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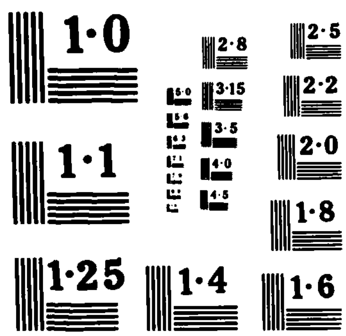
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A PERTURBATION SOLUTION FOR RIGID DUMBBELL SUSPENSIONS IN STEADY SHEAR FLOW

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ABSTRACT

The orientation distribution function of a dumbbell undergoing rotary Brownian motion (with time constant λ) in steady shear flow, and the viscosity and normal stress coefficients are computed by a perturbation expansion in small, dimensionless shear rates $\lambda\dot{\gamma}$. It is found that the series expansions for both the viscosity and the first normal stress coefficient have identical radii of convergence at $\lambda\dot{\gamma} \doteq 0.81$. By using analytical continuation, the solution was extended to $\lambda\dot{\gamma} = 1.5$, and checked with established results. Our results agree with earlier perturbation calculations of Kirkwood and Plock (1956), Bird and Warner (1971) and numerical calculations of Stewart and Sorenson (1972).

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SIGNIFICANCE AND EXPLANATION

Polymeric solutions play a central role in the manufacture of many plastics and especially, artificial fibres. A large research effort over decades has therefore been directed towards the prediction of the mechanical properties of such solutions which are important in manufacture, in particular, their viscosity and their normal stress.

It has turned out that many features found in a plot of the viscosity and normal stress coefficients vs. shear rate for polymeric solutions can be modeled qualitatively by a suspension of rigid dumbbells. Thus this model has been quite popular. Despite many attempts, exact analytical solutions have never been found for this problem although numerical and asymptotic results are available.

The following investigation establishes that the asymptotic solution for weak flows (or strong Brownian diffusion) is accurate only for dimensionless shear rates $\lambda\dot{\gamma}$ less than 0.81 where $\dot{\gamma}$ is the shear rate and λ is a material time constant for the rigid dumbbell model.

The responsibility for the wording and views expressed in this descriptive summary lies with MRC, and not with the authors of this report.

A PERTURBATION SOLUTION FOR RIGID DUMBBELL SUSPENSIONS IN STEADY SHEAR FLOW

Sangtae Kim[*,1] and Xijun Fan[**,2]

INTRODUCTION

The rigid dumbbell in a Newtonian solvent under hydrodynamic and Brownian forces is a simple model of solutions of rigid macromolecules with both theoretical and pedagogical applications.[1,2] In this note, we show that expansion solutions in small, dimensionless shear rates, $\lambda\dot{\gamma}$, have a finite radius of convergence. We also show that these solutions can be analytically continued to a much larger domain by standard techniques for accelerating the convergence of series.

STATEMENT OF THE PROBLEM

Consider a dilute suspension (number of particles per unit volume, $n \ll 1$) of rigid axisymmetric particles, where hydrodynamic interaction is negligible between particles. The material functions can be determined from the orientation distribution function, $\psi(\theta,\phi)$, where $\psi(\theta,\phi)\, d\theta d\phi$ gives the fraction of particles with the axis oriented between $(\theta, \theta + d\theta)$ and $(\phi, \phi + d\phi)$. θ and ϕ are the usual spherical azimuthal and longitudinal angles. The equation of continuity and the equations of motion combine to give the "diffusion equation" for ψ, which for steady shear flow becomes[2]

$$\hat{\Lambda}\left(\frac{\psi}{\sin\theta}\right) - 6\lambda\dot{\gamma}\hat{\Omega}\left(\frac{\psi}{\sin\theta}\right) = 0 \quad (1)$$

with the operators $\hat{\Lambda}$, and $\hat{\Omega}$ defined as

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$$\hat{\Lambda}\psi = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

$$\hat{\Omega}\psi = \frac{\sin\phi\cos\phi}{\sin\theta}\frac{\partial}{\partial\theta}(\sin^2\theta\cos\theta\ \psi) - \frac{\partial}{\partial\phi}(\sin^2\phi\ \psi) \quad .$$

We have defined our coordinate system such that $\frac{\partial v_x}{\partial y} = \dot{\gamma}$ is the only non-vanishing element of the velocity gradient tensor $\nabla \underline{v}$. For rigid dumbbells of length L, and bead friction coefficient ζ, the rotational time constant is given by $\lambda = \zeta L^2/(12kT)$. The expression for λ for other axisymmetric shapes is given by Brenner.[3]

