analysis(Constantinides, 1987). The comparison of viscometric functions of the proposed model with the existing functions of White-Metzner and Oldroyd 3-constant models is also aimed. The material parameters determined for simple shear flow will be used for shear free flow for the solution of the reduced differential equations along the centerline of these three models(Kopaç et al., 1997; Kopaç and Arıkol, 1997). The solution of differential equations for shear free flow are obtained using 4th order Runge-Kutta Integration technique(Mathews, 1992).

Flow conditions

The two types of flow often used to characterize polymeric liquids are simple shear flow and shear free flow. For the periodic contractions and expansions channel shown in Fig. 1, only two-dimensional flow is considered and all changes in the 3-direction are neglected. Flow conditions have been presented by Kopaç et al.(1997) and Kopaç and Arıkol(1997) for both flow type.

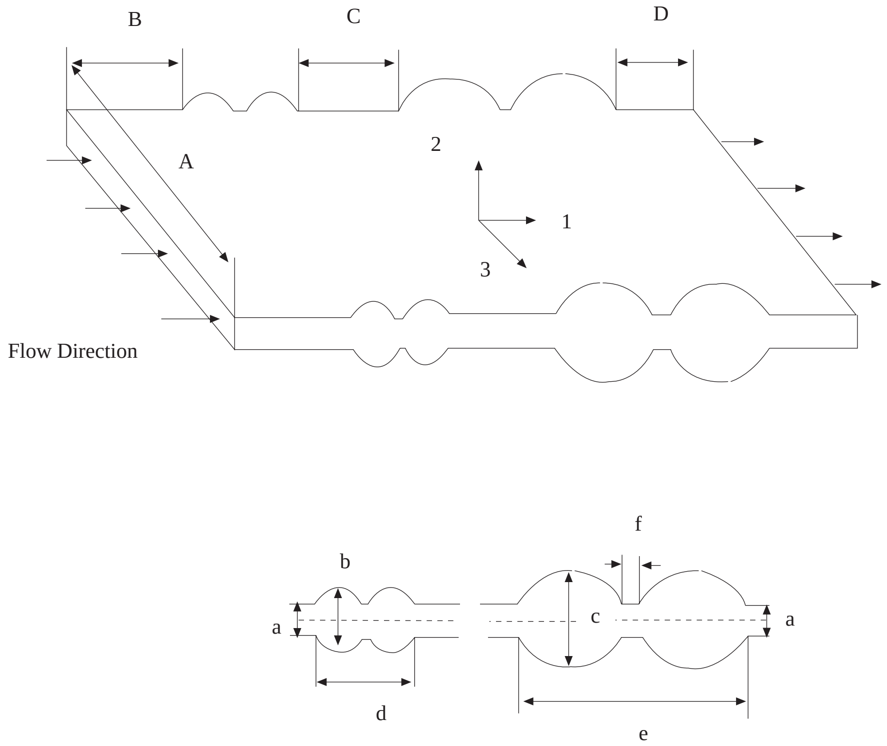

Figure 1. General and side views of the flow channel. Dimensions(metres): A=0.06; B=0.02; C=0.2; D=0.17; a=0.00207∓0.00005; b=0.00445∓0.00005; c=0.00695∓0.00005; d=0.00875∓0.0001; e=0.0175∓0.0001; f=0.0095∓0.00005

Governing equations

Continuity equation:

$$\frac{D\rho}{Dt} + \rho divV = 0 \tag{1}$$

(1) Equation can be written for incompressible liquids as follows;

$$divV = 0 \quad or \quad \frac{\partial V_1}{\partial x_1} + \frac{\partial V_2}{\partial x_2} = 0 \tag{2}$$

where V_1 and V_2 are velocities in 1- and 2- directions respectively.
The rate of strain and vorticity tensors can be written as follows;

$$\Delta_{ij} = (V_{i,j} + V_{j,i}) \tag{3}$$

$$\Omega_{ij} = (V_{j,i} - V_{i,j}) \tag{4}$$

Modified model

The non linear derivative operator constitutive equation proposed for the shear free flow in the previous study(Kopaç and Arıkol, 1997) is used for simple shear flow. This is a modified form of Jeffreys model. The relaxation time and viscosity which are constants at Jeffreys model are used in this model to be dependent of 2nd invariant of rate of strain tensor. Retardation time was used as a constant parameter as in Jeffreys (or Oldroyd) model. The derivative operator in this model is as in Jeffreys Model(Bird et al., 1987; Williams and Bird, 1962). For retardation time and viscosity, the expressions proposed by White and Metzner(1965) were used. This modified model has been defined as follows;

