CONFERENCE ON "COMPLEX FLOWS OF COMPLEX FLUIDS"

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SOME THOUGHTS ON DIFFERENTIAL VISCOELASTIC MODELS AND THEIR NUMERICAL SOLUTION

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UBI

TOPICS

- Derivation of a “generalized” Oldroyd-B model
- The traceless stress tensor formulation
- Law-of-the-wall for viscoelastic flows

DERIVATION OF GENERALISED MODEL

First TOPIC

GOVERNING EQUATIONS

$$\nabla \bullet \boldsymbol{u} = 0$$

$$\rho \frac{D\boldsymbol{u}}{Dt} = -\nabla p + \nabla \bullet \boldsymbol{\tau}_{tot} = -\nabla p + \eta_s \nabla^2 \boldsymbol{u} + \nabla \bullet \boldsymbol{\tau}$$

OLDROYD-B EQUATIONS

Differential formulation

Original:

$$\tau_{tot} + \lambda \overset{\nabla}{(\tau_{tot})} = 2\eta_0 \left(\boldsymbol{D} + \lambda_r \overset{\nabla}{\boldsymbol{D}} \right)$$

Alternative:

$$\tau_{tot} = \tau_s + \tau_p = 2\eta_s \boldsymbol{D} + \tau$$

$$\boxed{\tau + \lambda \overset{\nabla}{(\tau)} = 2\eta_p \boldsymbol{D}}$$

With:

$$\eta_0 = \eta_s + \eta_p$$

$$\beta = \frac{\eta_s}{\eta_0} = \frac{\lambda_r}{\lambda}$$

OLDROYD-B: molecular formulation

$$\overset{\nabla}{\boldsymbol{A}} = -\frac{(\boldsymbol{A}-\boldsymbol{I})}{\lambda} \qquad \textbf{(1)}$$

$$\boldsymbol{\tau} = \frac{\eta_p}{\lambda}(\boldsymbol{A}-\boldsymbol{I}) \qquad \textbf{(2)}$$

$$\lambda \overset{\nabla}{\boldsymbol{\tau}} = \eta_p\left(\overset{\nabla}{\boldsymbol{A}} - \overset{\nabla}{\boldsymbol{I}}\right) = \eta_p\left(-\frac{(\boldsymbol{A}-\boldsymbol{I})}{\lambda} + 2\boldsymbol{D}\right)$$

with: $\overset{\nabla}{\boldsymbol{I}} = -2\boldsymbol{D}$

$$\Rightarrow \lambda \overset{\nabla}{\boldsymbol{\tau}} = \eta_p\left(-\frac{\boldsymbol{\tau}}{\eta_p} + 2\boldsymbol{D}\right) \Rightarrow \boxed{\lambda \overset{\nabla}{\boldsymbol{\tau}} + \boldsymbol{\tau} = 2\eta_p \boldsymbol{D}}$$

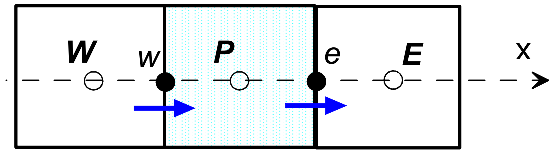
(λ and η_p are constants)

Equations with "conservative" property

• Idea based on conservativeness property (at continuum level)
• Convected variables should appear inside derivative:

$$\frac{D(\lambda\tau)}{Dt} = \frac{\partial(\lambda\tau)}{\partial t} + div(\lambda \boldsymbol{u} \tau)$$

so that balances of fluxes (out-in):



$$\Rightarrow \frac{V_P\left[(\lambda\tau)_P^{n+1} - (\lambda\tau)_P^{n}\right]}{\Delta t} + \Bigg(\lambda \underbrace{\boldsymbol{u}\bullet \boldsymbol{A}\tau}_{flux-e}\Bigg)_e - \Bigg(\lambda \underbrace{\boldsymbol{u}\bullet \boldsymbol{A}\tau}_{flux-w}\Bigg)_w = \ldots.$$

Example of "Conservative" stress models

FENE-MCR: not conservative

$$\tau + \frac{\lambda}{f}\left(\overset{\nabla}{\tau}\right) = 2\eta_p \boldsymbol{D}$$

FENE-CR: conservative

$$\tau + \overset{\nabla}{\left(\frac{\lambda}{f}\tau\right)} = 2\eta_p \boldsymbol{D}$$

PTT: not conservative (apparently)

$$f\tau + \lambda\left(\overset{\nabla}{\tau}\right) + = 2\eta_p \boldsymbol{D}$$

FENE-P: original equation also apparently not conservative

$$\lambda\left(\overset{\nabla}{\tau}\right) + Z\tau - \frac{D \ln Z}{Dt}\left[\lambda\tau + (1-\varepsilon b)nkT\lambda\boldsymbol{I}\right] = 2(1-\varepsilon b)nkT\lambda\boldsymbol{D}$$

Example of "Conservative" stress models: FENE-P (cont)

with function: $$Z = 1 + \frac{3}{b}\left[\left(1-\varepsilon b\right) + \frac{tr(\tau)}{3nkT}\right] \qquad \varepsilon = \frac{2}{b(b+2)}$$

But re-arrangement shows conservativeness:

$$\boldsymbol{\tau} + \left(\frac{\lambda}{f}\boldsymbol{\tau}\right)^{\nabla} = 2\frac{a\eta_p}{f}\boldsymbol{D} - \frac{D\left(a\eta_p / f\right)}{Dt}\boldsymbol{I}$$

with: $$f \equiv Z \qquad a = \frac{b+5}{b+2} \qquad \eta_p = nkT\lambda\frac{b}{b+5}$$

CONCLUSION

So, in general all previous equations can be cast in terms of variable relaxation times and viscosity coefficients:

$$\frac{\eta_p}{f} \qquad\qquad \frac{\lambda}{f}$$

as:

$$\tau + \left(\frac{\lambda}{f}\tau\right)^{\nabla} = 2\frac{\eta_p}{f}\boldsymbol{D} + \ldots..$$

with different functions for the various models:

TYPICAL STRESS FUNCTIONS:

FENE-CR:

$$f\left[\tau\right]=\frac{L^2+(\lambda_0/\eta_{p0})Tr(\tau)}{L^2-3}$$

FENE-P:

$$f\left[\tau\right]=1+\frac{3}{b+2}\left[1+\frac{\lambda_0}{3a\eta_{p0}}Tr(\tau)\right]$$

PTT:

$$f\left[\tau\right]=1+\left(\frac{\lambda_0\varepsilon}{\eta_{p0}}\right)Tr(\tau)$$

GENERALISATION:

Now, both viscosity and relaxation time are variable, functions of invariants of τ:

$$\eta_p = \eta_p(\tau) \qquad\qquad \lambda = \lambda(\tau)$$

We shall use for the constant zero-shear rate values: η_{p0} $\qquad$ λ_0

In general:

$$\overset{\nabla}{(fA)} = \left(\frac{Df}{Dt}\right)A + f\left(\overset{\nabla}{A}\right)$$

DERIVATION OF "GENERALISED" MODEL:

Assume as still valid:

$$\overset{\nabla}{\boldsymbol{A}} = -\frac{(\boldsymbol{A}-\boldsymbol{I})}{\lambda}$$

