Stress singularities of some common kernel transformed viscoelastic models

JD Evans^{a,*}, IL Palhares Junior^b, AM Afonso^{c,d}

^aDepartment of Mathematical Sciences, University of Bath, Bath, BA2 7AY, United Kingdom

^bDepartamento de Matemática e Computa cão, Faculdade de Ciências e Tecnologia, Universidade Estadual

Paulista 'Júlio de Mesquita Filho' 19060-900 Presidente Prudente, Sao Paulo, Brazil

^cDepartamento de Engenharia Mecânica, Centro de Estudos de Fenómenos de Transporte, CEFT,

Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465, Porto,

Portugal.

^dALiCE, Associate Laboratory in Chemical Engineering, Faculdade de Engenharia, Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal

Abstract

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 the numerical scheme results for the two common particular 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.

Keywords:

sec:1 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 [4, 11], simplified PTT [5, 2, 12] and Giesekus [9] 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

$$\mathbf{T} \sim \lambda(\psi) \mathbf{u} \mathbf{u}^T$$
 as $r \to 0$, (1) eq:T

*Corresponding author

Email addresses: masjde@bath.ac.uk (JD Evans), irineu.palhares@unesp.br (IL Palhares Junior), aafonso@fe.up.pt (AM Afonso)

Preprint submitted to Elsevier

November 20, 2024

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

$$\psi = C_0 r^m f(\theta), \qquad \lambda(\psi) = C_1 \left(\frac{\psi}{C_0}\right)^n,$$
(2)

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

$$\mathbf{T} = O(\lambda |\mathbf{u}|^2) = O(r^{m(n+2)-2}), \qquad \nabla \mathbf{v} = O(r^{m-2}) \qquad \text{as } r \to 0.$$
 (3)

Results for the re-entrant corner [10, 13, 6, 7] and extrudate-swell [<empty citation>] are summarised 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 no of vortices at the boundaries, such as lip vortices.

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°. 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 transcendental equations to the determine the λ_0 eigenvalue are

$$\sin\left(\frac{\lambda_0 \pi}{\alpha}\right) = -\lambda_0 \sin\left(\frac{\pi}{\alpha}\right) \tag{4} \quad \text{eq:terc}$$

for the re-entrant corner and

$$\sin\left(\frac{2\lambda_0\pi}{\alpha}\right) = \lambda_0 \sin\left(\frac{2\pi}{\alpha}\right) \tag{5}$$

for extrudate-swell.

The dimensionless model equations we are considering are

$$\nabla \cdot \mathbf{u} = 0, \qquad \operatorname{Re} \frac{D\mathbf{u}}{Dt} = -\nabla p + \beta \nabla^{2}\mathbf{u} + (1 - \beta)\nabla \cdot \mathbf{T},$$

$$\mathbf{T} + \operatorname{Wi} \left(\overset{\triangledown}{\mathbf{T}} + \mathbf{g} \left(\mathbf{T} \right) \right) = 2\mathbf{D}, \qquad \mathbf{g} \left(\mathbf{T} \right) = \begin{cases} \mathbf{0}, & \operatorname{UCM/Oldroyd-B}, \\ \epsilon \operatorname{tr}(\mathbf{T})\mathbf{T}, & \operatorname{PTT}, \\ \hat{\alpha}\mathbf{T}^{2}, & \operatorname{Giesekus}, \end{cases}$$
(6) GovEq

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 $\text{Re} = \rho U L/\eta_0$, Weissenberg number $\text{Wi} = \lambda_p U/L$, 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,

Model	$\psi \ \mathrm{m}$	$\lambda(\psi)$ n	T = m(n+2)-2	D q=m-2	p
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° is $\alpha = 2/3$. For sPTT and Giesekus, λ_0 is the smallest positive root of the transcendental equation (4). The sPTT and Giesekus results also hold for extrudate-swell, where π/α now represents the angle of separation with $1/3 < \alpha <$ and λ_0 is the smallest positive root of (5).

Table1

 $\eta_0 = \eta_s + \eta_p$ 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.

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.

sec:2

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

$$\mathbf{u}\mathbf{u}^T = \mathbf{O} \begin{pmatrix} |\mathbf{u}|^2 & 0\\ 0 & 0 \end{pmatrix} \mathbf{O}^{\mathbf{T}} \tag{7}$$

with

$$\mathbf{O} = \frac{1}{|\mathbf{u}|} \begin{bmatrix} u & -v \\ v & u \end{bmatrix},\tag{8}$$

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 **O** is proper orthogonal.