$$\tau_{ij} + \theta J(\tau_{ij}) = \mu[\Delta_{ij} + \lambda J(\Delta_{ij})] \tag{5}$$

where θ, μ and λ are relaxation time parameter, viscosity and retardation time parameter respectively. J is nonlinear derivative operator. θ and μ have been presented such as White and Metzner (1965) as follows;

$$\theta = \frac{1}{\theta_0 + \theta_1 |II_\Delta|^{r/2}} \quad ; \quad \mu = \frac{\eta_0}{1 + d_1 |II_\Delta|^{r/2}} \tag{6}$$

where θ_0, θ_1, r and d_1 are constant parameters; η_0 is zero viscosity; II is second invariant.
Nonlinear derivative operator, J, can be written as follows;

$$J()_{ij} \equiv \mathcal{D}/\mathcal{D}t()_{ij} - 1/2[\Delta_i^k()_{jk} + \Delta_j^k()_{ik}] \\ +1/3()_{kn}\Delta^{kn}g_{ij} \tag{7}$$

where $\mathcal{D}/\mathcal{D}$t is Jaumann derivative and have been presented as follows;

$$\mathcal{D}/\mathcal{D}t()_{ij} \equiv \partial/\partial t()_{ij} + V^k()_{ij,k} + \frac{1}{2} \\ [\Omega_i^k()_{kj} - ()_{ik}\Omega_j^k] \tag{8}$$

The compenents of rate of strain and vorticity tensors have been reduced for simple shear flow as follows;

$$\bar{\Delta}_{ij} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \dot{\gamma} \\ \bar{\Omega}_{ij} = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \dot{\gamma} \tag{9}$$

where $\dot{\gamma}$ (shear rate) $= \frac{\partial V_1}{\partial x_2}$

Derivations of viscometric functions

Viscosity function ($\eta(\dot{\gamma})$), first and second normal stress coefficients $[\Psi_1(\dot{\gamma}), \Psi_2(\dot{\gamma})]$ are defined generally as follows(Bird et al., 1987);

$$\eta = \frac{\tau_{12}}{\dot{\gamma}}; \quad \Psi_1 = \frac{\tau_{11} - \tau_{22}}{\dot{\gamma}^2}; \quad \Psi_2 = \frac{\tau_{22} - \tau_{33}}{\dot{\gamma}^2} \tag{10}$$

Compenents of J() of stress and rate of strain tensors obtained used Eqs(7 to 9) have been reduced as follows;

$$\bar{J}(\tau_{ij}) = \dot{\gamma} \begin{bmatrix} -\frac{4}{3}\tau_{21} & -\tau_{22} & 0 \\ -\tau_{22} & \frac{2}{3}\tau_{21} & 0 \\ 0 & 0 & \frac{2}{3}\tau_{21} \end{bmatrix} \\ \bar{J}(\Delta_{ij}) = \dot{\gamma}^2 \begin{bmatrix} -\frac{4}{3} & 0 & 0 \\ 0 & \frac{2}{3} & 0 \\ 0 & 0 & \frac{2}{3} \end{bmatrix} \tag{11}$$

Inserting equation (11) in equation (5), the components of stress were found as follows with the asummption of τ_{21}=τ_{12};

$$\tau_{11} = (-4/3)\mu\lambda\dot{\gamma}^2 + (4/3)\theta\dot{\gamma}\tau_{12}; \tag{12}$$
$$\tau_{12} = \mu\dot{\gamma} + \theta\dot{\gamma}\tau_{22} \tag{13}$$
$$\tau_{22} = (2/3)\mu\lambda\dot{\gamma}^2 - (2/3)\theta\dot{\gamma}\tau_{12}; \tag{14}$$
$$\tau_{33} = (2/3)\mu\lambda\dot{\gamma}^2 - (2/3)\theta\dot{\gamma}\tau_{12}; \tag{15}$$

