A Priori DNS Development of a Closure for The Nonlinear Term of The Evolution Equation of The Conformation Tensor for FENE-P Fluids

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Abstract. A closure is developed for the time-averaged cross correlation between fluctuating conformation and rate of strain tensors appearing in the evolution equation of the conformation tensor for the polymer stress of the FENE-P fluid. The closure was calibrated against DNS data pertaining to the low and high drag reduction regimes.

Keywords: drag reduction, polymer solutions, FENE-P, turbulence model, closure of NLT_{ij}.
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INTRODUCTION

The addition of small amounts of polymer additives to a Newtonian solvent is a powerful drag and heat transfer reducer in turbulent flow [1]. The rheology of dilute polymer solutions can be described by the Finitely-Extensible-Nonlinear-Elastic constitutive equation with Peterlin's approximation (FENE-P). The extensive use of these fluids in engineering applications requires the capability to predict accurately their flow characteristics at low cost using Reynolds-average Navier-Stokes (RANS) methods that can be developed using DNS data [2,3]. In RANS, the Reynolds- average evolution equation (RACE) for the conformation tensor (C_{ij}) requires a closure for the cross-correlation between the fluctuating conformation and rate of strain tensors, denoted NLT_{ij}. NLT_{ij} also appears in the closure for the viscoelastic stress work [4], a term in the transport equation of turbulent kinetic energy (k). The development of a closure for NLT_{ij} is carried out with the help of DNS for a Reynolds number of $Re_{\tau 0}$=395, a maximum molecular extensibility of L^2=900 and a solvent to total zero-shear-rate viscosities ratio of β=0.9 at Weissenberg numbers of $We_{\tau 0}$= 25 and 100.

MODELLING NLT$_{IJ}$

All equations are written in the indicial notation of Einstein. Upper-case letters and overbars denote time-average, lower-case letters denote fluctuations and ^ is used for instantaneous quantities. The momentum equation for turbulent flow of FENE-P fluids needs the time-averaged polymer stress ($\overline{\tau}_{ik,p}$) given by the Reynolds-averaged FENE-P equation (1), where λ is the relaxation time and η_p the polymer viscosity coefficient. It also requires the calculation of C_{ij} in the RACE equation (2).

$$\overline{\tau}_{ij,p} = \frac{\eta_p}{\lambda}\left[f(C_{kk})C_{ij} - f(L)\delta_{ij}\right] + \frac{\eta_p}{\lambda}\overline{f(C_{kk}+c_{kk})c_{ij}} \text{ with } f(C_{kk}) = \frac{L^2-3}{L^2-C_{kk}} \text{ and } f(L)=1 \quad (1)$$

$$\left(\frac{\partial C_{ij}}{\partial t} + U_k\frac{\partial C_{ij}}{\partial x_k} - C_{jk}\frac{\partial U_i}{\partial x_k} - C_{ik}\frac{\partial U_j}{\partial x_k}\right) + \overline{u_k\frac{\partial c_{ij}}{\partial x_k}} - \left(\overline{c_{kj}\frac{\partial u_i}{\partial x_k}} + \overline{c_{ik}\frac{\partial u_j}{\partial x_k}}\right) = -\frac{\overline{\tau}_{ij,p}}{\eta_p} \quad (2)$$

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Here, U_i is the mean velocity vector, $\overline{f\left(C_{kk}+c_{kk}\right)c_{ij}}$ and $CT_{ij}=-\overline{u_k\,\partial c_{ij}/\partial x_k}$ are negligible [3-5], and a closure for $NLT_{ij}\equiv\overline{c_{kj}\,\partial u_i/\partial x_k}+\overline{c_{ik}\partial u_j/\partial x_k}$ is required.

A quasi-exact expression for NLT_{ij} was derived by Pinho [6] given here as equation (3), where NLT_{ij} is contained in the boxed term under the approximation of equation (4) as corroborated by DNS data [4].

