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Stress singularities of some common kernel transformed viscoelastic models

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The kernel conformation tensor is a powerful generic transformation for a large class of differential constitutive models. We derive its stress singularity associated with the stretching solution of the viscoelastic extra-stress tensor. This is relevant to re-entrant corner flows in contraction/expansion flows and the separation of a free-surface from a solid surface at the die lip in extrudate swell. The theoretical asymptotic results are compared to numerical scheme results for the two common kernel conformation cases of natural logarithm and square-root. These results are presented for the viscoelastic models in which the asymptotic stress-tensor singularity is currently known.

Key words:

MSC Codes 76A10, 76M45

1. Introduction

We will be concerned here with deriving the stress singularities of the kernel-conformation tensor for the common viscoelastic models of UCM, Oldroyd-B Bird *et al.* (1987); Larson (1988), simplified PTT Davoodi *et al.* (2022); Alves *et al.* (2003*a*); Phan-Thien & Tanner (1977) and Giesekus Giesekus (1982) relevant to steady planar contraction/expansion and extrudate swell flows. In these situations, the local asymptotic behaviour of the viscoelastic extra-stress has been determined to take the generic form

$$\mathbf{T} \sim \lambda(\psi)\mathbf{u}\mathbf{u}^T \qquad \text{as } r \to 0, \tag{1.1}$$

where r denotes the radial distance to the singularity, ψ is the planar streamfunction, $\mathbf{u}$ the velocity field and the scalar function λ is constant along streamlines. Near to the above

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mentioned singularities, the velocity and stress is self-similar, taking separable forms

$$\psi = C_0 r^m f(\theta), \qquad \lambda(\psi) = C_1 \left(\frac{\psi}{C_0}\right)^n, \tag{1.2}$$

where the amplitudes C_0, C_1 and exponents m, n are all constant. These give the estimates

$$\mathbf{T} = O(\lambda|\mathbf{u}|^2) = O(r^{m(n+2)-2}), \qquad \nabla\mathbf{v} = O(r^{m-2}) \qquad \text{as } r \to 0. \tag{1.3}$$

Results are flow problem and model dependent. They are summarised for both the re-entrant corner and extrudate-swell in Table 1. The angle of flow is π/α in both cases, where $\alpha \in (1/2, 1)$ for re-entrant corners and $\alpha \in (2/3, 1)$ for extrudate-swell. These implicitly assume an absence of vortices at the boundaries, such as lip vortices. In both geometries $\theta = 0$ represents the upstream wall and $\theta = \pi/\alpha$ is either the re-entrant corner downstream wall or extrudate-swell free-surface. The transcendental equations to determine the λ_0 eigenvalue are

$$\sin\left(\frac{\lambda_0\pi}{\alpha}\right) = -\lambda_0 \sin\left(\frac{\pi}{\alpha}\right) \tag{1.4}$$

for the re-entrant corner and

$$\sin\left(\frac{2\lambda_0\pi}{\alpha}\right) = \lambda_0 \sin\left(\frac{2\pi}{\alpha}\right) \tag{1.5}$$

for extrudate-swell.

The results in Table 1 have been built up in a serious of works. The re-entrant corner behaviour was deteremined for UCM/Oldroyd-B in Hinch (1993); Renardy (1995); Rallison & Hinch (2004); Evans (2005, 2008*a*,*b*), sPTT in Renardy (1997); Evans (2010*b*) and Giesekus in Evans (2010*a*). Extrudate-swell behaviour for sPTT and Giesekus has been studied in Evans & Evans (2019, 2024*b*,*a*). In the re-entrant corner case, UCM and Oldroyd-B take the same potential flow solutions. The elastic stress dominates the solvent stress for all corner angles greater than 180^o. Thus the effect of adding a solvent viscosity to UCM does not change the nature of the singularity. However, this is not the same for sPTT and Giesekus, where currently results are known only when a solvent viscosity is present, the solvent stress then dominating the elastic stress. In the absence of a solvent, results are incomplete Evans & Sibley (2008, 2009). As regards extrudate-swell, the singularity is currently only known for sPTT and Giesekus models in the presence of a solvent, and again the solvent stress dominates the elastic stress.

