

# The White-Metzner model – Then and Now

K. Walters<sup>a</sup>, M.F. Webster<sup>b</sup>, and H.R.Tamaddon-Jahromi<sup>b</sup>

<sup>a</sup> Institute of Mathematics and Physics, University of Aberystwyth, Aberystwyth, SY23 3BZ, UK

<sup>b</sup> Institute of Non-Newtonian Fluid Mechanics, Swansea University, School of Engineering,  
Singleton Park, Swansea, SA28PP, UK

## Abstract

There is no doubt that the publication of the 1963 *Journal of Applied Polymer Science* paper of J.L.White and A.B.Metzner was an important landmark in constitutive modelling, with important consequences in process modelling and related fields.

The paper appeared after a period of research by others that emphasised the need for ‘generality’ in constitutive modelling. As important as such studies were at the time, the resulting constitutive equations were too complex to be used in ‘earthy’ practical rheological problems of the sort encountered in process modelling.

So, the 1958 *Proc Roy Soc* paper of J.G.Oldroyd and, more particularly, the White-Metzner 1963 paper were timely additions to the literature, especially for those working in practical fields such as polymer processing. The original White-Metzner model had constitutive equations of the form:

$$\sigma_{ik} = -p\delta_{ik} + T_{ik},$$
$$T_{ik} + \frac{\eta}{G} \overset{\nabla}{T}_{ik} = 2\eta d_{ik},$$

where  $\sigma_{ik}$  is the stress tensor,  $p$  is an arbitrary isotropic pressure (for incompressible fluids),  $\delta_{ik}$  is the Kronecker delta and the overscore triangle denotes the upper convective time derivative introduced by Oldroyd in his seminal 1950 paper. As originally introduced,  $\eta$  was ‘a function of the invariants of stress matrix’ and  $G$  was ‘a constant modulus’.

Various simple modifications to the original White-Metzner model began to appear in the rheological literature and the current authors have recently carried out simulations for what we might call ‘the Generalized White Metzner model’. This has equations of state of the form:

$$T_{ik} + \lambda \overset{\nabla}{T}_{ik} = 2\eta d_{ik},$$

where  $\lambda$  and  $\eta$  are now functions of  $II_2$  and  $III_3$ , the second and third invariants of the rate-of strain tensor.

We shall trace the evolution of such an equation, paying particular attention to important contributions by Debbaut et al. in 1988.

The remainder of the presentation will illustrate how various forms of the Generalized White-Metzner model can be used to explain, amongst other things, the competing influences of normal stress differences and extensional viscosity in some complex flows of importance in process modelling.

## 1. Introduction

In rheology, the twenty five years following the Second World War were noted above all for advances in theoretical rheology, particularly constitutive modelling, and several innovative papers appeared in that period. The names of J.G. Oldroyd, R.S. Rivlin, J.L. Ericksen, A.E. Green, M. Reiner, B.D. Coleman and W. Noll in particular are associated with the most important contributions (see, for example, Tanner and Walters 1998).

It soon became apparent that the search for complete generality (as is provided, for example, by the Navier-Stokes equations for a Newtonian fluid) led to constitutive equations of prohibitive complexity, except in the case of some simple flows. In consequence, rheologists, particularly those involved in process modelling, sought simple *approximate* equations with a predictive capability. This resulted in the appearance of a plethora of constitutive equations, many of which had their faithful adherents and supporters, although it must be said that the popularity of a given simple constitutive model has often been ephemeral. This observation cannot be levelled at the so-called White-Metzner model, which appeared in 1963 and is still being used in numerical simulations for complex viscoelastic flows today. Indeed, the current authors have found the use of variants of the White-Metzner model to be extremely useful in some recent computational studies (Walters et al. 2009).

In their original paper, White and Metzner (1963) proposed a constitutive equation, which we can write in the form:

$$\sigma_{ik} = -p\delta_{ik} + T_{ik}, \quad (1)$$

$$T_{ik} + \frac{\eta}{G} T_{ik}^{\nabla} = 2\eta d_{ik}, \quad (2)$$

where  $\sigma_{ik}$  is the stress tensor,  $p$  is an arbitrary isotropic pressure (for incompressible fluids),  $\delta_{ik}$  is the Kronecker delta and the overscore triangle denotes the upper convective time derivative introduced by Oldroyd in his seminal 1950 paper (Oldroyd, 1950). As originally introduced,  $\eta$  was ‘a function of the invariants of stress matrix’ and  $G$  was ‘a constant modulus’.

We note that it is customary to write  $\lambda = \eta/G$  and to define  $\lambda$  as the relaxation time.

For a steady simple shear flow with constant shear rate  $\dot{\gamma}$ , the model defined by (1) and (2) predicts the following rheometrical functions:

$$\begin{aligned} \sigma &= \eta\dot{\gamma}, \\ N_1 &= \frac{2\sigma^2}{G}, \quad N_2 = 0, \end{aligned} \quad (3)$$

where  $\sigma$  is the shear stress and  $N_1$  and  $N_2$  are the first and second normal stress differences, respectively.

$N_2=0$  corresponds to the so-called Weissenberg hypothesis, which was very much in vogue in 1963 when White and Metzner wrote their paper. Subsequent research has shown that, for many polymeric liquids,  $N_2$  is negative and much smaller than  $N_1$  (cf. Barnes et al. 1989). So, the conclusion reached by White and Metzner that “most experimental measurements point to either the predicted equality or to a near equality of  $\tau_{22}$  and  $\tau_{33}$ ” is still valid\*.

Hence, the *zero* second normal stress difference is not taken to be a major disadvantage of the White-Metzner model. Indeed, the so-called Oldroyd-B model, which has been so extensively used in computational rheology, has the same prediction.

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\* In modern notation,  $N_2 = \tau_{22} - \tau_{33}$

In assessing the relationship between  $N_1$  and  $\sigma$  implied in (3), White and Metzner (1963) concluded that it worked reasonably well for some polymeric systems (like a high molecular weight polystyrene solution in toluene) but not so well for others (e.g. a low molecular weight polystyrene solution). Of course, for the latter, this simply suggested relaxing the constancy of  $G$  and writing

$$T_{ik} + \lambda T_{ik}^{\vee} = 2\eta d_{ik}, \quad (4)$$

with  $\lambda$  and  $\eta$  as independent functions of the invariants of the stress matrix (tensor) [see, for example, Baid and Metzner (1977), Agrawal et al. (1977)].