(1) Equilibrium between rotation/stretching and relaxation

$$\tau = \frac{\eta_p}{\lambda}(\boldsymbol{A}-\boldsymbol{I})$$

(2) Kramers expression

Upper convected derivative of Eq. (2) gives:

$$\overset{\nabla}{(\lambda\tau)} = \overset{\nabla}{(\eta_p \boldsymbol{A})} - \overset{\nabla}{(\eta_p \boldsymbol{I})} = \frac{D\eta_p}{Dt}\boldsymbol{A} + \eta_p \overset{\nabla}{\boldsymbol{A}} - \frac{D\eta_p}{Dt}\boldsymbol{I} + 2\eta_p \boldsymbol{D}$$

DERIVATION OF "GENERALISED" EQUATION

Substituting Eq. (1):

$$\Rightarrow \left(\overset{\nabla}{\lambda\tau}\right) = 2\eta_p \boldsymbol{D} + \frac{D\eta_p}{Dt}\left(\boldsymbol{A}-\boldsymbol{I}\right) - \eta_p \frac{\left(\boldsymbol{A}-\boldsymbol{I}\right)}{\lambda}$$

Eq. (2) again:

$$\Rightarrow \left(\overset{\nabla}{\lambda\tau}\right) + \tau = 2\eta_p \boldsymbol{D} + \frac{\lambda\tau}{\eta_p}\frac{D\eta_p}{Dt}$$

Finally:

$$\Rightarrow \boxed{\left(\overset{\nabla}{\lambda\tau}\right) + \tau\left(1 - \frac{\lambda}{\eta_p}\frac{D\eta_p}{Dt}\right) = 2\eta_p \boldsymbol{D}}$$

GENERALISED EQUATION – SPECIAL CASE

Recall:

$$\eta_p = \frac{\eta_{p0}}{f} \qquad \lambda = \frac{\lambda_0}{f}$$

assume same function $f[\tau]$ **for** η_p **and** λ **.**

$$\left(\lambda \overset{\nabla}{\tau}\right) + \tau\left(1 - \frac{\lambda}{\eta_p}\frac{D\eta_p}{Dt}\right) = 2\eta_p \boldsymbol{D}$$

Gives:

$$\Rightarrow \lambda \overset{\nabla}{\tau} + \tau\frac{D\lambda}{Dt} + \tau\left(1 - \frac{\lambda_0}{\eta_{p0}}\frac{D\eta_p}{Dt}\right) = 2\eta_p \boldsymbol{D}$$

MANIPULATION FOR SPECIAL CASE:

$$\Rightarrow \frac{\lambda_0}{f}\overset{\nabla}{\tau}+\tau\frac{D\left(\lambda_0/f\right)}{Dt}+\tau\left(1-\frac{\lambda_0}{\eta_{p0}}\frac{D\left(\eta_{p0}/f\right)}{Dt}\right)=2\frac{\eta_{p0}}{f}\boldsymbol{D}$$

$$\Rightarrow \lambda_0\overset{\nabla}{\tau}+f\tau=2\eta_{p0}\boldsymbol{D}$$

… the PTT equation!!

COMPARISON WITH FENE-P:

FENE-P under conservative form:

$$\overset{\nabla}{(\lambda\tau)} + \tau = 2\eta_p \boldsymbol{D} - \frac{D\eta_p}{Dt}\boldsymbol{I}$$

with:

$$\lambda = \lambda_0 / f$$
$$\eta_p = a\eta_{p0} / f$$

or in a more "compact" and conservative form:

$$\overset{\nabla}{(\lambda\tau)} + \tau = -\overset{\nabla}{(\eta_p I)}$$

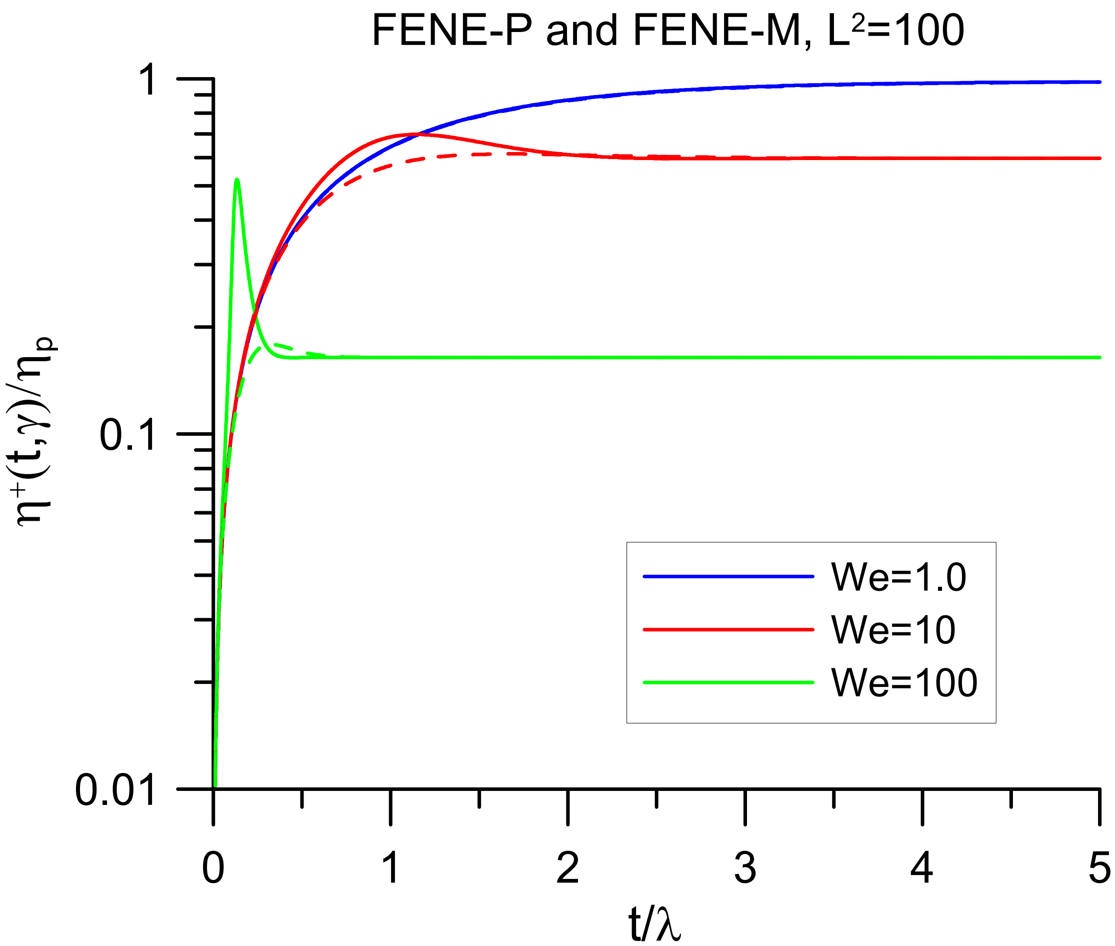
Present model:

$$\overset{\nabla}{(\lambda\tau)} + \tau = 2\eta_p \boldsymbol{D} + \frac{\lambda\tau}{\eta_p}\frac{D\eta_p}{Dt}$$