The dimensionless model equations we are considering are

$$\begin{aligned} &\nabla \cdot \mathbf{u} = 0, \qquad \mathrm{Re}\frac{D\mathbf{u}}{Dt} = -\nabla p + \beta\nabla^2\mathbf{u} + (1-\beta)\nabla\cdot\mathbf{T}, \\ &\mathbf{T} + \mathrm{Wi}\left(\overset{\triangledown}{\mathbf{T}} + \mathbf{g}(\mathbf{T})\right) = 2\mathbf{D}, \qquad \mathbf{g}(\mathbf{T}) = \begin{cases} \mathbf{0}, & \text{UCM/Oldroyd-B}, \\ \epsilon \mathrm{tr}(\mathbf{T})\mathbf{T}, & \text{PTT}, \\ \hat{\alpha}\mathbf{T}^2, & \text{Giesekus}, \end{cases} \end{aligned} \tag{1.6}$$

with pressure p, D/Dt denoting the material or substantive derivative and the upper convective stress derivative in the elastic constitutive equation. The usual dimensionless parameters are the Reynolds number $\mathrm{Re} = \rho U L/\eta_0$, Weissenberg number $\mathrm{Wi} = \lambda_p U/L$, solvent viscosity fraction $\beta = \eta_s/\eta_0$ and model parameters ϵ in PTT and $\hat{\alpha}$ in Giesekus. Here, U and L are characteristic velocity and length scales, η_s is the solvent viscosity, η_p the polymer viscosity, $\eta_0 = \eta_s + \eta_p$ the total viscosity and ρ the density. The dimensional pressure, solvent and elastic stresses have been scaled with $\eta_0 U/L$, $\eta_s U/L$ and $\eta_p U/L$ respectively.

Model	ψ m	$\lambda(\psi)$ n	**T** p=m(n+2)-2	**D** q=m-2
UCM/Oldroyd-B	$\alpha(3-\alpha)$	$-\frac{2(1-\alpha)}{(3-\alpha)}$	$-2(1-\alpha)$	$-(1-\alpha)(2-\alpha)$
sPTT (with solvent)	$1+\lambda_0$	$-\frac{2(2+\lambda_0)}{(5+\lambda_0)}$	$-\frac{4((1-\lambda_0))}{(5+\lambda_0)}$	$-(1-\lambda_0)$
Giesekus (with solvent)	$1+\lambda_0$	$-\frac{(3+\lambda_0)}{4}$	$-\frac{(1-\lambda_0)(3-\lambda_0)}{4}$	$-(1-\lambda_0)$

Table 1: Summary by model of singularity exponents for re-entrant corners of angle π/α with $1/2 < \alpha < 1$. The benchmark case of 270^o is $\alpha = 2/3$. For sPTT and Giesekus, λ_0 is the smallest positive root of the transcendental equation (1.4). The sPTT and Giesekus results also hold for extrudate-swell, where π/α now represents the angle of separation with $2/3 < \alpha < 2$ and λ_0 is the smallest positive root of (1.5).

The Weissenberg number is usually scaled from the local singularity problems and set to unity. The results in Table 1 hold not only for Weissenberg order one, but large as well. As regards the Reynolds number, the results hold generally for order one values, although the main application is the creeping flow regime with Reynolds number small.

2. Kernel-conformation singular behaviour

We begin by remarking that the dyadic product $\mathbf{u}\mathbf{u}^T$ has eigenvalues 1 and 0 with associated eigenvectors in the directions parallel and perpendicular to $\mathbf{u}$ respectively. This affords the diagonalisation

$$\mathbf{u}\mathbf{u}^T = \mathbf{O}\begin{pmatrix}|\mathbf{u}|^2 & 0\\ 0 & 0\end{pmatrix}\mathbf{O}^\mathbf{T} \tag{2.1}$$

with

$$\mathbf{O} = \frac{1}{|\mathbf{u}|}\begin{bmatrix} u & -v\\ v & u\end{bmatrix}, \tag{2.2}$$

being composed of the unitary eigenvectors, the one in the velocity direction we denote by $\hat{\mathbf{u}} = \mathbf{u}/|\mathbf{u}|$. As long as the velocity does not vanish, then $\mathbf{O}$ is proper orthogonal.