In their original paper, White and Metzner worked with invariants of the stress tensor, but they also suggested that invariants of the rate-of-strain tensor could be used instead. Indeed, as the model has been introduced in standard text books and employed by others in process modelling, the most common expression of the White-Metzner model involves  $\lambda$  and  $\eta$  being functions of the second invariant of the rate-of-strain tensor:

$$\mathbf{II}_d = \frac{1}{2} \text{tr}(\mathbf{d}^2) \quad (5)$$

For incompressible fluids, the first invariant is zero and the third invariant, defined by

$$\mathbf{III}_d = \det(\mathbf{d}), \quad (6)$$

is zero in two-dimensional flows, which presumably accounts for the early restriction to the second invariant of the rate-of-strain tensor. However, some have ‘kept the door open’ to a dependence on  $\mathbf{III}_3$ . For example, in their influential text, Bird et al. (1987) comment: “There are of course other ways in which invariants could be introduced into the model. There is no reason, other than preserving simplicity, to include the invariant  $\mathbf{II}_2$  of  $d_{ik}$  but not  $\mathbf{III}_3$  in the model.”

As a result of these developments and suggestions, we now write down what we can readily call the ‘Generalised White-Metzner model’:

$$T_{ik} + \lambda T_{ik}^{\vee} = 2\eta d_{ik}, \quad (7)$$

where  $\lambda$  and  $\eta$  are functions of  $\mathbf{II}_2$  and  $\mathbf{III}_3$ .

Such a model allows us to:

- (i) Choose the dependence of  $\eta$  on  $\mathbf{II}_2$  so as to match the experimental shear-viscosity data for any polymeric liquid of interest.
- (ii) Choose the dependence of  $\lambda$  on  $\mathbf{II}_2$  so as to match the first normal stress difference data for the polymeric liquid.
- (iii) Choose the dependence of  $\lambda$  and  $\eta$  on the third invariant in such a manner as to match any *extensional viscosity*  $\eta_E$  data which may be available. We shall give examples of the usefulness of this dependence on  $\mathbf{III}_3$  in later sections.
- (iv) As we have already noted,  $N_2=0$  for the model.

(i) - (iv) are some of the reasons for the continued popularity of the White-Metzner models in process modelling and similar studies, some forty-six years after the publication of the original paper! Its relative simplicity is another factor of importance.

Of course, these advantages are offset somewhat by the fact that the model has only one relaxation time, while it is well known that virtually all polymeric systems require a spectrum of relaxation times to represent their dynamic data. As a result, there must clearly be some situations where this limitation has to be taken seriously. However, there are other flow situations where the simple model (7) is likely to be more than adequate to predict real behaviour, at least in a qualitative or semi-quantitative sense.

For two specific, but very different reasons, it is often convenient to add a ‘Newtonian’ contribution  $T_{ik}^{(1)}$  to equation (7) and to write

$$T_{ik} = T_{ik}^{(1)} + T_{ik}^{(2)}, \quad (8)$$

where

$$T_{ik}^{(1)} = 2\eta_1 d_{ik}, \quad (9)$$

$$T_{ik}^{(2)} + \lambda T_{ik}^{\nabla(2)} = 2\eta_2 d_{ik}. \quad (10)$$

*Computational* rheologists have often found that the introduction of the Newtonian component can greatly assist in the numerical simulation of complex flows, and *experimental* rheologists, particularly those working with dilute solutions of high molecular weight polymers in a Newtonian solvent, have also found the modification to be useful. They invariably associate  $\eta_1$  with the solvent viscosity and  $\eta_2$  with the ‘polymer’ contribution to the total viscosity. (In the following, we shall assume that equations (8) to (10) now describe what we have called the ‘Generalized White-Metzner model’).

As an example of this stress splitting, consider the well-known Oldroyd B model, with constitutive equations given by

$$T_{ik} + \lambda_1 T_{ik}^{\nabla} = 2\eta_0 \left[ d_{ik} + \lambda_2 d_{ik}^{\nabla} \right]. \quad (11)$$

It is often convenient to write this equation in the form:

$$T_{ik}^{(1)} = 2\eta_0 \beta d_{ik}, \quad (12)$$

$$T_{ik}^{(2)} + \lambda_1 T_{ik}^{\nabla(2)} = 2\eta_0 (1 - \beta) d_{ik}, \quad (13)$$

where  $\beta = \lambda_2 / \lambda_1$ .

For the popular Boger fluids, which have been used in many fundamental experimental studies (see, for example, Boger and Walters 1993), the polymer contribution to the total viscosity is very low. This is dominated by the solvent contribution, so that  $\beta$  is usually in the range 0.9 to 0.95, or even higher.

## 2. A later development of interest

Twenty five years after the publication of the original White-Metzner paper, Debbaut, Crochet, Barnes and Walters studied a special *inelastic* version of equation (7), with constitutive equations of the form (see Debbaut et al. 1988, Debbaut and Crochet 1988):

$$T_{ik} = 2\eta(\dot{\gamma}, \dot{\epsilon}) d_{ik}. \quad (14)$$

The symbols  $\dot{\gamma}$  and  $\dot{\epsilon}$  in equation (14) now denote the following invariants of the rate-of-deformation tensor  $d_{ik}$  :

$$\dot{\gamma} = 2\sqrt{\mathbf{\Pi}_d}, \quad \dot{\epsilon} = 3\mathbf{\Pi}_d / \mathbf{\Pi}_d. \quad (15)$$

In their work, there was no reference to a Newtonian solvent contribution and they compared their numerical simulations with those for the so-called Upper Convected Maxwell (UCM) model, which can be considered either as a special case of the Oldroyd B model with  $\lambda_2 = 0$  or a special case of the original White- Metzner model (2) with constant  $\eta$ .

We note that the important rheometrical functions for the UCM model are:

$$\begin{aligned} \eta(\dot{\gamma}) &= \eta_0, \\ N_1(\dot{\gamma}) &= 2\eta_0\lambda\dot{\gamma}^2, \quad N_2(\dot{\gamma}) = 0, \\ \eta_E(\dot{\epsilon}) &= \frac{3\eta_0}{1 - \lambda\dot{\epsilon} - 2\lambda^2\dot{\epsilon}^2}. \end{aligned} \quad (16)$$

Note that, even for finite values of  $\lambda$ , infinite extensional viscosities are predicted for relatively high (finite, order unity) extensional-strain rates.