A general analytic solution of (1) has never been found although exact solutions of related equations such as Boeder's equation are known.[4] Our objective is to solve equation (1) for ψ using a perturbation series in $\lambda\dot{\gamma}$ and to use the results to calculate the viscosity η and the first normal-stress coefficient Ψ_1 (Ψ_2 vanishes for this rigid dumbbell model):

$$\eta - \eta_s = \frac{1}{2} nkT\lambda \langle 2(P_0^0 - P_2^0) - P_2^2 \cos 2\phi \rangle_\psi \qquad (2)$$

$$\Psi_1 = \frac{nkT\lambda}{\dot{\gamma}} \langle P_2^2 \sin 2\phi \rangle_\psi \qquad (3)$$

THE PERTURBATION SOLUTION

We expand ψ in powers of $\lambda\dot{\gamma}$

$$\psi(\theta,\phi) = \frac{1}{4\pi}\sum_{k=0}^{\infty} (6\lambda\dot{\gamma})^k\ \phi_k(\theta,\phi) \qquad (4)$$

and substitute into the diffusion equation (1) to get the following hierarchy of equations for the ϕ_k:

$$\frac{\eta-\eta_s}{nkT\lambda} = \sum_{k=0}^{\infty} \left[A(1,1,2k) - \frac{1}{5}A(1,2,2k) - \frac{6}{5}A(2,2,2k)\right](6\lambda\dot{\gamma})^{2k}$$

$$\equiv \sum_{k=0}^{\infty} (-1)^k \, a_k (\lambda\dot{\gamma})^{2k} \tag{8}$$

$$\frac{5\Psi_1}{6nkT\lambda^2} = \sum_{k=0}^{\infty} 12A(2,2,2k+1)(6\lambda\dot{\gamma})^{2k}$$

$$\equiv \sum_{k=0}^{\infty} (-1)^k \, b_k (\lambda\dot{\gamma})^{2k} \tag{9}$$

The first twenty coefficients, a_k and b_k, are given in Table 1. The values for a_0, a_1 and a_2 agree with Kirkwood and Plock[5] and Bird and Warner.[6]

DISCUSSION

We note that the ratios a_{k+1}/a_k and b_{k+1}/b_k approach an asymptotic value with large k, i.e. approximately 1.521006. This result was tested by generating a_k and b_k up to k = 85, and it was found to hold for these higher coefficients as well. Therefore, the coefficients approach asymptotically to the coefficients of a geometric series in $(\lambda\dot{\gamma})^2$ with a radius of convergence of $(1.521006)^{-1/2} \doteq 0.81$. Therefore, our series solution converges only for $\lambda\dot{\gamma} < 0.81$. However, since the coefficients approach those of a geometric series, we tried analytical continuation.

First, we replace the higher coefficients a_k and b_k for $k > N+1$ with their asymptotic counterparts $\bar{a}_k$ and $\bar{b}_k$:

Table 1

Coefficients for the Series Solutions

k	a_k	b_k
0	1	1
1	0.5142 8571	1.0857 143
2	0.6888 3117	1.5475 724
3	1.0173 986	2.3156 606
4	1.5354 447	3.5063 866
5	2.3303 602	5.3265 547
6	$0.3542\ 3678 \times 10^1$	$0.8098\ 9823 \times 10^1$
7	$0.5387\ 1583 \times 10^1$	$0.1231\ 7694 \times 10^2$
8	$0.8193\ 7480 \times 10^1$	$0.1873\ 5352 \times 10^2$
9	$0.1246\ 2985 \times 10^2$	$0.2849\ 7327 \times 10^2$
10	$0.1895\ 6859 \times 10^2$	$0.4334\ 6025 \times 10^2$
11	$0.2883\ 4481 \times 10^2$	$0.6593\ 1852 \times 10^2$
12	$0.4385\ 8958 \times 10^2$	$0.1002\ 8628 \times 10^3$
13	$0.6671\ 2099 \times 10^2$	$0.1525\ 4144 \times 10^3$
14	$0.1014\ 7310 \times 10^3$	$0.2320\ 2467 \times 10^3$
15	$0.1543\ 4667 \times 10^3$	$0.3529\ 2344 \times 10^3$
16	$0.2347\ 7055 \times 10^3$	$0.5368\ 1773 \times 10^3$
17	$0.3571\ 0009 \times 10^3$	$0.8165\ 3198 \times 10^3$
18	$0.5431\ 7067 \times 10^3$	$0.1241\ 9941 \times 10^4$
19	$0.8261\ 9517 \times 10^3$	$0.1889\ 1476 \times 10^4$
20	$0.1256\ 6924 \times 10^4$	$0.2873\ 5068 \times 10^4$

$$\phi_1 = \frac{1}{12} P_2^2 \sin 2\phi$$

$$\hat{\Lambda}\phi_k = \hat{\Omega}\phi_{k-1} \qquad k = 2, 3, 4 \ldots \tag{5}$$