For stabilisation reasons, numerical simulations are performed with the kernel-conformation tensor Afonso *et al.* (2011), which can be any continuous, invertible and differentiable matrix transformation function $\Bbbk(\mathbf{A})$ of the conformation tensor $\mathbf{A}$. The extra-stress tensor is related by

$$\mathbf{A} = \mathrm{Wi}\mathbf{T} + \mathbf{I}, \tag{2.3}$$

and we take $\mathrm{Wi} = 1$ without loss of generality. Consequently, the form (1.1) becomes

$$\mathbf{A} = \mathbf{O}\begin{pmatrix}\lambda|\mathbf{u}|^2+1 & 0\\ 0 & 1\end{pmatrix}\mathbf{O}^\mathbf{T}, \tag{2.4}$$

and for the kernel-conformation

$$\mathbb{k}(\mathbf{A}) = \mathbf{O}\begin{pmatrix} \mathbb{k}(1+\lambda|\mathbf{u}|^2) & 0 \\ 0 & \mathbb{k}(1) \end{pmatrix}\mathbf{O}^{\mathbf{T}}. \tag{2.5}$$

Near singularities $\lambda|\mathbf{u}|^2$ grows unboundedly and hence we have the asymptotic behaviour

$$\mathbb{k}(\mathbf{A}) \sim \mathbb{k}(\lambda|\mathbf{u}|^2)\ \mathbf{O}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\mathbf{O}^{\mathbf{T}} = \mathbb{k}(\lambda|\mathbf{u}|^2)\hat{\mathbf{u}}\hat{\mathbf{u}}^T \qquad \text{as } r \to 0. \tag{2.6}$$

Consequently

$$\mathbb{k}(\mathbf{A}) = O(\mathbb{k}(r^p)) \qquad \text{as } r \to 0, \tag{2.7}$$

where $p = m(n+2) - 2$ is negative. The common transformations for $\mathbb{k}$ of natural logarithm Fattal & Kupferman (2004) and square-root Balci *et al.* (2011) have the effect of significantly reducing the singularity of $\mathbb{k}(\mathbf{A})$ compared to $\mathbf{A}$. This gives an additional computational benefit to the kernel transformed conformation formulation.

3. Numerical verification

Here we verify (2.7) with exponent p in Table 1 for the natural log and square-root transformations. The numerical methodology employed for all simulations is based on a finite-difference approach to discretize the system of equations (1.6). A projection method is applied to (1.6) to decouple the velocity and pressure fields. Explicit time discretization is utilized for solving the constitutive equations, with the convective terms approximated using an upwind scheme Alves *et al.* (2003*b*). For further details about the numerical code, refer to Evans *et al.* (2022).

3.1. *Re-entrant corner*

We take the standard benchmark case of 270^o, so that $\alpha = 2/3$ with corner angle $\pi/\alpha = 3\pi/2$. Table 2 summarises the theoretical singular radial behaviours for UCM/Oldroyd-B, sPTT and Giesekus. The sPTT and Giesekus results require the presence of a solvent viscosity and hold for $0 < \beta < 1$, with any non-zero value of the extensibility parameter ϵ for sPTT or non-zero value of the mobility parameter $\hat{\alpha}$ (and bounded by unity) for Giesekus.

Figures 1 and 2 show the results for the contraction and expansion respectively, for the three models in the parameter case Wi $= 1, \beta = 0.5$ and $\epsilon = \hat{\alpha} = 0.1$. These are plotted along the ray $\theta = \pi/2$, where $\theta = 0$ is the upstream wall and $\theta = 3\pi/2$ is the downstream wall.

3.2. *Extrudate-swell*

The separation angle has to be estimated as the tangent angle of the free-surface. This will vary with model, β, Wi and model parameter ϵ or $\hat{\alpha}$. We obtain numerically the following results

sPTT: Wi=1, $\beta = 0.5$, ϵ=0.1,: $\pi/\alpha =$, $\lambda_0 \approx 0.440$, p=-0.412 ,

Giesekus: Wi=1, $\beta = 0.5$, $\hat{\alpha} = 0.1$: $\lambda_0 \approx 0.442$, p=-0.357,

where the λ_0 values are obtained from (1.5) using the estimated value of the free-surface separation angle from a numerical scheme simulation. Table 3 summarises the singularity behaviours and these are compared in Figure 3 to the numerical scheme behaviours.