Debbaut et al. (1988) chose the  $\eta$  function in equation (14) such that the functions for  $\eta(\dot{\gamma})$  and  $\eta_E(\dot{\epsilon})$  were the same as those for the UCM model (i.e. those in equation (16)). The normal stress difference  $N_1$  was of course zero for this inelastic model. Debbaut et al. (1988) referred to the resulting inelastic model as GNM1.

By carrying out finite-element simulations for the viscoelastic UCM and inelastic GNM1 models, Debbaut et al. (1988) were able to study the distinctive influence of ‘viscoelasticity’ (as manifested through the normal stress differences) and of ‘extensional viscosity’ *per se*. They concentrated largely on pressure-driven flow through axisymmetric contractions with particular interest in the ‘resistance to flow’ as measured by the so-called Couette correction C, expressed as a function of a suitable non-dimensional flow variable such as the Deborah number  $D_e (= \lambda\dot{\gamma})$  (see, for example, Walters et al. 2009, where there are choices over the characteristic shear-rate, this being either sampled at the geometry wall or an “average” value based on the average velocity and length scale in the constriction region).

In their paper, Debbaut and Crochet (1988) also modified the UCM model and generated the UCM1 model, which possessed the same behaviour as the UCM model in steady simple shear flow, but for which the extensional viscosity  $\eta_E$  was independent of extensional strain rate  $\dot{\epsilon}$  and possessed a constant value  $3\eta_0$ . We can write the equations of state for the UCM1 model in the form:

$$T_{ik}^{(1)} = 0, \quad (17)$$

$$T_{ik}^{(2)} + \lambda_1 \overset{\nabla}{T}_{ik}^{(2)} = 2\eta(\dot{\epsilon})d_{ik}, \quad (18)$$

with

$$\eta(\dot{\epsilon}) = \eta_0(1 - \lambda_1\dot{\epsilon} - 2\lambda_1^2\dot{\epsilon}^2). \quad (19)$$

The rheometrical functions for this model are:

$$\begin{aligned} \eta(\dot{\gamma}) &= \eta_0, \\ N_1(\dot{\gamma}) &= 2\eta_0\lambda_1\dot{\gamma}^2, \quad N_2(\dot{\gamma}) = 0, \\ \eta_E &= 3\eta_0. \end{aligned} \quad (20)$$

We reproduce in Figure 1 important numerical simulations for the UCM, UCM1 and GNM1 models, which are taken from the Debbaut and Crochet (1988) paper. (This extended a similar figure in the earlier Debbaut et al. (1988) work, which limited attention to the UCM and GNM1 models).

From a comparison of the simulations for the UCM and GNM1 models, it was possible for Debbaut et al. to argue that, whereas increasing extensional viscosity levels can give rise to substantial increases in the resistance to flow through contractions, these can be hidden and indeed reversed by the influence of what we might refer to as the ‘normal stress effect’ associated with the viscoelasticity of the UCM model.

In a very recent paper, Walters et al. (2009) argue that such a conclusion is consistent with the conclusions of Binding, who in the second of two influential papers on the subject (Binding 1988, 1991) presented arguments along the same lines as those expressed above.

Referring again to Figure 1, we see that the Debbaut and Crochet (1988) simulations for the UCM and UCM1 models help to confirm the above conclusion. The simulations for the UCM model clearly lie above those for the UCM1 model. The two models have the same response in a steady shear flow, but have markedly different responses to an extensional deformation. So, the message is now clear – high extensional viscosities lead to increases in the Couette correction, but this can be damped and indeed reversed by the ‘normal stress’ effect.

We are left with one very provocative question: Why haven’t the many numerical simulations for constitutive equations like the Oldroyd B and UCM models led to the observed increases in flow resistance found experimentally, even though these models seemed to capture the essential features of rheometrical behaviour? We shall address this and related questions in the next section.

### 3. A very recent use of the Generalized White-Metzner model

We have seen in the preceding section that extensional viscosity and normal stress differences are opposing influences in determining the Couette correction in axisymmetric contraction flows. One consequence of this is that contraction flows should be used with caution as a means of estimating extensional-viscosity levels, unless that is the normal-stress-difference effect is relatively small. This is important, since ‘contraction flows’ have often been seen as providing a relatively simple experimental means of estimating extensional viscosity levels, ever since the pioneering work of Cogswell (1972) [see also James and Walters (1993)].

There is another consequence of the conclusion reached in the last section. This relates especially to those working in Computational Rheology and involves the growing interest in so-called Boger fluids, these being very dilute solutions of high molecular polymers in very viscous solvents [see, for example, Boger and Walters (1993)].

When Boger fluids have been studied in flow through axisymmetric contractions, there is universal acknowledgment that the Couette correction, or some other convenient measure of ‘resistance to flow’ such as the ‘extra pressure difference, *epd*’ [see, for example, Binding et al. (2006), Walters et al. (2009)], can become very large as a suitable variable such as the Deborah number increases [see, for example, Nigen and Walters (2002)].

There has also been a consensus that, from a computational standpoint, the Oldroyd B model is a useful ‘first approximation’ for Boger fluids. It is *relatively* simple and seems to possess the ability to simulate rheometrical data reasonably well. The problem has been that, when numerical simulations have been carried out for Oldroyd B fluids flowing through axisymmetric contractions, using a low solvent/high solute viscosity fraction ( $\beta=1/9$ ), significant *decreases* in the Couette correction with increasing Deborah number have been predicted (see, for example, Figure 2).

The initial reaction of workers in the field to such a situation was to question the accuracy of the numerical schemes being employed. However, as time has progressed and the subject of Computational Rheology has come of age, this is no longer viewed as a valid criticism and simulations of the sort shown in Figure 2 are now viewed as trustworthy.

As a result, doubt has been cast on the suitability of the choice of constitutive equation, and the present authors have recently singled out the implied dependence of the first normal stress difference  $N_1$  on shear rate  $\dot{\gamma}$  as the most likely cause of the problem so far as the Oldroyd B model is concerned (Walters et al. 2009).