As pointed out by Kirkwood and Plock[5] and by Bird and Warner[6] the ϕ_k may be expressed as a linear combination of the spherical harmonics, due to the fact that

$$\hat{\Lambda}\left(P_n^m \begin{Bmatrix} \sin m\phi \\ \cos m\phi \end{Bmatrix}\right) = -n(n+1)\, P_n^m \begin{Bmatrix} \sin m\phi \\ \cos m\phi \end{Bmatrix} \tag{6}$$

$$\hat{\Omega}\left(P_n^m \begin{Bmatrix} \sin m\phi \\ \cos m\phi \end{Bmatrix}\right) = \sum_{j=m-2}^{m+2} \sum_{k=n-2}^{n+2} a_{nk}^{mj} P_k^j \begin{Bmatrix} \cos m\phi \\ -\sin m\phi \end{Bmatrix} \tag{7}$$

The a_{nk}^{mj} are tabulated in Table 1 of reference (6) and Table 11.4-1 of reference (2). Furthermore, from (7) it follows that cos $m\phi$ terms appear only in the ϕ_k with k even, while sin $m\phi$ terms appear only with k odd. Therefore, the material functions given by equations (2) and (3) reduce to a power series in $(\lambda\dot{\gamma})^2$ because of the orthogonality with respect to the ϕ integration. The perturbation results up to ϕ_4 are given in reference (2).

We have programmed this procedure (i.e. equations 4, 6 and 7), by generating a recursion formula for A(m,n,k), where the m,n,k element is the coefficient of $P_{2(n-1)}^{2(m-1)}$ for ϕ_k. The coefficients generated by the program for ϕ_1, ϕ_2 and ϕ_3 matched those given in reference (2). Because of orthogonality, only a few terms make a contribution to the material functions, i.e.:

$$\frac{\eta-\eta_s}{nkT\lambda} = \sum_{k=0}^{N} (-1)^k a_k(\lambda\dot{\gamma})^{2k} + \sum_{k=N+1}^{\infty} (-1)^k \bar{a}_k(\lambda\dot{\gamma})^{2k} \tag{10}$$

$$\frac{5\Psi_1}{6nkT\lambda^2} = \sum_{k=0}^{\infty} (-1)^k b_k(\lambda\dot{\gamma})^{2k} + \sum_{k=N+1}^{\infty} (-1)^k \bar{b}_k(\lambda\dot{\gamma})^{2k} \tag{11}$$

with $\bar{a}_k = c_1 p^{-2k-2}$, $c_1 = 0.1879...$

$p = 0.8108...$

$\bar{b}_k = c_2 p^{-2k-2}$, $c_2 = 0.3582...$

$p = 0.8108...$

In the key step, the series is replaced by the equivalent continuation functions so that

$$\frac{\eta-\eta_s}{nkT\lambda} = \sum_{k=0}^{N} (-1)^k [a_k-\bar{a}_k](\lambda\dot{\gamma})^{2k} + c_1[p^2 + (\lambda\dot{\gamma})^2]^{-1} \tag{12}$$

$$\frac{5\Psi_1}{6nkT\lambda^2} = \sum_{k=0}^{N} (-1)^k [b_k-\bar{b}_k](\lambda\dot{\gamma})^{2k} + c_2[p^2 + (\lambda\dot{\gamma})^2]^{-1} \tag{13}$$

By comparing with the exact numerical (collocation) solutions of Stewart and Sørensen[7] we found that N = 10 was the optimum value. However, N = 8, 9, 11, and 12 also gave results which were accurate to four significant figures for $\lambda\dot{\gamma} < 1$. Table 2 shows the comparison between their collocation solution and

Table 2

Comparison of Stress Functions

$\lambda\dot{\gamma}$	$(\eta-\eta_s)/nkT\lambda$ equation (12) N = 10	$(\eta-\eta_s)/nkT\lambda$ exact solution[a]	$\Psi_1/nkT\lambda^2$ equation (13) N = 10	$\Psi_1/nkT\lambda^2$ exact solution[a]
0	1	1	6/5	6/5
0.1	0.9949	0.9949	1.1872	1.1872
0.125	0.9921	0.9921	1.1801	1.1801
0.25	0.9703	0.9703	1.1252	1.1252
0.3333	0.9502	0.9502	1.0749	1.0749
0.5	0.9029	0.9029	0.9588	0.9588
0.75	0.8306	0.8306	0.7874	0.7874
1.0	0.7676	0.7676	0.6467	0.6467
1.5	0.6604	0.6735	0.4596	0.4565
2.0833	-9.2	0.5998	-5.5	0.3289

[a]Collocation calculations of Stewart and Sørensen.[7]

our extended solution (with $N = 10$, $c_1 = 0.18799972$, $c_2 = 0.35822745$, and $p = 0.81082443$).

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