Finally, Figure 4 shows the eigenvalues of $\mathbf{A}$ for the preceeding simulations, confirming the growth of a dominant eigenvalue and hence verifying (2.6).

Model	$\mathbf{A}$	$\ln \mathbf{A}$	$\mathbf{A}^{\frac{1}{2}}$
UCM/Oldroyd-B	$r^{-\frac{2}{3}}$	$-\frac{2}{3}\ln r$	$r^{-\frac{1}{3}}$
sPTT (with solvent)	$r^{-0.3286}$	$-0.3286\ln r$	$r^{-0.1643}$
Giesekus (with solvent)	$r^{-0.2796}$	$-0.2796\ln r$	$r^{-0.1398}$

Table 2: Summary by model of singularity exponents for re-entrant corners of angle π/α with $1/2 < \alpha < 1$. For sPTT and Giesekus, λ_0 is the smallest positive root of the transcendental equation (1.4).

Model	$\frac{\pi}{\alpha}$	λ_0	$\mathbf{A}$	$\ln \mathbf{A}$	$\mathbf{A}^{\frac{1}{2}}$
sPTT (with solvent)	3.3568	0.4404	$r^{-0.4114}$	$-0.4114\ln r$	$r^{-0.2052}$
Giesekus (with solvent)	3.3521	0.4415	$r^{-0.3572}$	$-0.3572\ln r$	$r^{-0.1774}$

Table 3: Summary of the singularity behaviours for extrudate-swell in the specific parameter cases of $\mathrm{Wi} = 1, \beta = 0.5, \epsilon = \hat{\alpha} = 0.1$. The angle of separation π/α is estimated by regression and then λ_0 determined from (1.5).

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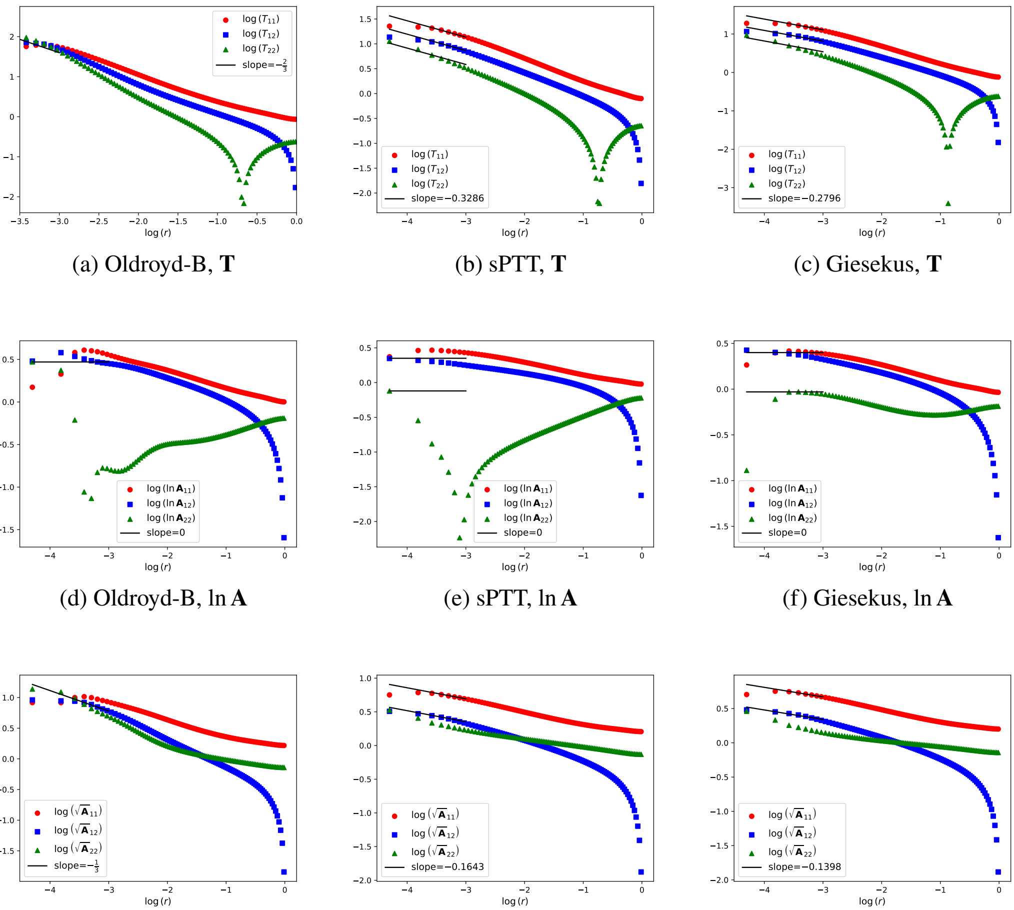