From a *continuum mechanics* standpoint, the initial dependence of the first normal stress difference  $N_1$  on shear rate  $\dot{\gamma}$  has to be quadratic and there is *experimental* evidence that this quadratic dependence can persist over a reasonable range of shear rates. However, there is also rheometrical evidence available that the dependence of  $N_1$  on  $\dot{\gamma}$  ultimately becomes weaker than quadratic as the shear rate increases further. For example, from an extensive study of the rheometrical behaviour of a series of Boger fluids, Jackson et al. (1984) state: “It will be seen that over a range of shear rates,  $\sigma$  is a linear function of  $\dot{\gamma}$  and  $N_1$  is a quadratic function of  $\dot{\gamma}$ , but that there is a departure from this ‘second-order’ behaviour at the high shear rates”.

To accommodate such behaviour, the present authors (Walters et al. 2009) employed a Generalized White-Metzner model that they called the J model. This had the following constitutive equations:

$$\begin{aligned} \mathbf{T}^{(1)} &= 2\eta_0\beta\mathbf{d}, \\ \mathbf{T}^{(2)} + \lambda_1\phi_4(\dot{\gamma})\mathbf{T}^{(2)\nabla} &= 2\eta_0(1-\beta)\phi_5(\dot{\epsilon})\mathbf{d}. \end{aligned} \quad (21)$$

$$\begin{aligned} \phi_4(\dot{\gamma}) &= \left[ \frac{1}{1+J\dot{\gamma}^2} \right], \\ \phi_5(\dot{\epsilon}) &= \left[ \frac{1-\lambda_1\phi_6(\dot{\epsilon})\dot{\epsilon}-2\lambda_1^2\phi_6^2(\dot{\epsilon})\dot{\epsilon}^2}{1-\lambda_1\dot{\epsilon}-2\lambda_1^2\dot{\epsilon}^2} \right], \\ \phi_6(\dot{\epsilon}) &= \left[ \frac{1}{1+3J\dot{\epsilon}^2} \right]. \end{aligned} \quad (22)$$

The relevant rheometrical functions for the J model are:

$$\begin{aligned} \eta &= \beta\eta_0 + \eta_0(1-\beta), \\ N_1 &= \frac{2\eta_0(1-\beta)\lambda_1\dot{\gamma}^2}{1+J\dot{\gamma}^2}, \\ \eta_E &= 3\beta\eta_0 + 3(1-\beta)\eta_0 \left[ \frac{1}{1-\lambda_1\dot{\epsilon}-2\lambda_1^2\dot{\epsilon}^2} \right], \end{aligned} \quad (23)$$

where J is a positive constant. Note that the Oldroyd B model is given by  $J = 0$ . Some of the relevant rheometry is contained in Figure 3. Of course, the extensional viscosity  $\eta_E$  is independent of J.

A hybrid finite volume/element (*fe/fv*) scheme was used to study the behaviour of the J model in the contraction/expansion geometry with rounded corners shown schematically in Figure 4. The choice of geometry was driven by several factors which we do not need to go into here. Sufficient to say that we felt that results for this geometry have immediate relevance for the more conventional contraction geometry with sharp corners.

The finite volume/element numerical scheme we employed has been shown to be second-order accurate [see, for example, Wapperom and Webster (1998) and Webster et al. (2005)]. In brief, the hybrid scheme consists of a Taylor-Galerkin (predictor-corrector) finite element discretisation in conjunction with and a cell-vertex fluctuation-distribution finite volume stencil. The finite element approximation is applied to the momentum-continuity set of equations, whilst the hyperbolic constitutive equation is treated via the finite volume discretisation. The combined *fe/fv(sc)* scheme forms a time-stepping process, with a three fractional-staged *pc*-formulation per time-step. On each time-step cycle, the first stage solves a set of equations for stress-velocity update, subject to the current pressure state (and past state for incremental-*pc*) in the momentum equation. Secondly, the forward time-step pressure is updated by imposing the continuity constraint through a Poisson equation (suitably adjusted with time derivative of density for compressible flow). At a third stage, the first fractional-stage velocity field is corrected to be compliant with the updated pressure field.

Figure 5 from Walters et al. (2009) contains simulations for various values of  $J$  obtained using the above numerical techniques. The graphs tell their own story, namely that damping the quadratic dependence of  $N_1$  on  $\dot{\gamma}$  ultimately leads to positive values of the *epd*, something that is required to match *even qualitatively* the published experimental axisymmetric contraction- flow data for Boger fluids.

#### 4. Some new computational solutions

To conclude, we shall show how a comparison of numerical simulations for three constitutive models of the White-Metzner type can elucidate further the various influences on the dynamics of flow through contraction/expansion geometries. For convenience, we shall label the three models as A, B and C.

All the models have the usual structure, given by

$$\begin{aligned}\mathbf{T} &= \mathbf{T}^{(1)} + \mathbf{T}^{(2)}, \\ \mathbf{T}^{(1)} &= 2\eta_0\beta\mathbf{d} .\end{aligned}\tag{24}$$

For model A, we have Newtonian behaviour, i.e.

$$\mathbf{T}^{(2)} = 2\eta_0(1-\beta)\mathbf{d} .\tag{25}$$

In the case of model B,  $\mathbf{T}^{(2)}$  is given by

$$\mathbf{T}^{(2)} = \frac{2\eta_0(1-\beta)\mathbf{d}}{(1-\lambda_1\dot{\epsilon} - 2(\lambda_1\dot{\epsilon})^2)} .\tag{26}$$

This is essentially the Generalized Newtonian Model we have already discussed, with rheometrical functions given by

$$\begin{aligned}\eta &= \eta_0, \\ N_1 &= 0,\end{aligned}\tag{27}$$

$$\eta_E = 3\beta\eta_0 + 3(1-\beta)\eta_0 \left[ \frac{1}{1-\lambda_1\dot{\epsilon} - 2\lambda_1^2\dot{\epsilon}^2} \right],$$

Model C is a Generalized White-Metzner type model, given by

$$\begin{aligned}\mathbf{T}^{(2)} + \lambda_1 \overset{\nabla}{\mathbf{T}}^{(2)} &= 2\eta(\dot{\gamma}, \dot{\epsilon})\mathbf{d}, \\ \eta(\dot{\gamma}, \dot{\epsilon}) &= \eta_0(1-\beta)(1-\lambda_1\dot{\epsilon} - 2(\lambda_1\dot{\epsilon})^2),\end{aligned}\tag{28}$$



with rheometrical functions given by

$$\begin{aligned}\eta &= \eta_0, \\ N_1 &= 2\eta_0(1-\beta)\lambda_1\dot{\gamma}^2, \\ \eta_E &= 3\eta_0.\end{aligned}\tag{29}$$

It is clear from the various rheometrical functions that a comparison of models A and B allows us to investigate extensional-viscosity effects, while a comparison of models A and C permits us to isolate normal stress effects.