$$\boxed{\overline{f\left(\hat{C}_{mm}\right)c_{kj}\frac{\partial u_i}{\partial x_k}}+\overline{f\left(\hat{C}_{mm}\right)c_{ik}\frac{\partial u_j}{\partial x_k}}}+C_{kj}\overline{f\left(\hat{C}_{mm}\right)\frac{\partial u_i}{\partial x_k}}+C_{ik}\overline{f\left(\hat{C}_{mm}\right)\frac{\partial u_j}{\partial x_k}}+\lambda\left[\overline{\frac{\partial u_i}{\partial x_k}\frac{\partial c_{kj}}{\partial t}}+\overline{\frac{\partial u_j}{\partial x_k}\frac{\partial c_{ik}}{\partial t}}+\frac{\partial C_{kj}}{\partial x_n}\overline{u_n\frac{\partial u_i}{\partial x_k}}+\frac{\partial C_{ik}}{\partial x_n}\overline{u_n\frac{\partial u_j}{\partial x_k}}\right]$$
$$+\lambda\left[\overline{\frac{\partial\left(U_n c_{kj}\right)}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{\frac{\partial\left(U_n c_{ik}\right)}{\partial x_n}\frac{\partial u_j}{\partial x_k}}+\overline{u_n\frac{\partial c_{kj}}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{u_n\frac{\partial c_{ik}}{\partial x_n}\frac{\partial u_j}{\partial x_k}}\right]-\lambda\left[\frac{\partial U_k}{\partial x_n}\left(\overline{c_{jn}\frac{\partial u_i}{\partial x_k}}+\overline{c_{in}\frac{\partial u_j}{\partial x_k}}\right)+\frac{\partial U_j}{\partial x_n}\overline{c_{kn}\frac{\partial u_i}{\partial x_k}}+\frac{\partial U_i}{\partial x_n}\overline{c_{kn}\frac{\partial u_j}{\partial x_k}}\right]$$
$$-\lambda\left[C_{kn}\left(\overline{\frac{\partial u_j}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{\frac{\partial u_i}{\partial x_n}\frac{\partial u_j}{\partial x_k}}\right)+C_{jn}\overline{\frac{\partial u_k}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+C_{in}\overline{\frac{\partial u_k}{\partial x_n}\frac{\partial u_j}{\partial x_k}}+\overline{c_{jn}\frac{\partial u_k}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{c_{in}\frac{\partial u_k}{\partial x_n}\frac{\partial u_j}{\partial x_k}}+\overline{c_{kn}\frac{\partial u_j}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{c_{kn}\frac{\partial u_i}{\partial x_n}\frac{\partial u_j}{\partial x_k}}\right]=0 \qquad (3)$$

$$\overline{f\left(\hat{C}_{mm}\right)c_{kj}\frac{\partial u_i}{\partial x_k}}+\overline{f\left(\hat{C}_{mm}\right)c_{ik}\frac{\partial u_j}{\partial x_k}}\approx f\left(C_{mm}\right)\left(\overline{c_{kj}\frac{\partial u_i}{\partial x_k}}+\overline{c_{ik}\frac{\partial u_j}{\partial x_k}}\right)=f\left(C_{mm}\right)NLT_{ij} \qquad (4)$$

Near walls molecules are stretched, $f\left(\hat{C}_{kk}\right)$ is larger than its equilibrium value of 1 and C_{kk} and $\sqrt{\overline{c_{kk}^2}}$ are large, but $\sqrt{\overline{c_{kk}^2}}<<C_{kk}$. Elsewhere $\sqrt{\overline{c_{kk}^2}}$ approaches C_{kk}, but since both are small $f\left(\hat{C}_{kk}\right)\simeq f\left(C_{kk}\right)\simeq 1$. Hence, $\overline{f\left(\hat{C}_{mm}\right)}\approx f\left(C_{mm}\right)$ and $\overline{f\left(\hat{C}_{kk}\right)a_ib_{jl}}\simeq f\left(C_{kk}\right)\overline{a_ib_{jl}}$ holds everywhere [4].

Several standard assumptions in turbulence modelling are invoked together with approximations justified by DNS. CT_{ij}-like terms are similarly neglected. Invoking homogeneous turbulence, terms like turbulent diffusion of k are neglected ($\overline{u_n\,\partial u_j/\partial x_k}=0$). Invariance requires that convective terms are null except as part of a material derivative, hence all terms multiplying U_n, and likewise triple correlations involving u_n, are set to zero.