(a) Oldroyd-B, **T** (b) sPTT, **T** (c) Giesekus, **T**

(d) Oldroyd-B, $\ln \mathbf{A}$ (e) sPTT, $\ln \mathbf{A}$ (f) Giesekus, $\ln \mathbf{A}$

(g) Oldroyd-B, $\sqrt{\mathbf{A}}$ (h) sPTT, $\sqrt{\mathbf{A}}$ (i) Giesekus, $\sqrt{\mathbf{A}}$

Figure 1: Numerical verification of the asymptotic results for the 4:1 contraction flow along $\theta = \frac{\pi}{2}$.

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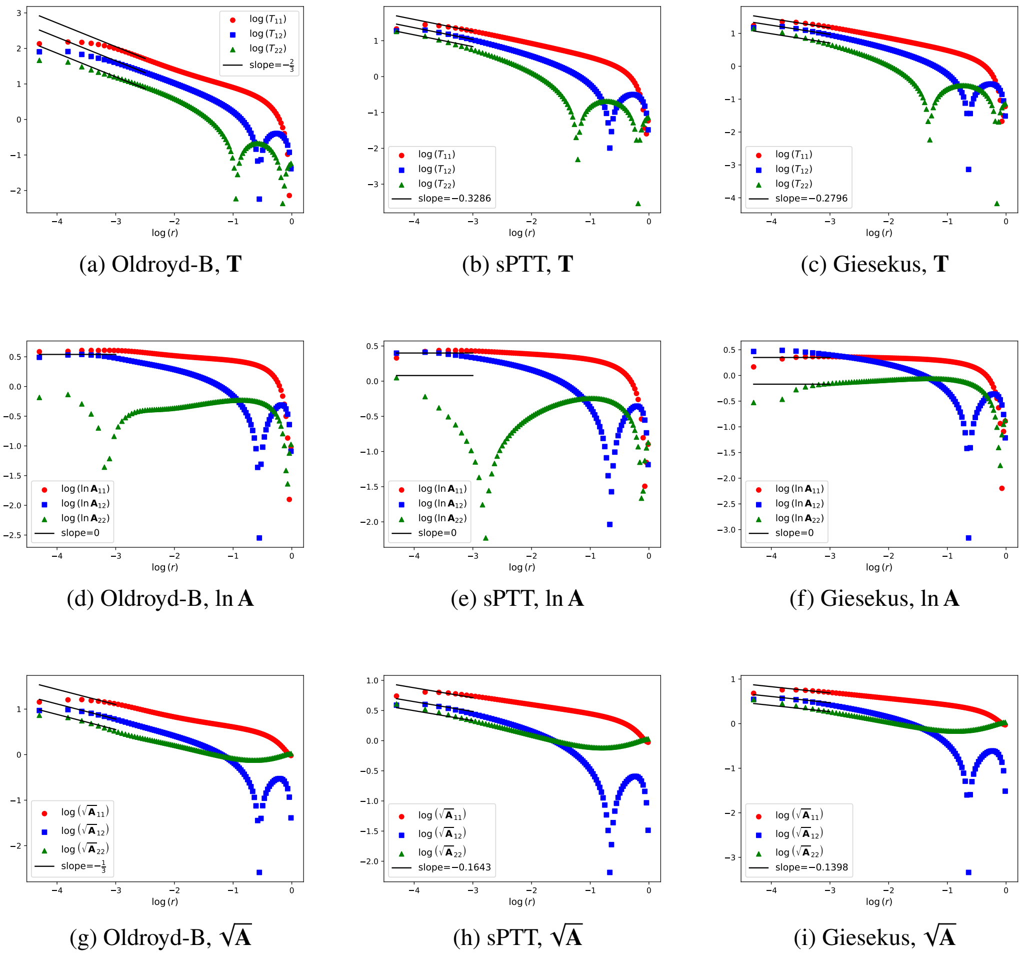

