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COUPLING DNS WITH POLYMER MODELS FOR FLOW CONTROL

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Abstract

This paper discusses the coupling of polymer models with direct numerical simulation (DNS) toward understanding, modeling, and controlling turbulent boundary layer flows for drag reduction. Experiments have demonstrated that a dilute polymer solution injected into a turbulent flow can result in up to 80% drag reduction. Pipe, channel, and flat plate experiments are summarized to highlight similarities and differences in the flows associated with the polymer-induced drag reduction process. Constitutive and kinetic approaches to polymer modeling are then discussed with their respective couplings to DNS.

1. Introduction

Discussions concerning our physical understanding of the fluid dynamics phenomena we call turbulence are extremely controversial mainly because of our lack of irrefutable evidence to explain the flow. However, a couple of schools of thought have formed to explain the flow. One explanation follows a statistical evolution of flow based on averaged quantities and a that of energy cascades.[1] The second view describes turbulence within a deterministic coherent structures process that can be described by dynamical systems or flow stability analysis.[2] More recently, a workshop was held on the subject to further discuss the essence of turbulence.[3] These two schools still exist but with added insight brought about by research on the topic. Now, one school can be described as a *parent-offspring* vortex mechanism whereby the parent (initial) vortex interacts with the wall to induce secondary (offspring) vortices. The second mechanism involves a *flow instability* cyclic process, whereby streamwise vortices collect low speed streaks that cause inviscidly unstable velocity profiles. These views on turbulence serve as an introduction to this paper which focuses on the complex phenomena of non-Newtonian turbulent flows and flow control.

Specifically, our non-Newtonian flows are viscoelastic fluids.[4] The study of these flows involve both material science and fluid mechanics because it requires an understanding of rheological and mechanical properties and complex fluid flows. The rheological properties of the material determine the manner of deformation (or flow) subject to forces; the imposed deformation leads to internal stresses in the material. Typically this material flow, albeit non-

Newtonian, can be considered in many cases as a continuum flow. Such material flows may include toothpaste, paint, blood, oil, cookie dough, soap solutions, and cosmetic flows. Here, for brevity, we will "glaze over" all details associated with particular materials and their properties and resulting influence of these properties on the resulting fluid dynamics. Here, our focus is on non-Newtonian turbulent polymer/water solutions from the fluid mechanics point of view for viscous drag reduction.

This paper is not intended to be a review or summary of the many important papers that have used polymer solutions for skin friction drag reduction. The reader can refer to a bibliography for some 4900 publications on the topic[5] and the excellent texts by Bird et al.[6,7] Instead, only some of the key physical phenomena found from the various experiments will be emphasized for benefit of the modeling activities. All researchers currently agree that the mechanism for drag reduction by polymers remains illusive.

1.1 Polymer Pipe Experiments:

Although many studies of particles and polymers in fluids were documented well before the observations of Toms[8] in 1948, skin friction reductions associated with dilute polymer solutions in turbulent pipe flow are typically referred to as Toms phenomena. By looking at the number of publications since Toms observation, it is clear that much progress has been made toward the understanding of the phenomena. There are some commonly observed features in such flows that are highlighted in this introduction.

For pipe flows, a significant advancement was made by Virk,[9,10] whereby experimental data was analyzed to arrive at a universal asymptote (that is applicable for all polymer solutions). This asymptote reflects the maximum drag reduction possible for pipe flows. Three connected regions across the pipe were identified. The "viscous" zone near the wall was postulated to be essentially the same for both Newtonian and non-Newtonian flows. Near the center of the pipe, the "Newtonian turbulent" zone is shifted upward with increased drag reduction. Finally, the "interactive" (or buffer) zone connects the two other zones and is extended upward with increased drag reduction. Maximum drag reduction occurs when the interactive zone extends to the pipe axis. Concerning turbulence statistics, laser Doppler velocimetry measurements (rms) show that the axial velocity component increased, the radial velocity component decreased, and the Reynolds stress decreased, while the peak profile moved away from the wall.[11] The movement of the peak corresponds to an increase in the size of the buffer region.

Finally, pipe drag reduction can take two forms.[12] This discussion so far has focused on homogeneous drag reduction. The second form is termed heterogeneous and involves drag reduction associated with injecting polymer solutions into the core of the pipe. Little mixing is observed and the drag reduction is not associated with polymers influencing the wall region.