Advantage: permits to control functions separately

COMPARISON WITH FENE-P: material functions

Stress growth upon inception of shear flow: viscosity

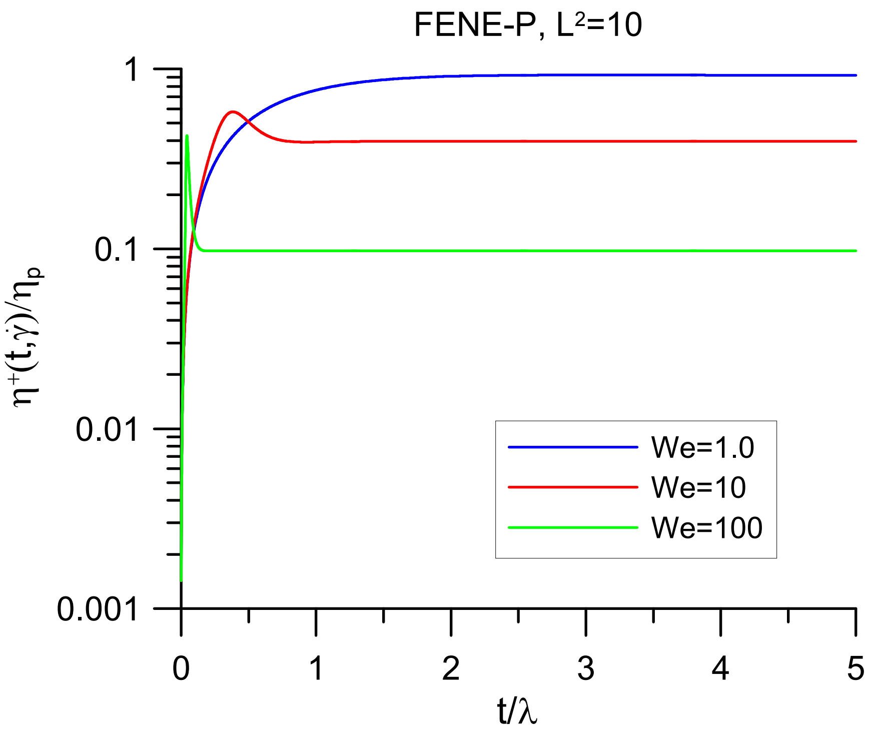


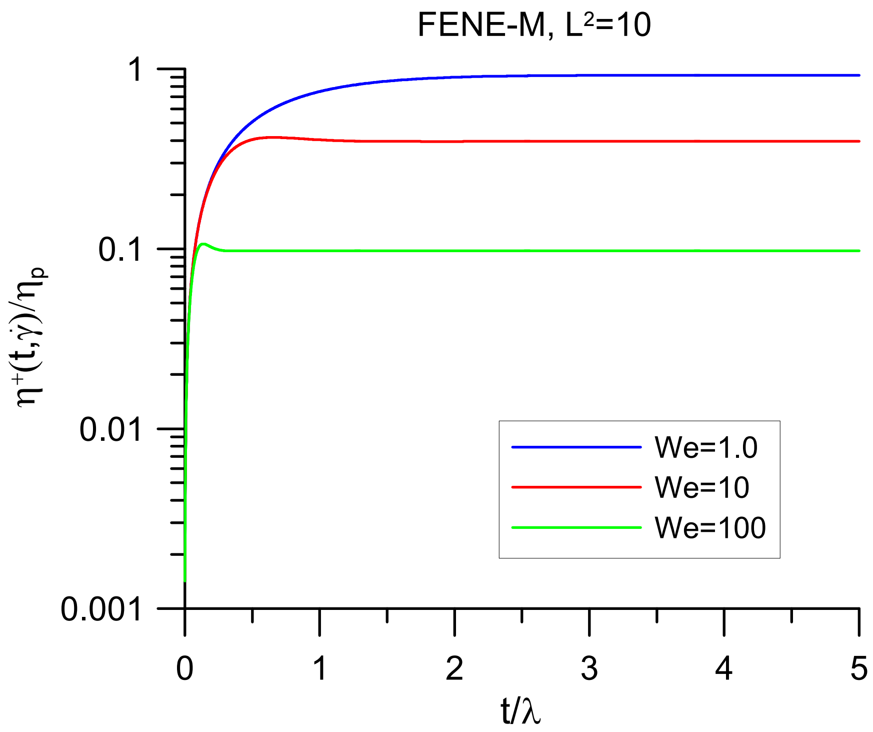
$$\boxed{L^2 = b + 3}$$

FENE-P (solid lines) goes beyond the linear viscoelastic limit envelope; cf. DeAguiar (1983)