(a) Oldroyd-B, $\mathbf{T}$ (b) sPTT, $\mathbf{T}$ (c) Giesekus, $\mathbf{T}$

(d) Oldroyd-B, $\ln \mathbf{A}$ (e) sPTT, $\ln \mathbf{A}$ (f) Giesekus, $\ln \mathbf{A}$

(g) Oldroyd-B, $\sqrt{\mathbf{A}}$ (h) sPTT, $\sqrt{\mathbf{A}}$ (i) Giesekus, $\sqrt{\mathbf{A}}$

Figure 2: Numerical verification of the asymptotic results for the 1:4 expansion flow along $\theta = \frac{\pi}{2}$.

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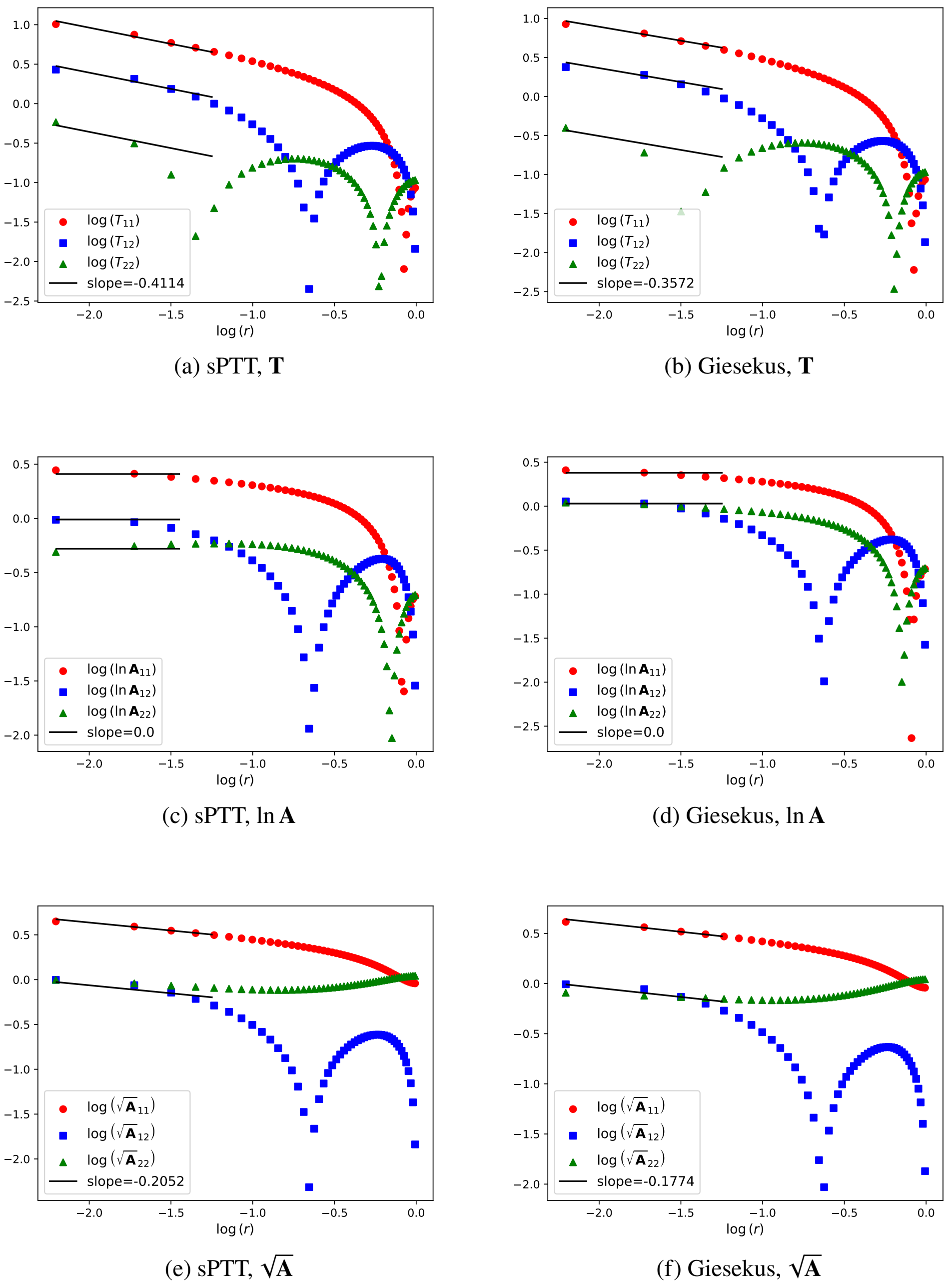