A comparison similar to that which we are proposing was contained in the early work of Debbaut and Crochet (1988) for flow through a 4:1 contraction. As we have already indicated, their work was limited to UCM-type models.

We show in Figure 6, numerical simulations for models A, B and C, and, in Figure 7, we also include simulations for the Oldroyd B model. Notice that we have included a Newtonian *reference line* in both figures, although we are aware that  $\lambda = 0$  for a Newtonian liquid and that, in that sense, a Deborah number of zero is strictly the only relevant one in that case.

The curves for models B and C give further convincing evidence of the relative effects of normal-stress differences and extensional viscosity in determining the flow resistance in the contraction/expansion geometry shown in Figure 4.

Close inspection of the curve for the Oldroyd B model in Figure 7 allows us to offer an alternative interpretation of the seeming inability of models of the UCM/Oldroyd B type to predict the increases in *epd* found experimentally for Boger fluids.

In describing these developments, we can do no better than quote from a general review of Computational Rheology, published in 1993. In referring to the schematic figure of Couette correction against Deborah number, which we have reproduced in Figure 8, Crochet and Walters (1993) observed:

“The slight drop in the Couette correction at low values of the Deborah number is difficult to measure experimentally, but most respectable numerical codes testify to its existence. The large increase in the Couette correction at high Deborah number is very easy to measure experimentally but provides significant challenges to numerical simulators as they attempt to model contraction flows for highly-elastic liquids”.

As a digression, we remark that the above is a good example of the frustration encountered in the field, namely that the flow phenomena which can be easily predicted at low values of the Deborah number, are at the same time difficult to measure experimentally. At the same time, the extravagant changes in flow characteristics, which are easily demonstrated experimentally at high values of the Deborah number, present major challenges to even the most adept numerical algorithm.

In many ways, this remains a valid observation, but, with the passage of time and improvement in computer facilities and numerical techniques, it is now possible to reach higher values of the Deborah number, and our simulations for the Oldroyd B model contained in Figure 7 are a case in point. We now see a behaviour which is in qualitative agreement with that shown schematically in Figure 8. The curve for the *epd* is clearly going to reach positive values – although we are currently unable to reach the Deborah numbers required for this to happen. However, we have been able to reach an *epd* value of 0.999792 for  $De=5.1$ ! Furthermore, some of our previously published solutions for  $\beta = 0.95$  shown in Figure 9 do exhibit the elusive positive values of *epd* (see Aguayo et al. (2008)).

So, it seems that simulations for even the original Oldroyd B model would be able to supply the increases in *C* or *epd* that we are seeking, if and when we are able to reach sufficiently high values of the Deborah number in the computational solutions. On reflection, this is entirely reasonable,

since the positive effect from ever-increasing extensional-viscosity levels must ultimately dominate the negative influence of the normal stresses. Obviously, the departure from the quadratic dependence of  $N_1$  on  $\dot{\gamma}$  found in most, if not all, Boger fluids at high shear rates will hasten this domination, as our simulations have shown.

## 5. Conclusions

In this paper, we have attempted to show how generalizations of the original White-Metzner model are still proving useful some forty six years after its introduction. In particular, we have argued that such generalizations are still helping rheologists to understand the competing influence of various rheometrical functions on important flow characteristics. We have concentrated on axisymmetric contraction and contraction/expansion flows, but we know that related work is also proceeding on some axisymmetric free surface flows (Tomé et al. 2009).

Finally, we need to reissue a warning first expressed by Debbaut et al. (1988) and Debbaut and Crochet (1988). It concerns an important limitation of the introduction of a  $III_3$  dependence into the constitutive equation. In particular, such a dependence has no influence in two-dimensional flows, since  $III_3$  is zero in such flows. So, the introduction of a dependence on both  $II_2$  and  $III_3$  in the model must be seen simply as a very useful means of investigating various rheological influences in *three*-dimensional flows, as we have attempted to illustrate in this paper.

Clearly, the above warning is irrelevant for models with a dependence only on the *second* invariant  $II_2$ , and these will continue to be useful as a means of studying complex flows in both two and three dimensions.

## Dedication

This paper is dedicated to Professor James Lindsay White on the occasion of his 70<sup>th</sup> birthday. Hopefully, the research we have described will be seen as a fitting tribute to the relevance of just one of his many research publications.

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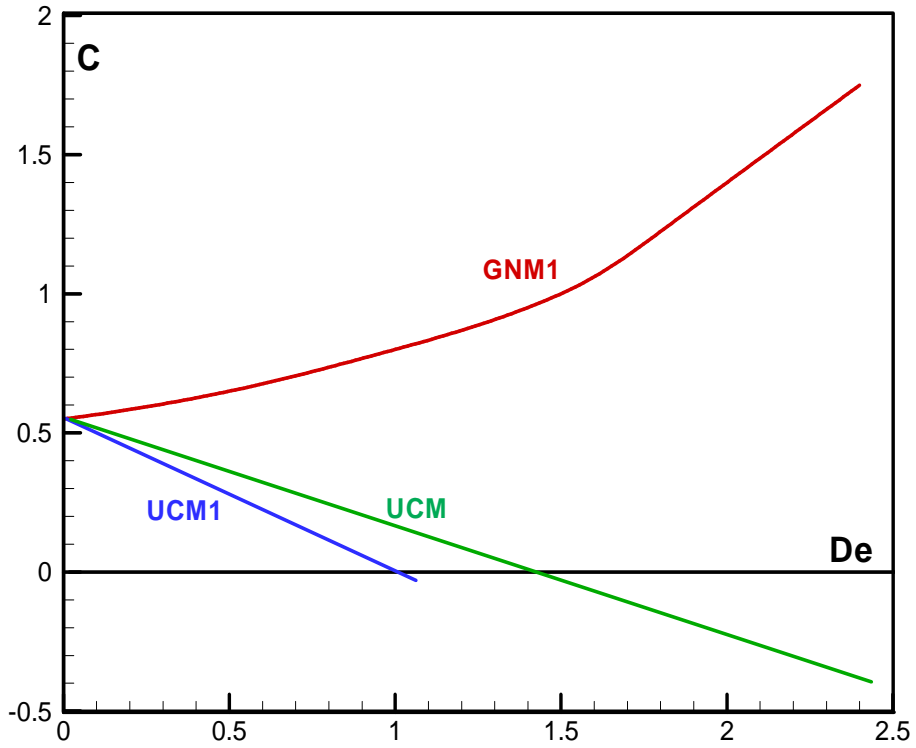