The term in equation (5) is modeled on the basis of homogeneous isotropic turbulence arguments involving Taylor's longitudinal micro-scale and the dissipation of k, denoted ε (see [7] for details).

$$C_{kn}\left(\overline{\frac{\partial u_j}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{\frac{\partial u_i}{\partial x_n}\frac{\partial u_j}{\partial x_k}}\right)+C_{jn}\overline{\frac{\partial u_k}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+C_{in}\overline{\frac{\partial u_k}{\partial x_n}\frac{\partial u_j}{\partial x_k}}\approx C_{\varepsilon_F}\frac{4}{15}\times\frac{\varepsilon}{\beta\times We_{\tau 0}\times\nu_s}C_{mm}\times f_{F2}\times\delta_{ij} \qquad (5)$$

For cross-correlations terms like $\overline{c_{kn}\,\partial u_i/\partial x_k}$ modelling was based on symmetry and invariance, plus a decoupling of higher-order correlations into products of lower order terms. We introduced a viscous length scale $L\approx\nu_0\Big/\sqrt{\left|\overline{u_iu_m}\right|}$ and, for convenience, a Reynolds shear stress ($\overline{u_iu_n}$) to model normal components of NLT_{ij}. Invoking also increased anisotropy of Reynolds stress and conformation tensors with DR, this led to the model of equation (6).

$$\frac{\partial U_k}{\partial x_n}\left(\overline{c_{jn}\frac{\partial u_i}{\partial x_k}}+\overline{c_{in}\frac{\partial u_j}{\partial x_k}}\right)+\frac{\partial U_j}{\partial x_n}\overline{c_{kn}\frac{\partial u_i}{\partial x_k}}+\frac{\partial U_i}{\partial x_n}\overline{c_{kn}\frac{\partial u_j}{\partial x_k}}=\approx C_{F3}\times\left[\left|\frac{\partial U_j}{\partial x_k}\frac{\partial U_m}{\partial x_n}\right|C_{kn}\frac{\overline{u_iu_m}}{\nu_0\sqrt{2S_{pq}S_{pq}}}+\left|\frac{\partial U_i}{\partial x_k}\frac{\partial U_m}{\partial x_n}\right|C_{kn}\frac{\overline{u_ju_m}}{\nu_0\sqrt{2S_{pq}S_{pq}}}\right] \qquad (6)$$

$C_{kj}\overline{f\left(\hat{C}_{mm}\right)\partial u_i/\partial x_k}$ was decoupled, together with the assumption $O(u)\sim O(U)$, leading to

$$C_{kj}\overline{f\left(\hat{C}_{mm}\right)\frac{\partial u_i}{\partial x_k}}+C_{ik}\overline{f\left(\hat{C}_{mm}\right)\frac{\partial u_j}{\partial x_k}}\approx C_{F2}\left[C_{kj}f\left(C_{mm}\right)\frac{\partial U_i}{\partial x_k}+C_{ik}f\left(C_{mm}\right)\frac{\partial U_j}{\partial x_k}\right] \qquad (7)$$

The four triple correlations were also decoupled into a product of lower order terms as below.

$$\overline{c_{jn}\frac{\partial u_k}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{c_{in}\frac{\partial u_k}{\partial x_n}\frac{\partial u_j}{\partial x_k}}+\overline{c_{kn}\frac{\partial u_j}{\partial x_n}\frac{\partial u_i}{\partial x_k}}+\overline{c_{kn}\frac{\partial u_i}{\partial x_n}\frac{\partial u_j}{\partial x_k}}\approx -f_{F1}\times C_{F4}\left[C_{jn}\frac{\partial U_k}{\partial x_n}\frac{\partial U_i}{\partial x_k}+C_{in}\frac{\partial U_k}{\partial x_n}\frac{\partial U_j}{\partial x_k}+C_{kn}\frac{\partial U_j}{\partial x_n}\frac{\partial U_i}{\partial x_k}+C_{kn}\frac{\partial U_i}{\partial x_n}\frac{\partial U_j}{\partial x_k}\right] \qquad (8)$$

Finally, the model of NLT_{ij} in equation (9) was compared with DNS data and improved with the addition of an extra corrective term, as frequently done in turbulence modelling, because the assumptions invoked often oversimplify the physics. The added term is $-C_{F1}\times C_{ij}f(C_{mm})^2/\lambda$. The model coefficients are listed in Table 1 and the two damping functions $f_{F_1}=\left[1-0.8\exp\left(-y^+/30\right)\right]^2$ and $f_{F_2}=\left[1-\exp\left(-y^+/25\right)\right]^4$ account for low *Re* effects.