Rearrangement of Equations (12-15), according to Equation (10), viscometric functions of the modified model were derived as follows,

Viscosity function:

$$\eta = \frac{\tau_{12}}{\dot{\gamma}} = \mu \frac{1 + \frac{2}{3}\theta\lambda\dot{\gamma}^2}{1 + \frac{2}{3}\theta^2\dot{\gamma}^2} \tag{16}$$

First and second normal stress coefficients:

$$\Psi_1 = \frac{\tau_{11} - \tau_{22}}{\dot{\gamma}^2} = 2\mu \frac{\theta - \lambda}{1 + \frac{2}{3}\theta^2\dot{\gamma}^2} \tag{17}$$

$$\Psi_2 = \frac{\tau_{22} - \tau_{33}}{\dot{\gamma}^2} = 0 \tag{18}$$

Determination of material parameters and results

The experimental viscometric data of Leider and Lielleieht(1973) have been utilized in order to determine the material parameters. The material parameters of viscometric functions defined by equation (16, 17) have been determined using the nonlinear regression method developed by Constantinides(1987). Application of the algorithm to the equations has been given in detail in the previous studies(Kopaç, 1992; Kopaç et al., 1997; Kopaç and Arıkol, 1997; Kopaç et al., 1998). The material parameters determined for the modified model and the results for White-Metzner ve Oldroyd 3-constant models determined by Leider and Lielleleht(1973) have been given in Table 1.

Using the parameters given in Table 1 at the viscometric functions for 3 models, sum of square values with respect to the experimental data are given in Table 2.

Using the material parameters given in Table 1, comparison of the variation of viscometric functions with respect to shear rate with experimental data are presented in Figures 2 and 3.

Also, nonlinear differential equations reduced to symmetry axis were obtained for shear free flow in the previous studies(Kopaç, 1992; Kopaç et al., 1997; Kopaç and Arıkol, 1997; Kopaç et al., 1998) for each of three models used. The material parameters determined for simple shear flow were used as input in these equations. These equations were solved by the 4th order Runge-Kutta integration method and compared with the experimental data(Arıkol, 1976, 1985). Experimental stress difference values(Arıkol, 1976, 1985) and the results for each of 3 models were shown in Figure 4. Sum of square values of the errors for model results with respect to experimental values are summarized in Table 3.

Table 1. Numerical values of parameters of the viscoelastic models

Model	Parameters
Modified Model (This study)	η_0=66 dynes.sec/cm^2 θ_0=10.359000 sec^{-1} θ_1=0.3325100 sec$^{-1/r}$ λ=0.0199490 sec d_1=0.0054894 sec$^{-1/r}$ r=0.7000000
White-Metzner (Leider and Lilleleht, 1973)	η_0=66 dynes.sec/cm^2 θ_0=13.20 sec^{-1} θ_1=5.250 sec$^{-1/r}$ d_1=0.154 sec$^{-1/r}$ r=0.750
Oldroyd 3-constant (Leider and Lilleleht, 1973)	η_0=66 dynes.sec/cm^2 λ_1=0.1050 sec λ_2=0.0292 sec

Table 2. Comparison of viscometric functions of different constitutive equations

Model	Sum of squares	
	$\eta(x(0.1Pas)^2)$	$\Psi_1(x(0.1Pas^2)^2)$
Modified Model	12.4	0.107
Oldroyd 3-constant	47.3	0.236
White-Metzner	469.5	27.1

Table 3. Comparison of first normal stress difference predictions of different constitutive equations via fourth order Range-Kutta integration method

Model	Sum of squares $(x(0.1Pa)^2)$
Modified Model	2113
Oldroyd 3-constant	2237
Whiti-Metzner	3072

Discussion

In the previous studies(Kopaç et al., 1997), it has been shown that White-Metzner and Oldroyd 3-constant models seem to be more successful than the other existing models for shear free and simple shear type flows. For this reason in this study the modified model was compared with these two equations. For the determination of viscometric functions for these two existing models with respect to shear rate, η_0 value used is 66 dyn.s/cm^2 and the parameter values determined by Leider and Lilleleht(1973) were used.

It is seen in Table 2 that sum of squares of both viscometric functions for the modified model are lower than those of the other existing models. Sum of squares of White-Metzner model are much larger than the other two models. In other words it can be said that retardation time parameter (second time parameter) models fits to the experimental results with lower error than the models without retardation time.