Figure 1: Couette correction vs  $De (= \lambda \dot{\gamma}_w)$ , taken from Debbaut and Crochet (1988)

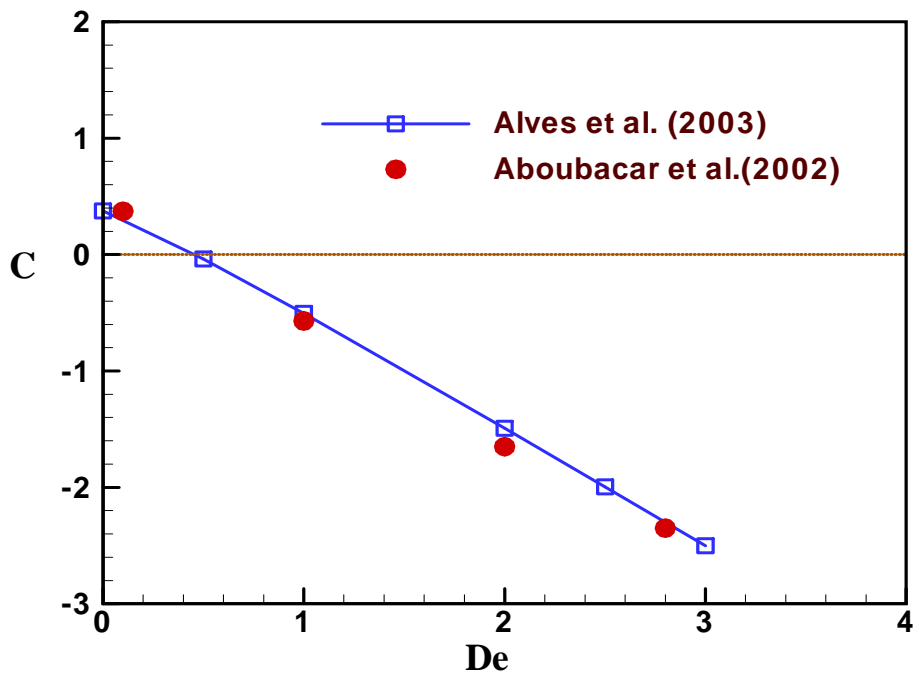


Figure 2: Couette correction (C) vs  $De (= \lambda \dot{\gamma}_{avg})$ , Oldroyd-B model,  $\beta=1/9$