COMPARISON WITH FENE-P: material functions

Stress growth upon inception of shear flow: viscosity

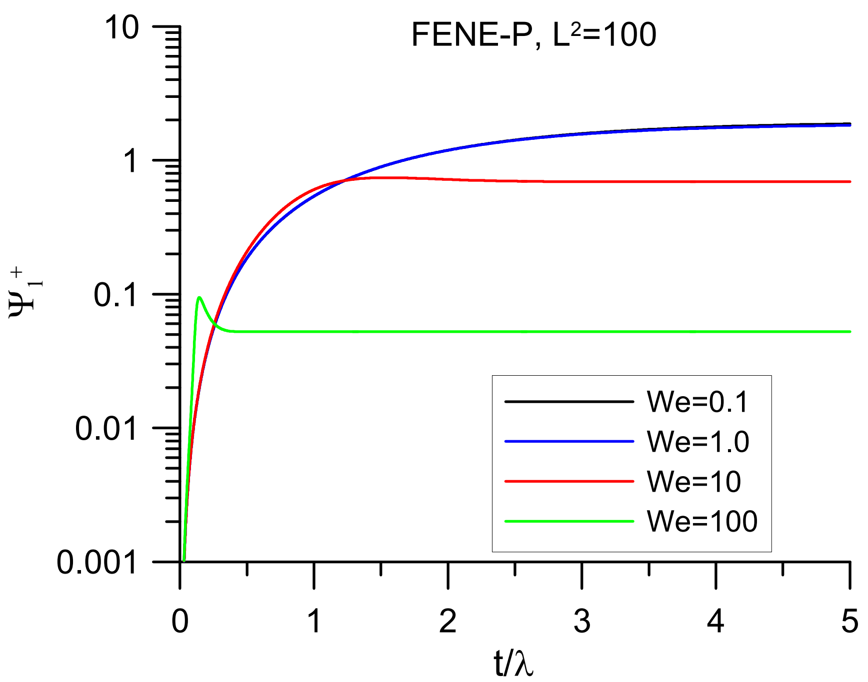


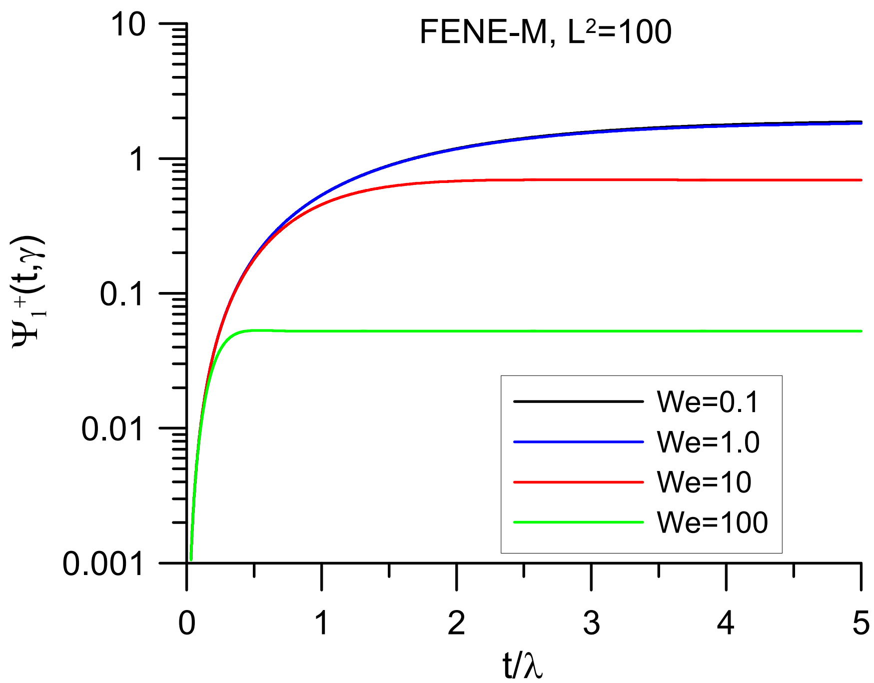


Same as before, for lower extensibility, L2=10

COMPARISON WITH FENE-P: material functions

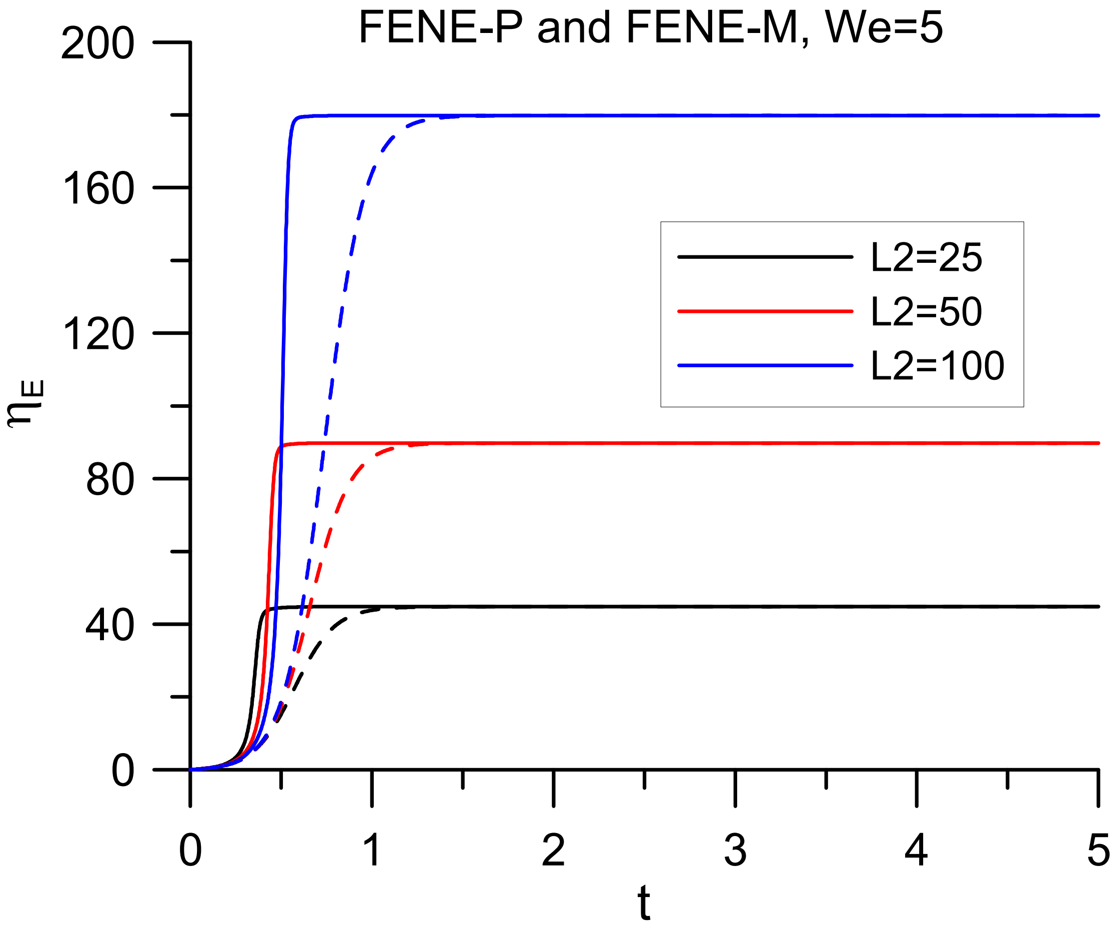
Similar for start up of first normal stress coefficient