As for viscosity function(η), all the viscoelastic models predict constant viscosity (zero viscosity) η_0 at low shear rate ($\dot{\gamma}$ <1) and decreasing viscosity function with slightly different slopes with increasing shear rate(Fig. 2). The predictions for the Oldroyd 3-constant and White-Metzner models deviate from the experimental data at high shear rates. Similar variation has been observed for the modified model and the Oldroyd 3-constant models for viscosity values in the range $0.1\leq \dot{\gamma} \leq 10$ for $\dot{\gamma}$ >10, the results of Oldroyd 3-constant model deviates from the results of the modified model.

In the whole range results of the modified model are in good agreement with the experimental viscosity function.

The first normal stress coefficient (Ψ_1) predicted by the modified model and Oldroyd 3-constant model are in good agreement with the experimental data throughout the shear rate range considered(Fig. 3). The predictions for the White-Metzner model deviate from the data at the shear rate range $0.1\leq \dot{\gamma} \leq 10$.

When the results of each of three models for shear free flow were compared with the experimental results of Arıkol(1985), the modified model is appeared to be more successful as seen in Figure 4. Oldroyd 3-constant model gives closer results with the modified model whereas White-Metzner model gives poorer results.

As a result for both flows, shear free and simple shear flows, the results of the modified model are in better agreement with the experimental results. It has been concluded that the models with retardation time and those of which material parameters are dependent on invariant of rate of strain tensor are more successful.

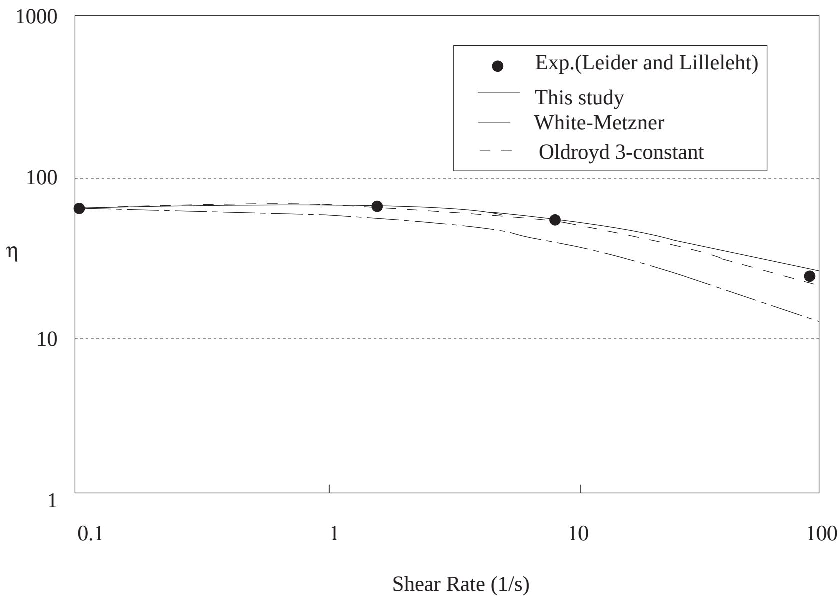

Figure 2. Comparison of the values of viscosity function of considered models with experimental data of Leider and Lilleleht(1973).