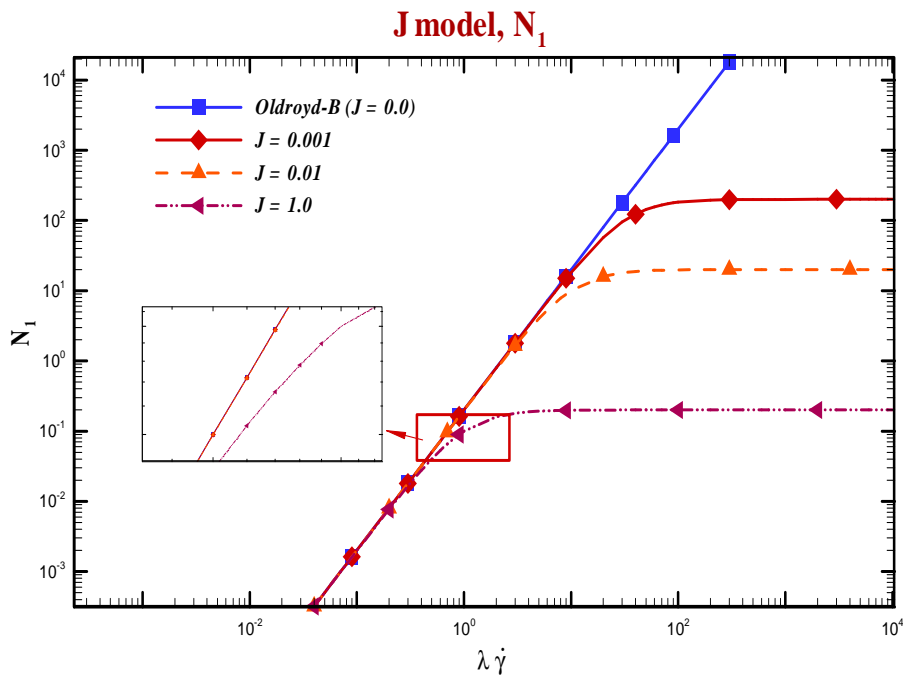


Figure 3: Representative normal stress data for the J model

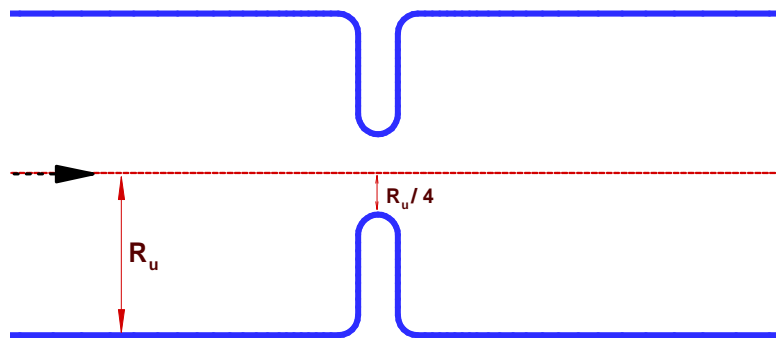


Figure 4: Schematic diagram of axisymmetric contraction/expansion geometry

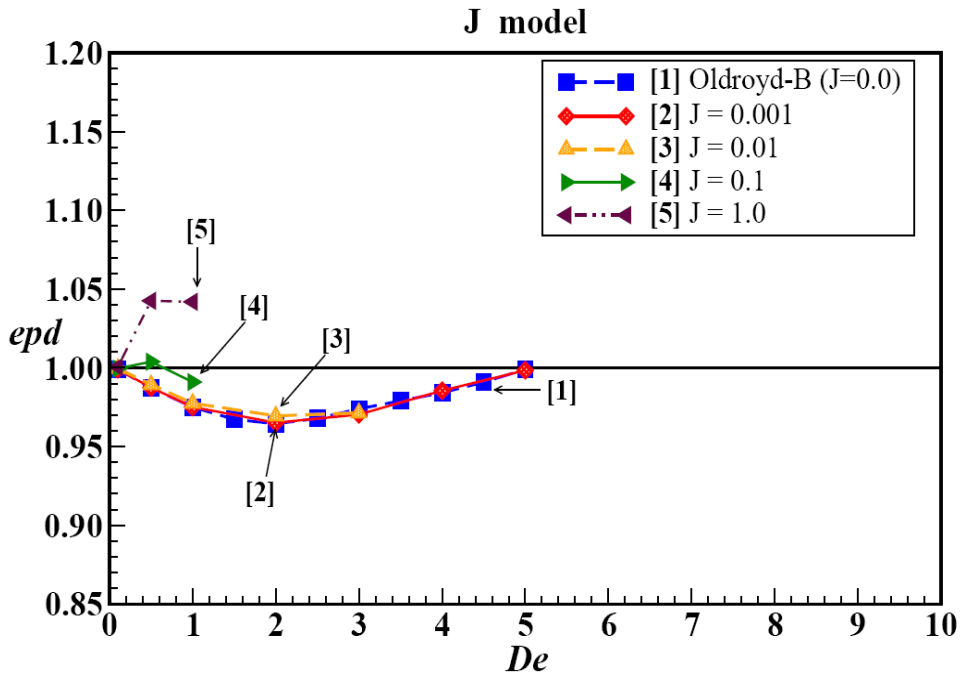


Figure 5: Normalised pressure-drop ( $epd$ ) vs  $De$  ( $=\lambda\dot{\gamma}_{avg}$ ) for the J model

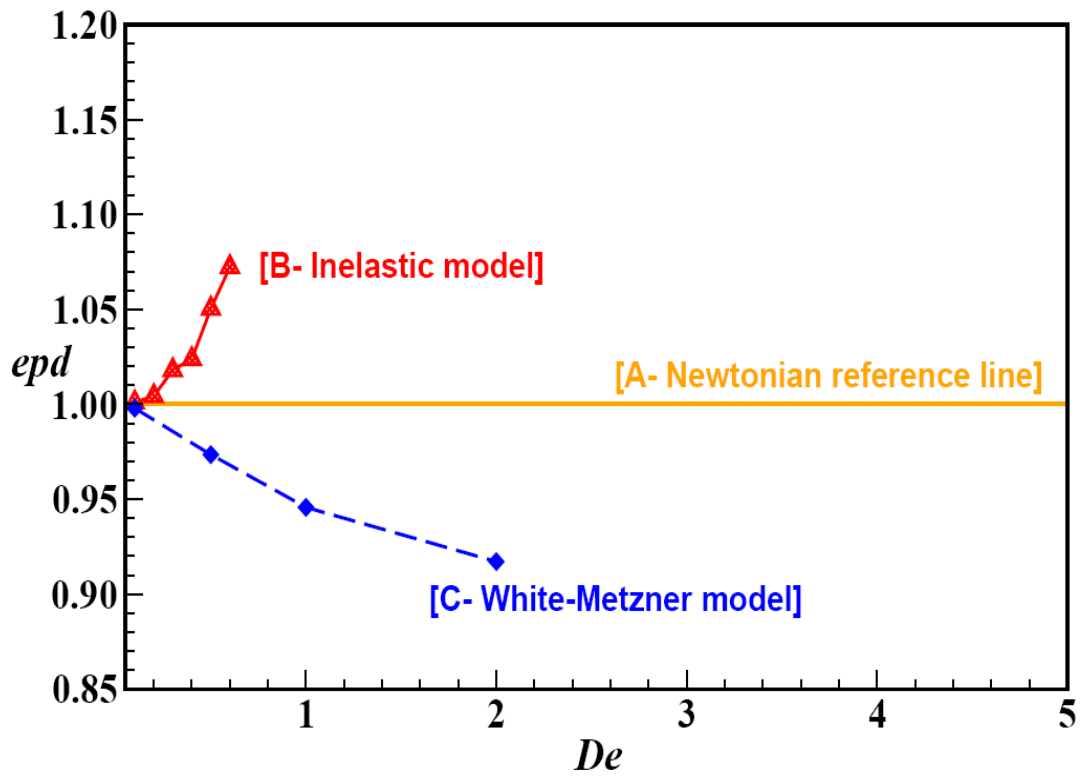


Figure 6: Normalised pressure-drop ( $epd$ ) vs  $De$  ( $=\lambda\dot{\gamma}_{avg}$ ) for A, B, and C models