For stabilisation reasons, numerical simulations are performed with the kernel-conformation tensor [1], which can be any continuous, invertible and differentiable matrix transformation function $k(\mathbf{A})$ of the conformation tensor \mathbf{A} . The extra-stress tensor is related by

$$\mathbf{A} = \text{Wi}\mathbf{T} + \mathbf{I},\tag{9}$$

and we take Wi = 1 without loss of generality. Consequently, the form (1) becomes

$$\mathbf{A} = \mathbf{O} \begin{pmatrix} \lambda |\mathbf{u}|^2 + 1 & 0 \\ 0 & 1 \end{pmatrix} \mathbf{O}^{\mathbf{T}},\tag{10}$$

and for the kernel-conformation

$$\mathbb{k}(\mathbf{A}) = \mathbf{O} \begin{pmatrix} \mathbb{k}(1+\lambda|\mathbf{u}|^2) & 0\\ 0 & \mathbb{k}(1) \end{pmatrix} \mathbf{O}^{\mathbf{T}}.$$
 (11)

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

$$\mathbb{k}(\mathbf{A}) \sim \mathbb{k}(\lambda |\mathbf{u}|^2) \mathbf{O} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \mathbf{O}^{\mathbf{T}} = \mathbb{k}(\lambda |\mathbf{u}|^2) \hat{\mathbf{u}} \hat{\mathbf{u}}^T \quad \text{as } r \to 0.$$
 (12)

Consequently

$$\mathbb{k}(\mathbf{A}) = O(\mathbb{k}(r^p))$$
 as $r \to 0$, (13) $\boxed{\text{eq:kA}}$

where p = m(n+2) - 2 is negative. The common transformations for k of natural logarithm [8] and square-root [3] have the effect of significantly reducing the singularity of $k(\mathbf{A})$ compared to \mathbf{A} . This gives an additional computational benefit to the kernel transformed conformation formulation.

sec:3 3. Numerical verification

Here we verify (13) with exponent p in Table 1 for the natural log and square-root transformations.

3.1. Re-entrant corner

We take the standard benchmark case of 270° , 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.

Figure 1 shows the results for the three models in the parameter case $\beta = 0.5$ 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 $\hat{\alpha}$.

sPTT: Wi=1, ϵ =0.1, β = 0.5: $\lambda_0 \approx 0.440$ (from estimated separation angle), p=-0.412 Giesekus: Wi=1, $\hat{\alpha}$ = 0.1, β = 0.5: $\lambda_0 \approx 0.442$ (from estimated separation angle), p=-0.357

Model	A	$\ln \mathbf{A}$	$\mathbf{A}^{rac{1}{2}}$
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 (4).

Model	A	$\ln {f A}$	$\mathbf{A}^{rac{1}{2}}$	
sPTT (with solvent) Giesekus (with solvent)	$\begin{vmatrix} r^{-0.3286} \\ r^{-0.2796} \end{vmatrix}$		$r^{-0.1643}$ $r^{-0.1398}$	

Table3

Table2

Table 3

4. Discussion

Acknowledgments

- J.D. Evans acknowledges financial support from FAPESP-SPRINT grants 2018/22242-0 and 2024/01651-0, and would like to thank the University of Bath for subbatical leave during 2023-2024.
- A. M. Afonso acknowledges FCT Fundação para a Ciência e a Tecnologia for financial support through LA/P/0045/2020 (ALiCE), UIDB/00532/2020 and UIDP/00532/2020 (CEFT), funded by national funds through FCT/MCTES (PIDDAC).
- I.L. Palhares Junior would like to acknowledge support from CEPID-CeMEAI (FAPESP grant no. 2013/07375-0) and FAPESP-SPRINT grant no. 2024/01651-0 and FAPESP-ANR grant no. 2024/04769-1.

References

fonso2011

[1] A.M. Afonso, F.T. Pinho, and M.A. Alves. "The kernel-conformation constitutive laws". In: Journal of Non-Newtonian Fluid Mechanics Not available (Oct. 2011), Not available. ISSN: 0377-0257. DOI: 10.1016/j.jnnfm.2011.09.008. URL: https://dx.doi.org/10.1016/j.jnnfm.2011.09.008.

Alves2003

[2] Manuel A. Alves, Paulo J. Oliveira, and Fernando T. Pinho. "Benchmark solutions for the flow of Oldroyd-B and PTT fluids in planar contractions". In: Journal of Non-Newtonian Fluid Mechanics 110 (Feb. 2003), pp. 45–75. ISSN: 0377-0257. DOI: 10.1016/s0377-0257(02)00191-x. URL: https://dx.doi.org/10.1016/s0377-0257(02)00191-x.