COMPARISON WITH FENE-P: material functions

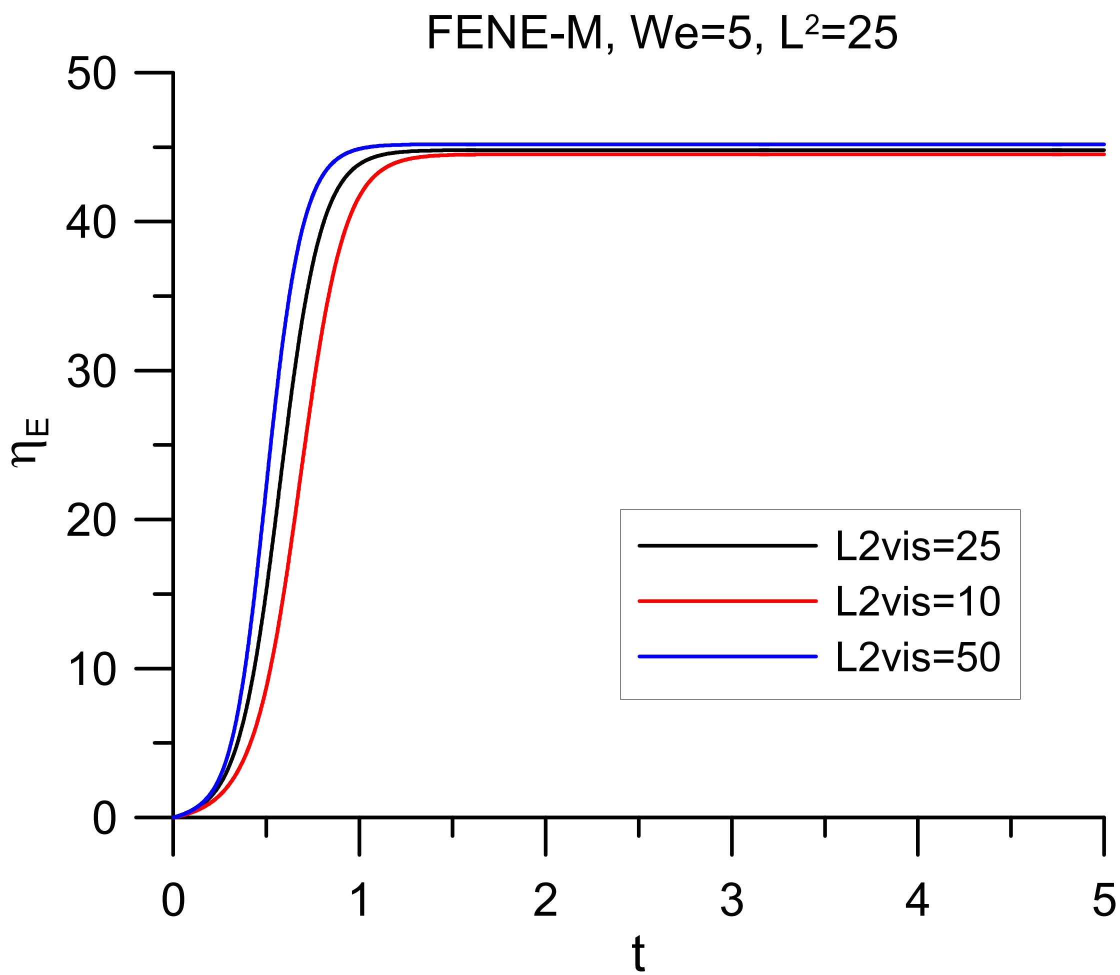
Start-up of uniaxial elongational flow



Modified model allows a less steep rise of extensional viscosity (more realistic??
cf. contrast FENE – FENE-P: Keunings 97; van Heel et al 98; Herrchen &Ottinger 97)

COMPARISON WITH FENE-P: material functions

Modified model in uniaxial elongational flow



Variation of L2 in viscosity funtion permits some control…

TRACELESS STRESS TENSOR FORMULATION

Second TOPIC

TRACELESS STRESS TENSOR FORMULATION

Standard equations of motion:

P-correction solver

$$\frac{\partial u_j}{\partial x_j} = 0$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

Coupling term

$\propto (1-\beta)De$

Traceless tensor:

$$\boxed{\tau'_{ij} = \tau_{ij} - \tfrac{1}{3}\tau_{kk}\delta_{ij}}$$

so that: $$Tr\left(\tau'\right) = \tau'_{kk} = 0$$

TRACELESS MOMENTUM EQ.

Substitution in original eqs. gives:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial \left(p - \frac{1}{3}\tau_{kk} \right)}{\partial x_i} + \frac{\partial \tau'_{ij}}{\partial x_j}$$

$$\Rightarrow \boxed{\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial p'}{\partial x_i} + \frac{\partial \tau'_{ij}}{\partial x_j}}$$

with: $$\boxed{p' = p - \frac{1}{3}\tau_{kk}}$$

(modified pressure)

TRACELESS STRESS: OLDROYD-B

Oldroyd-B equation, indicial notation:

$$\tau_{ij} + \lambda \frac{D\tau_{ij}}{Dt} = \eta_p \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda G_{ij}$$

with "generation" tensor term:

$$G_{ij} = \tau_{ik} \frac{\partial u_j}{\partial x_k} + \tau_{jk} \frac{\partial u_i}{\partial x_k}$$

Using the TST we get:

$$\boxed{\tau'_{ij} + \lambda \frac{D\tau'_{ij}}{Dt} = \eta'_p \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \lambda \left(G'_{ij} - \tfrac{2}{3} G' \delta_{ij} \right)}$$

TRACELESS STRESS TENSOR: increased viscosity

with: $$G'_{ij} = \tau'_{ik}\frac{\partial u_j}{\partial x_k} + \tau'_{jk}\frac{\partial u_i}{\partial x_k}$$

and: $$G'_{ll} = 2\tau'_{lk}\frac{\partial u_l}{\partial x_k} \equiv 2G'$$

(in turbulence modelling, $G = \tau_{lk}\frac{\partial u_l}{\partial x_k}$ **is the generation rate)**

An "increased" viscosity arises:

$$\boxed{\eta'_p = \eta_p + \tfrac{1}{3}\lambda\tau_{kk}}$$

… very high, where it matters!

(link with AVSS …)

Evolution of the trace

Relations for the evolution of the trace of the stress:

$$G = G' + \tfrac{1}{3}\tau_{kk} \underbrace{\frac{\partial u_j}{\partial x_j}}_{=0}$$

Contracting indices:

$$\tau_{kk} + \lambda \frac{D\tau_{kk}}{Dt} = 2\eta'_p \underbrace{\frac{\partial u_k}{\partial x_k}}_{=0} + 2\lambda G'$$

enabling calculation of the trace

TRACELESS STRESS TENSOR for OLDROYD-B

Resumé in tensor notation:

$$\boxed{\tau' + \lambda \overset{\nabla'}{(\tau')} = 2\eta'_p \boldsymbol{D}'}$$

$$\tau' = \tau - \tfrac{1}{3} Tr(\tau) I$$

$$\boldsymbol{D}' = \boldsymbol{D} - \tfrac{1}{3} Tr(\boldsymbol{D}) I$$

$$\eta'_p = \eta_p + \tfrac{1}{3} \lambda Tr\left(\tau\right)$$

and the extended definition:

$$\overset{\nabla'}{(\tau')} = \frac{D\tau'}{Dt} - \left\{ \tau' \bullet \nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T \bullet \tau' - \tfrac{2}{3} \left(\tau' : \nabla \boldsymbol{u} \right) \boldsymbol{I} \right\}$$