(a) sPTT, $\mathbf{T}$ (b) Giesekus, $\mathbf{T}$

(c) sPTT, $\ln \mathbf{A}$ (d) Giesekus, $\ln \mathbf{A}$

(e) sPTT, $\sqrt{\mathbf{A}}$ (f) Giesekus, $\sqrt{\mathbf{A}}$

Figure 3: Numerical verification of the asymptotic results for the extrudate flow along $\theta = \frac{\pi}{2}$.

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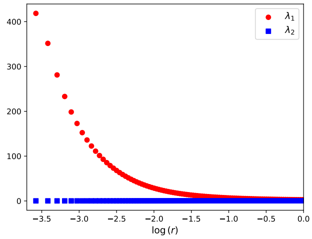
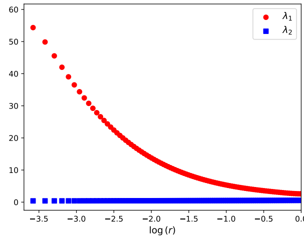
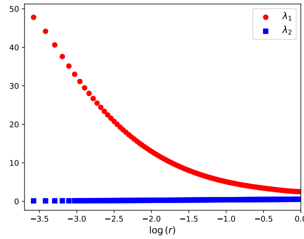


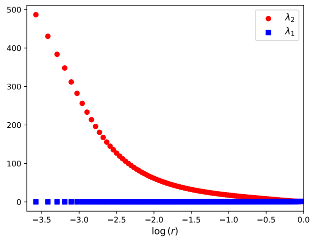
(a) Oldroyd-B, 4:1 Contraction



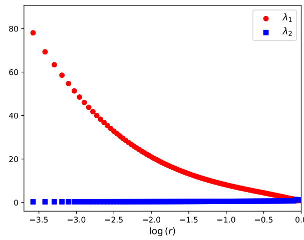
(b) sPTT, 4:1 Contraction



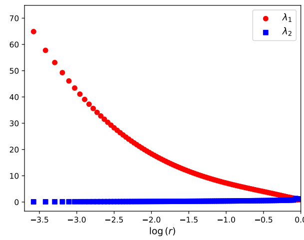
(c) Giesekus, 4:1 Contraction



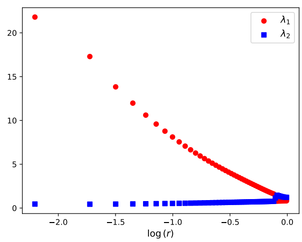
(d) Oldroyd-B, 1:4 Expansion



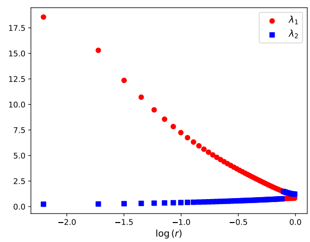
(e) sPTT, 1:4 Expansion



(f) Giesekus, 1:4 Expansion



(g) sPTT, Die-swell



(h) Giesekus, Die-swell

Figure 4: Numerical verification of the asymptotic results for the eigenvalues along $\theta = \frac{\pi}{2}$.

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