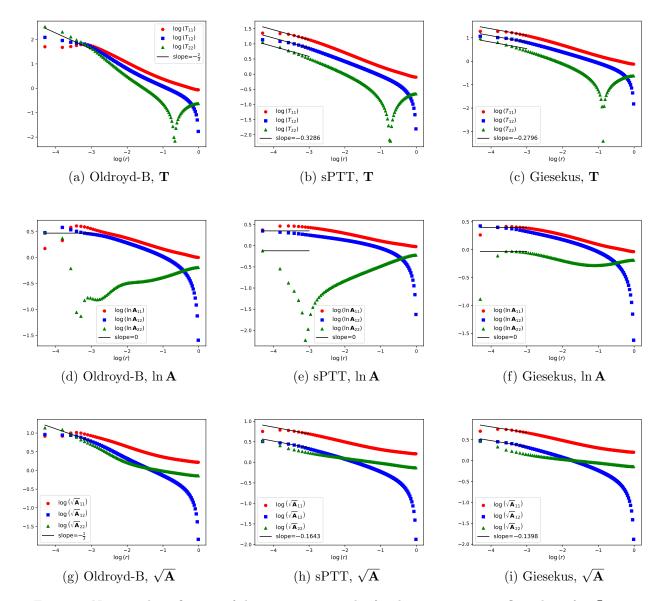


Figure 1: Numerical verification of the asymptotic results for the 4:1 contraction flow along $\theta = \frac{\pi}{2}$.

Balci2011

ntraction

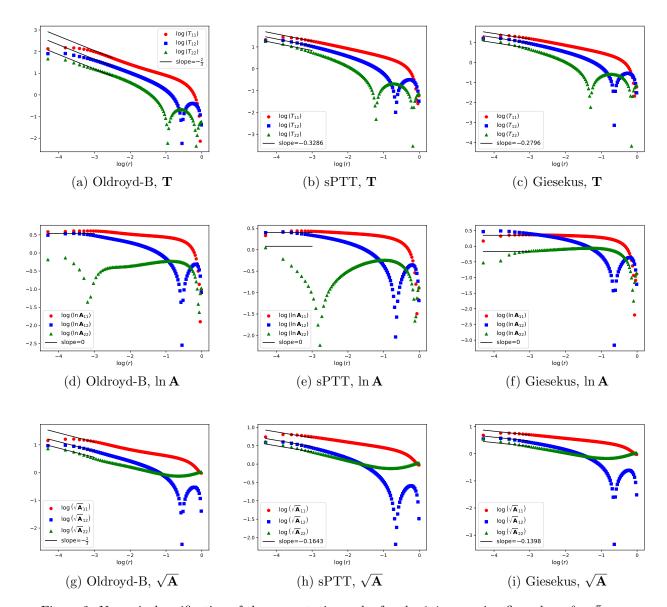
[3] Nusret Balci et al. "Symmetric factorization of the conformation tensor in viscoelastic fluid models". In: Journal of Non-Newtonian Fluid Mechanics 166 (June 2011), pp. 546-553. ISSN: 0377-0257. DOI: 10.1016/j.jnnfm.2011.02.008. URL: https://dx.doi.org/10.1016/j.jnnfm.2011.02.008.

Bird1987

[4] R. B. Bird, R. C. Armstrong, and O. Hassager. *Dynamics of polymeric liquids. Vol.1, Fluid mechanics*. 2nd ed. New York, 1987.

voodi2022

[5] Mahdi Davoodi, Konstantinos Zografos, and Robert J. Poole. "On the similarities of the sPTT and FENE-P models for polymeric fluids". In: Science Talks 2 (June 2022), p. 100015. ISSN: 2772-5693. DOI: 10.1016/j.sctalk.2022.100015. URL: https://dx.doi.org/10.1016/j.sctalk.2022.100015.



Expansion

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

Evans2005

[6] J. D. Evans. "Reâentrant corner flows of the upper convected Maxwell fluid". In: Proc. R. Soc. A. 461 (2053 Jan. 2005), pp. 117–142. DOI: 10.1098/rspa.2004.1335.

vans2005b

[7] J.D Evans. "Re-entrant corner flows of Oldroyd-B fluids". In: Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 461 (June 2005), pp. 2573-2603. ISSN: 1364-5021, 1471-2946. DOI: 10.1098/rspa.2004.1410. URL: https://dx.doi.org/10.1098/rspa.2004.1410.

attal2004

[8] Raanan Fattal and Raz Kupferman. "Constitutive laws for the matrix-logarithm of the conformation tensor". In: *Journal of Non-Newtonian Fluid Mechanics* 123 (Nov. 2004), pp. 281–285. ISSN: 0377-0257. DOI: 10.1016/j.jnnfm.2004.08.008. URL: https://dx.doi.org/10.1016/j.jnnfm.2004.08.008.

sekus1982

[9] H. Giesekus. "A simple constitutive equation for polymer fluids based on the concept of deformation-dependent tensorial mobility". In: Journal of Non-Newtonian Fluid Mechanics 11 (Jan. 1982), pp. 69–109. ISSN: 0377-0257. DOI: 10.1016/0377-0257(82)85016-7. URL: https://dx.doi.org/10.1016/0377-0257(82)85016-7.