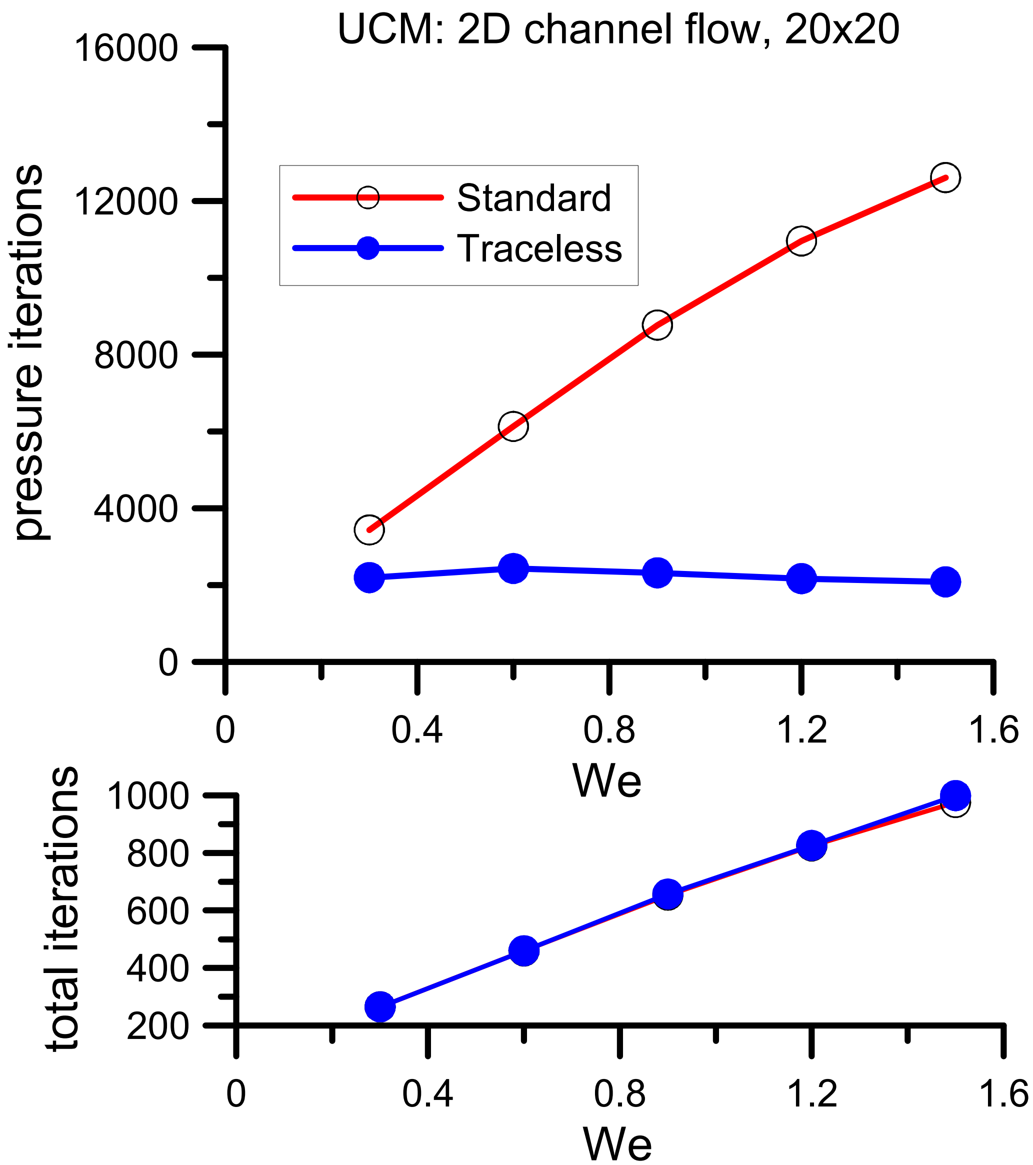
TRACELESS STRESS TENSOR: RESULTS (1)

UCM in channel flow, 20x20, L=10, H=1

Total number of iterations to solve pressure equation:

We	Outer iterations	Total number of inner iterations for pressure		
		Standard method	Traceless method	Ratio
0.3	265	3434	2193	1.6
0.6	459	6129	2428	2.5
0.9	653	8768	2316	3.8
1.2	824	10957	2163	5.1
1.5	975	12609	2080	6.1

TRACELESS STRESS TENSOR: RESULTS (1a)



TRACELESS STRESS TENSOR: RESULTS (2)

UCM, 4:1 plane contraction flow (mesh 2960 CV)

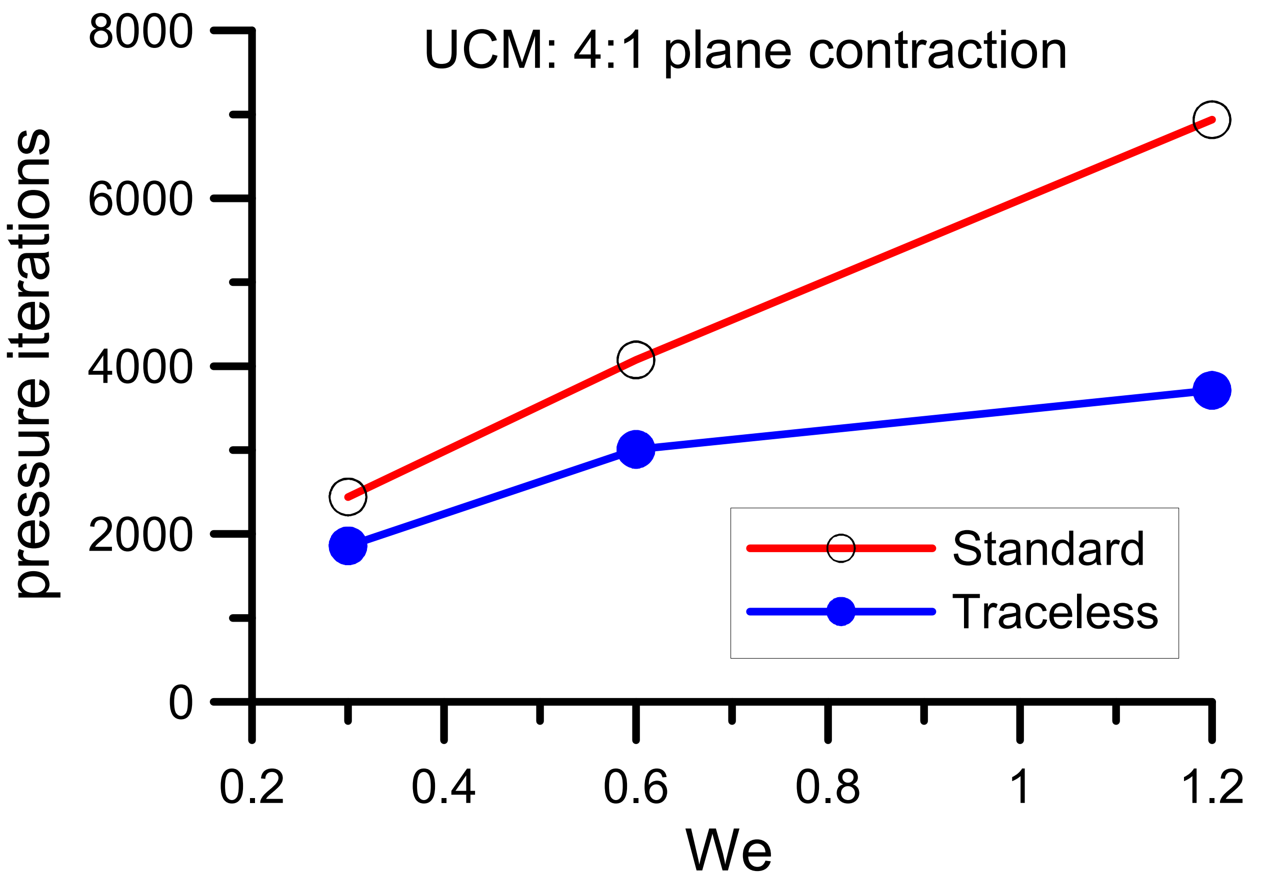
Total number of iterations to solve pressure equation:

We	Outer iterations	Total number of inner iterations for pressure		
		Standard method	Traceless method	Ratio
0.0	798	8641	--	
0.3	651	2442	1859	1.3
0.6	664	4074	3008	1.4
1.2	725	6935	3711	1.9

Ratio proportional to relative CPU times

TRACELESS STRESS TENSOR: RESULTS (2)

UCM, 4:1 plane contraction flow (mesh 2960 CV)



(ratio proportional to relative CPU times)

TRACELESS STRESS TENSOR: CONCLUSIONS

Advantages:
- TST offers better coupling and much less CPU
- Number of pressure iterations approximately constant

Problems:
- Creation of strong normal stress normal to a wall
- Difficulty to implement such BCs (oscillations)

e.g. UCM, channel aligned with x:

Standard: $\tau_{xx} = 2\lambda\eta\dot{\gamma}^2 \quad \tau_{yy} = 0 \quad \tau_{xy} = \eta\dot{\gamma}$