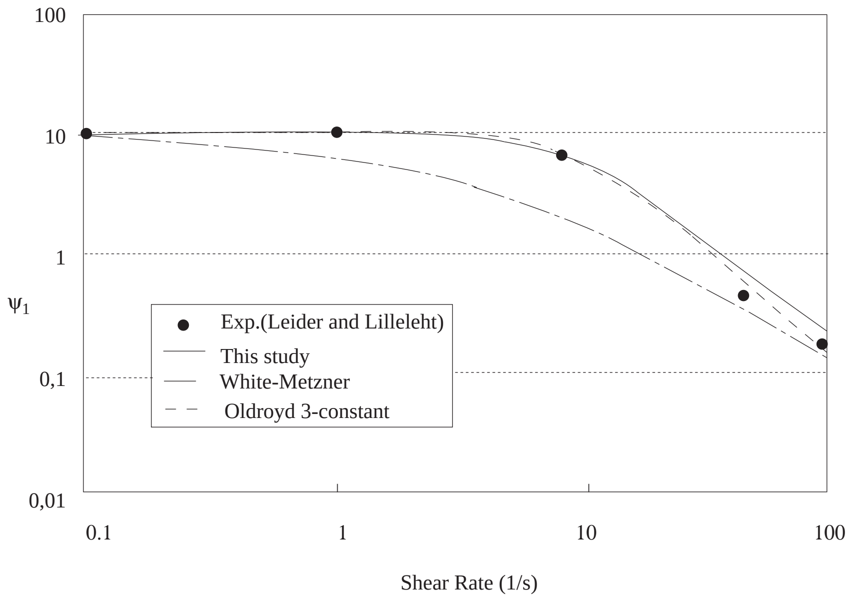

Figure 3. Comparison of the values of first normal stress coefficient of considered models with experimental data of Leider and Lilleleht(1973).

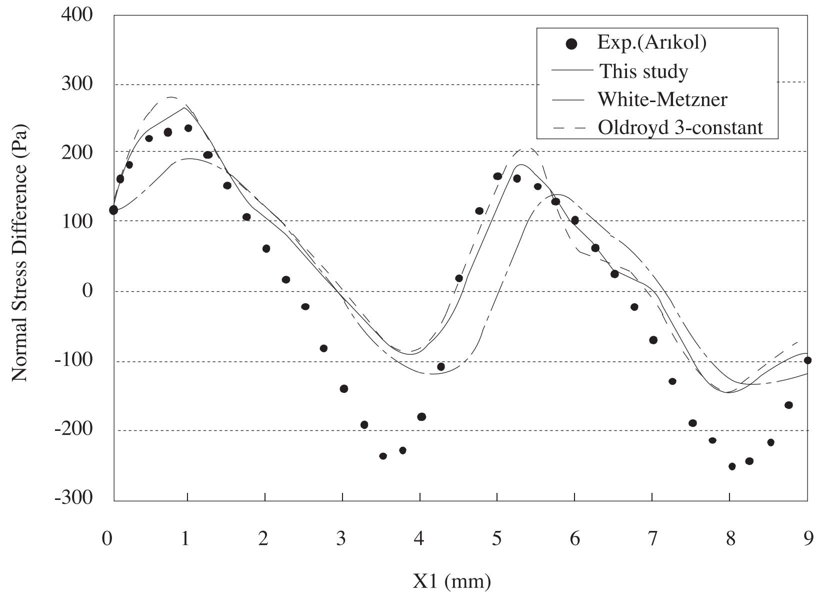

Figure 4. Comparison of the values of first normal stress difference of constitutive equations with experimental data of Arıkol(1985) for shear free flow.

Nomenclature

d_1 parameter for viscosity for White-Metzner and Modified Models

II_Δ second invariant of rate of strain tensor

r parameter for viscosity and relaxation time for White-Metzner and Modified Models

V_1 velocity in the 1 direction

V_2 velocity in the 2 direction

x_1 distance in the 1 direction
x_2 distance in the 2 direction

Greek letters

Δ_{ij} rate of strain tensor
$\bar{\Delta}_{ij}$ components of rate of strain tensor
$\dot{\gamma}$ shear rate
η viscosity function (in the simple shear flow)
η_0 zero viscosity
θ relaxation time for White-Metzner and Modified models
θ_0 parameter of relaxation time for White-Metzner and Modified Models
θ_1 parameter of relaxation time for White-Metzner and Modified Models
λ retardation time for Modified model
λ_1 relaxation time for Oldroyd 3-constant model
λ_2 retardation time for Oldroyd 3-constant model
μ viscosity for White-Metzner and Modified Models
τ_{ij} the stress tensor
Ψ_1 first normal stress coefficient(in the simple shear flow)
Ψ_2 second normal stress coefficient (in the simple shear flow)
Ω_{ij} the vorticity tensor
$\bar{\Omega}_{ij}$ compenents of the vortisity tensor

Other symbols and operators

D/Dt material derivative
$\mathcal{D}/\mathcal{D}$t Jaumann derivative
J() Oldroyd nonlinear time derivative
$()_{,j}$ derivative of quantity () with respect to the j coordinate direction

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