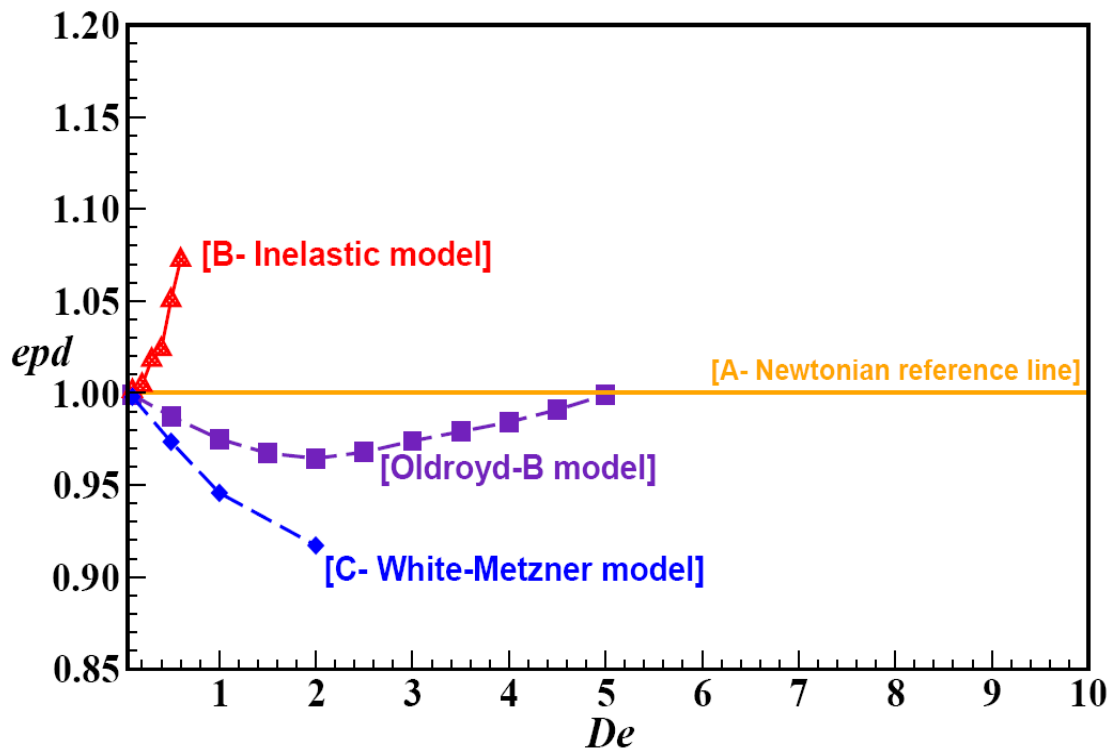


Figure 7: Normalised pressure-drop ( $epd$ ) vs  $De (= \lambda \dot{\gamma}_{avg})$  for A, B, C, and Oldroyd-B models

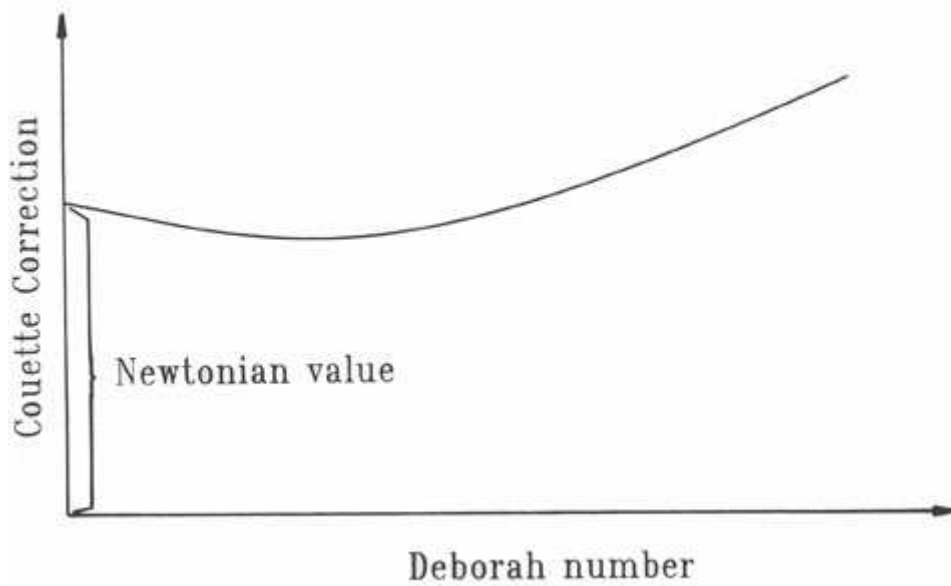


Figure 8: Couette correction vs  $De (= \lambda \dot{\gamma}_w)$ , taken from Crochet and Walters (1993)

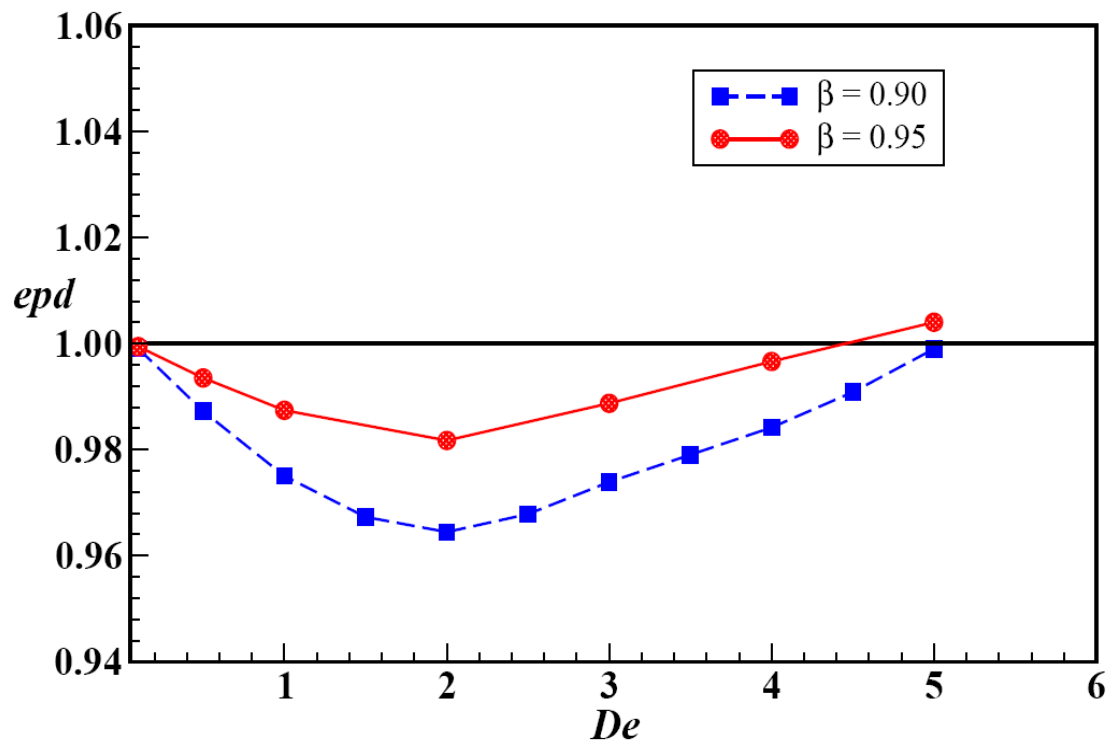


Figure 9: Normalised pressure-drop ( $epd$ ) vs  $De$  ( $=\lambda\dot{\gamma}_{avg}$ ) for the Oldroyd-B model