TST: $\tau'_{xx} = \frac{4}{3}\lambda\eta\dot{\gamma}^2 \quad \tau'_{yy} = -\frac{2}{3}\lambda\eta\dot{\gamma}^2 \quad \tau'_{xy} = \eta\dot{\gamma}$

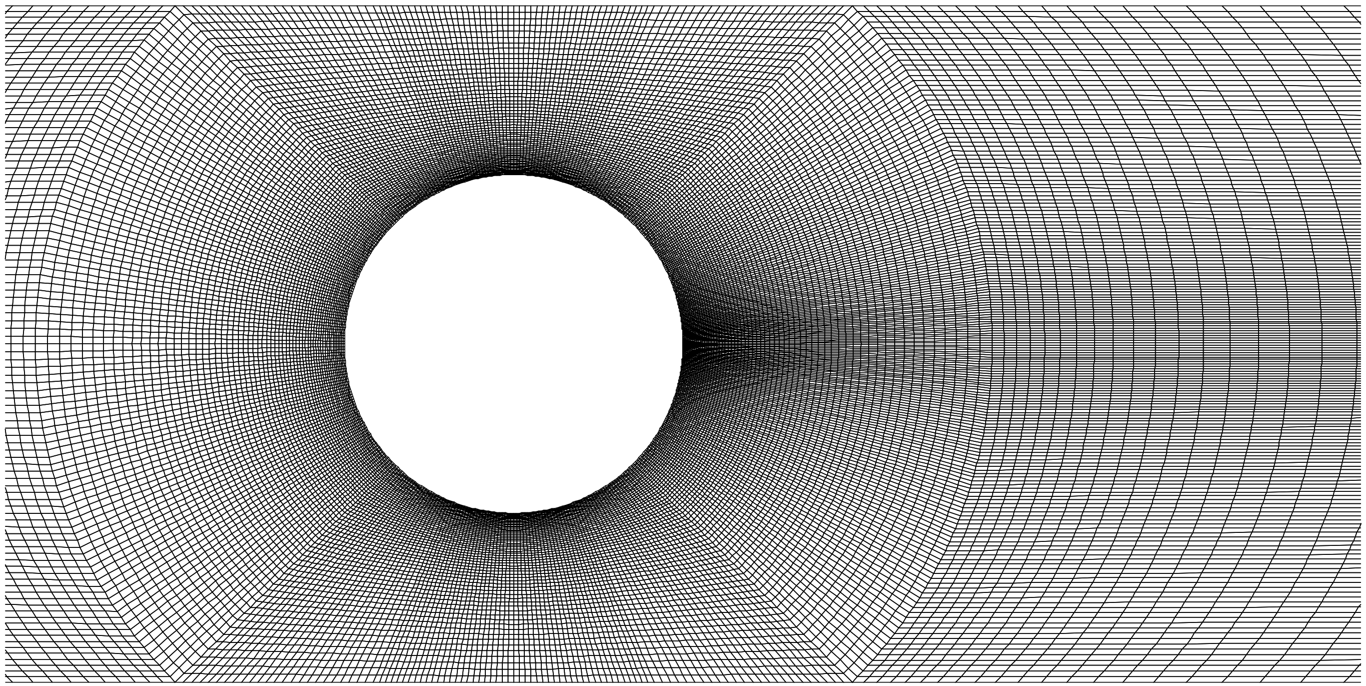
- Problems are particular to our FVM (collocated) (?)
- Would like to see other attempts with FEM

LAW-OF-WALL FOR VISCOELASTIC FLOWS

Third TOPIC

LAW-OF-WALL FOR VISCOELASTIC FLOWS

At present, 2D meshes are so fine that any attempt to extend to 3D is out of question… (ex: cylinder)



NC=44280; even a coarser mesh NC=11040x100=1.104.000

LAW-OF-WALL FOR TURBULENT FLOWS

Flow depends on: $y \quad \tau_w \quad \rho \quad \mu$

Dimensional analysis gives: $u_\tau \equiv \sqrt{\dfrac{\tau_w}{\rho}} \qquad y^+ \equiv \dfrac{\rho y u_\tau}{\mu}$

and a wall layer:

$$\frac{u}{u_\tau} = f_1(y^+) \qquad \frac{\partial u}{\partial y} = \frac{u_\tau}{y} f_2(y^+) \qquad \frac{-\overline{u'v'}}{{u_\tau}^2} = f_3(y^+)$$

Small acceleration implies: $\dfrac{\partial \tau}{\partial y} = 0 \Rightarrow \tau = \tau_l + \tau_t \cong const.$

(constant-stress layer)

Experiments show, for "large" y+:

$$f_3 \approx 1 \qquad u_\tau = \sqrt{-\overline{u'v'}} \qquad f_2 \approx const. = 1/\mathrm{K} \qquad \mathrm{K} = 0.41$$

$$\frac{\partial u}{\partial y} = \frac{u_\tau}{\mathrm{K} y} \qquad \Rightarrow \qquad \boxed{u^+ \equiv \frac{u}{u_\tau} = \frac{1}{\mathrm{K}} \ln(E y^+)}$$ (the log-law)

LAW-OF-WALL FOR VISCOELASTIC FLOWS

Carry same ideas for viscoleastic flows near walls

List of dependent variables includes relaxation time:

$$y \quad p'_x \quad \rho \quad \eta \quad \lambda$$

Giving the characteristic scales:

$$t_c = \lambda \qquad y_c = \frac{\eta}{\lambda p'_x} \qquad u_c = \frac{\eta}{\lambda^2 p'_x}$$

Instead of a logarithmic variation, power law attempts were followed in the next fittings of shear flows
(following Zagarola et al., Phy Fluids 1997)