$$\begin{aligned} NLT_{ij} &\equiv \overline{c_{kj}\frac{\partial u_i}{\partial x_k}}+\overline{c_{ik}\frac{\partial u_j}{\partial x_k}} \approx \frac{\lambda}{f(C_{mm})}\left[C_{\varepsilon_F}\frac{4}{15}\times\frac{\varepsilon}{\nu_s\times\beta\times We_{\tau 0}}C_{mm}\times f_{F2}\times\delta_{ij}\right]+C_{F1}\times\frac{C_{ij}\times f(C_{mm})}{\lambda}-\frac{C_{F2}}{We_{\tau 0}}\left[C_{kj}\frac{\partial U_i}{\partial x_k}+C_{ik}\frac{\partial U_j}{\partial x_k}\right] \\ &+\frac{\lambda}{f(C_{mm})}\left[C_{F3}\times\left(\left|\frac{\partial U_j}{\partial x_k}\frac{\partial U_m}{\partial x_n}\right|C_{kn}\frac{\overline{u_i u_m}}{\nu_0\sqrt{2S_{pq}S_{pq}}}+\left|\frac{\partial U_i}{\partial x_k}\frac{\partial U_m}{\partial x_n}\right|C_{kn}\frac{\overline{u_j u_m}}{\nu_0\sqrt{2S_{pq}S_{pq}}}\right)\right] \\ &-\frac{\lambda}{f(C_{mm})}\times f_{F1}\times C_{F4}\left(\frac{We_{\tau_0}}{25}\right)^{0.228}\left[C_{jn}\frac{\partial U_k}{\partial x_n}\frac{\partial U_i}{\partial x_k}+C_{in}\frac{\partial U_k}{\partial x_n}\frac{\partial U_j}{\partial x_k}+C_{kn}\frac{\partial U_j}{\partial x_n}\frac{\partial U_i}{\partial x_k}+C_{kn}\frac{\partial U_i}{\partial x_n}\frac{\partial U_j}{\partial x_k}\right] \end{aligned} \tag{9}$$

TABLE 1. Numerical value of the coefficients of the closure of NLT_{ij}.

C_{F_1}	C_{F_2}	C_{F_3}	C_{F_4}	C_{ε_F}
0.32	5	0.026	0.806	1.428

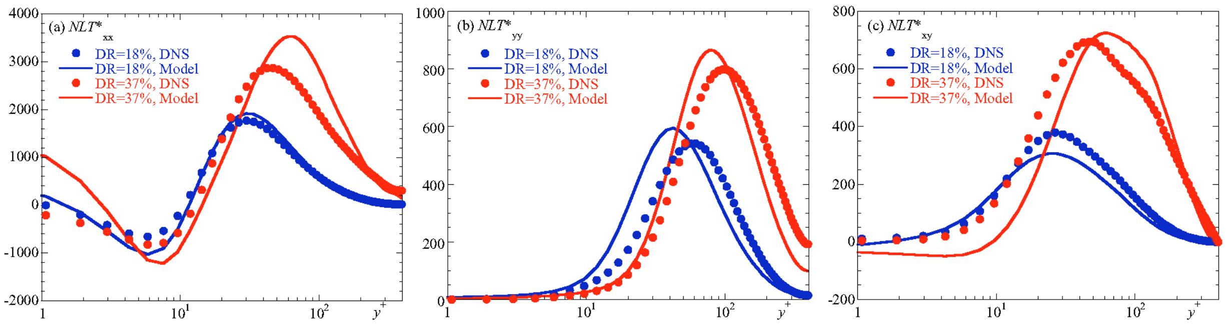

FIGURE 1. Comparison between the DNS data and the model of NLT_{ij} for $Re_{\tau 0}$= 395, L^2= 900 and β=0.9 for $We_{\tau 0}$= 25 (DR= 18%) and $We_{\tau 0}$= 100 (DR= 37%): (a) NLT_{11}; (b) NLT_{22}; (c) NLT_{12}.

The behavior of the model is compared in Figure 1 with DNS for DR=18% and 37%. The performance is better at DR= 18%, because some assumptions are more realistic. In assessing the model we must distinguish between the viscous sublayer and the buffer and log-law regions. Not shown for conciseness, NLT_{ij} in the viscous sublayer is not so important because the other terms in equation (2) are much larger [4,5]. Therefore, the discrepancies in the wall region seen in Figure 1 are of no consequence. The buffer and log-law regions are those that matter and here the model performs well, slightly over-predicting NLT_{11} and NLT_{kk} at high DR, predicting well NLT_{22} and NLT_{12}, with mixed results regarding the location of its peak value.

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