Hinch1993

[10] E.J. Hinch. "The flow of an Oldroyd fluid around a sharp corner". In: Journal of Non-Newtonian Fluid Mechanics 50 (2 Dec. 1993), pp. 161–171. ISSN: 0377-0257. DOI: 10.1016/0377-0257(93)80029-b. URL: https://dx.doi.org/10.1016/0377-0257(93)80029-b.

arson1988

[11] R. G. Larson. Constitutive Equations for Polymer Melts and Solutions. Oct. 1988. ISBN: 9780409901191.

Thien1977

[12] N. Phan-Thien and R. I. Tanner. "A new constitutive equation derived from network theory". In: Journal of Non-Newtonian Fluid Mechanics 2.4 (1977), pp. 353-365. ISSN: 0377-0257. DOI: https://doi.org/10.1016/0377-0257(77)80021-9. URL: https://www.sciencedirect.com/science/article/pii/0377025777800219.

nardy1995

[13] Michael Renardy. "A matched solution for corner flow of the upper convected Maxwell fluid". In: *J. Non-Newton. Fluid Mech.* 58 (1 1995), pp. 83–89. ISSN: 0377-0257. DOI: https://doi.org/10.1016/0377-0257(94)01339-J.

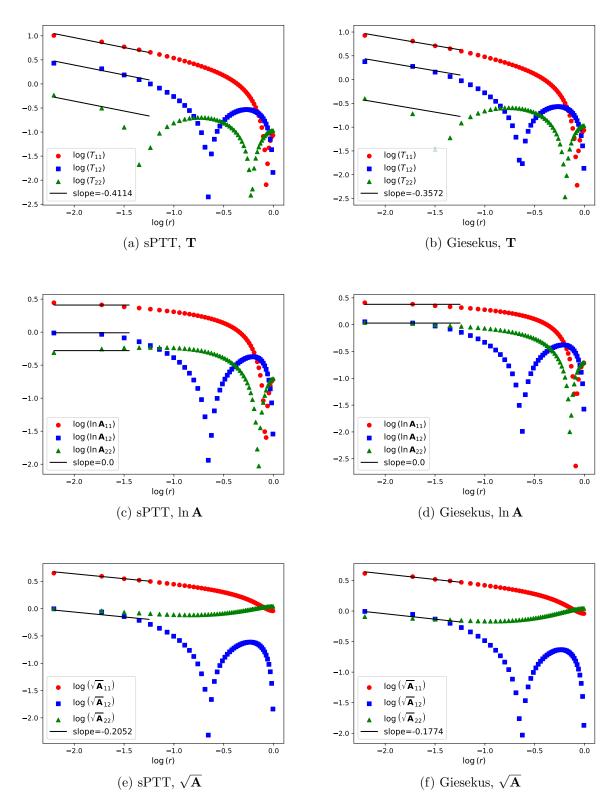


Figure 3: Numerical verification of the asymptotic results for the extrudate flow along $\theta = \frac{\pi}{2}$.

_DieSwell

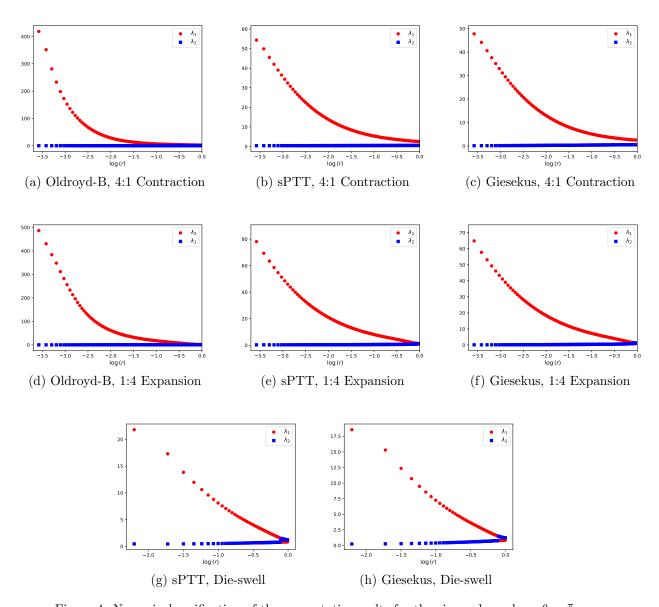


Figure 4: Numerical verification of the asymptotic results for the eigenvalues along $\theta = \frac{\pi}{2}$.

genvalues