LAW-OF-WALL FOR VISCOELASTIC FLOWS

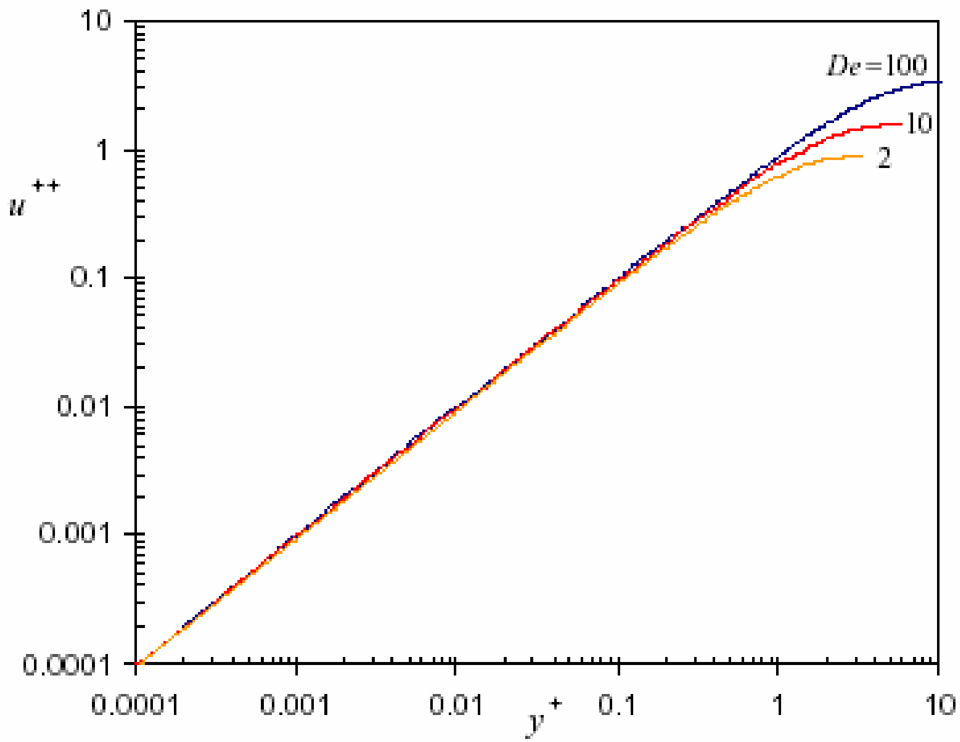
Pipe flow: Linear SPTT

$$u^{+} = \frac{u}{\eta / \lambda^{2} p'_{x}}$$

$$y^{+} = \frac{y}{\eta / \lambda \; p'_{x}}$$

$$u^{++} = u^{+} / 6De$$

$$\boxed{u^{++} = y^{+}}$$



LAW-OF-WALL FOR VISCOELASTIC FLOWS

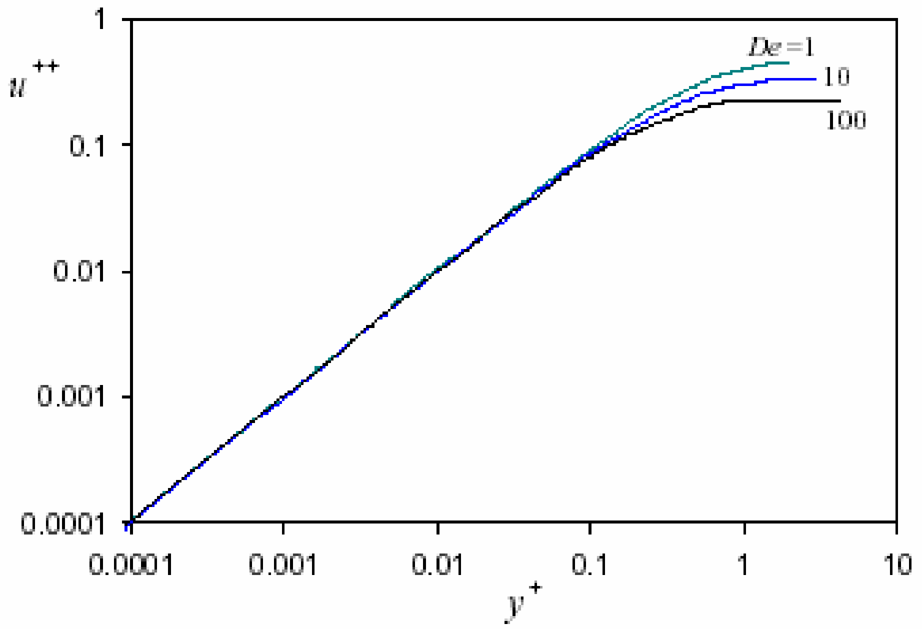
Pipe flow: Exponential SPTT

$$u^{+} = \frac{u}{\eta / \lambda^{2} p'_{x}}$$

$$y^{+} = \frac{y}{\eta / \lambda \; p'_{x}}$$

$$u^{++} = \frac{u^{+}}{De\left[6.66 + \ln(\varepsilon De^{2})\right]}$$

$$\boxed{u^{++} = y^{+}}$$



LAW-OF-WALL FOR VISCOELASTIC FLOWS

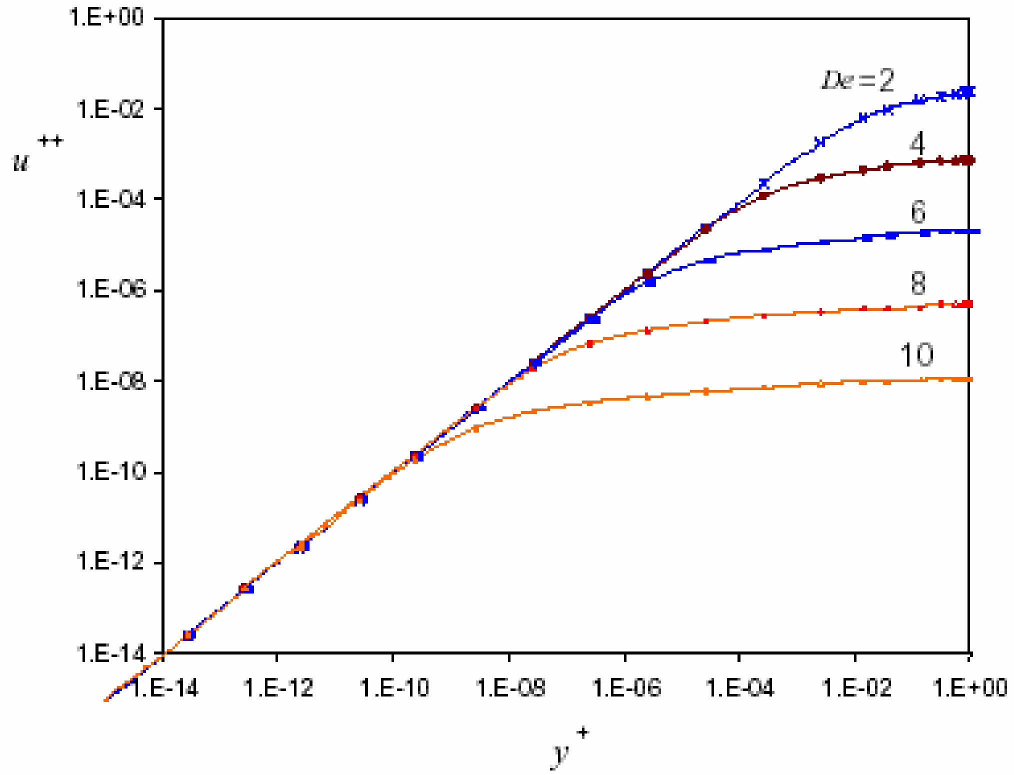
Channel flow: Leonov fluid

$$u^{+} = \frac{u}{\eta / \lambda^2 p'_x}$$

$$y^{+} = \frac{y}{\eta / \lambda \; p'_x}$$

$$u^{++} = \frac{u^{+}}{e^{2De+2}/4}$$

$$\boxed{u^{++} = y^{+}}$$



LAW-OF-WALL FOR VISCOELASTIC FLOWS

Lot to be done….

In future attempts, a wall law should be sought for the stresses (and not velocity), based on the notion of "local equilibrium"

CONCLUSIONS

- Theoretical (empirical): a “naive” derivation led to a modified FENE-P equation with some advantages for time-dependent flows. It is the PTT when functions are the same.

- Numerics: the traceless approach allows tighter coupling of equations in decoupled methods. Unsolved problems with normal stresses at wall.

- Pratical applications (3D): proposal for a “log-law”-like treatment to bridge the near wall BLs.

ACKNOWLEDGMENTS:

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(law-of-wall)

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