1.2 Polymer Channel Flow Experiments:

Particle image velocimetry measurements showed a 40% drag reduction in channel flow[13] using only 3.5 wppm (weight-part-per-million) solution and suggested that the streamwise vorticies are enlarged as a result of the addition of polymers. The streamwise fluctuation levels increased for low-drag reductions and decreased for high-drag reduction test cases. The increased drag reduction was achieved by increasing the polymer concentration.[14] Other experiments[15] showed increased streamwise velocity fluctuations and decreased Reynolds stress levels. With drag reduction, the bursting rate per unit area decreased and a total absence of small scale structure was observed during a burst event.[16] Measurements[17] indicate that the near-wall streaks can double, triple and even quadruple in spanwise extent and therefore the spanwise scaling indicates an increase in the size of the large-scale structures. Drag reduction phenomena for the channel is very much like the pipe flow problem. Experiments in the channel showing variation in concentration recorded a 69% drag reduction and velocity profiles that closely approached Virk's ultimate asymptote.[14]

1.3 Polymer Turbulent Flat Plate Experiments:

The flat plate boundary layer flow has many characteristics comparable to the pipe and channel flows. These include an increase in the streamwise rms velocity, decrease in the wall-normal rms velocity, and decrease in the Reynolds stress for polymer solutions.[18-20] However, the flat plate flow is an external flow so diffusion plays a significant role in the degradation of polymer-induced drag reduction. The drag reduction is decreased with distance downstream because of the movement of polymers away from the wall. The polymer concentration was shown to exponentially decrease with downstream distance.[21] For the boundary layer, initial, intermediate, transition and final zones can be outlined to classify the polymer-induced effects in the flow.[22] The initial zone is near the injector and is a region of large concentration gradients. Next, the intermediate zone has self-similar concentration profiles and lasts approximately 18 boundary-layer thicknesses downstream of the initial zone. The transition zone has non-similar concentration profiles and an increasing diffusion layer. Beginning about 60 boundary layer thicknesses downstream of the initial zone, the final zone has self-similar concentration profiles but the amount of drag reduction is continually decreasing with downstream distance. So although there are similarities between the pipe, channel and boundary layer, the boundary layer has an increased complexity because of diffusion.

1.4 Benefits:

Experimental results using polymers have demonstrated a drag reduction of 40-70% in turbulent pipe flows[23,24] and 50-70% for flows on flat plates.[18,25] The success in pipe flows has resulted in over 80 projects using polymers for oil pipe lines; the Trans Alaskan Pipeline uses polymers to reduce the required number of pumping stations from 12 to 10 to move oil over 1200 km.[23] For external flow applications, the projected benefits of drag reduction are enormous for military and commercial ships. For example, let us estimate the benefits to the M/V AIVIK, which operates around the world. The ship is over 109 m long, weighs some 7000 metric tons fully loaded, and has a top speed of 13 kts. With a 50% reduction in the drag, the speed of the vehicle increases to approximately 17-18 kts. A trip of 13,000 miles (say New York to South Africa) would take 26 days instead of 35 days, which saves 9 days (25%) in transport time. In addition there would be a fuel savings of 20-25%, somewhat offset by the polymer system.

1.5 Mechanisms for Drag Reduction:

As two schools exist to explain the physics of turbulent flows, two leading postulations exist for drag reduction caused by dilute polymer solutions. The first maintains that unraveling and elongation of the polymer chain (extension) is the key process affecting the turbulence and results in a drag reduction. The second claims that elasticity is the mechanism, whereby the stress of a viscoelastic fluid generally is not in phase with the strain rate. As with turbulence alone, no conclusive evidence exists (as yet) to support either postulation.

2. DNS

Some good analytical correlations with the experimental data have been developed for polymer solutions. However, for brevity and to remain in alignment with the focus of this conference, we proceed directly to the link between polymer models and direct numerical simulations (DNS).

The Navier-Stokes equations can be implemented in numerous forms.[26] Here, the velocity-pressure equations in full form are simply listed, including the affect of polymer models. The Navier-Stokes equations are given as

$$\frac{\partial u_i}{\partial x_i} = 0, \quad \rho\frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i}(\tau_{ij}) + F \qquad (1)$$

Any equation that assigns values to τ_{ij} is a *constitutive* equation; F may be a polymer-induced body force. The constitutive equation can be decomposed into Newtonian and non-Newtonian (polymer) contributions, such that $\tau_{ij} = \tau_{ij}^{N} + \tau_{ij}^{P}$. There are many publications documenting the DNS solutions and therefore we proceed directly into the polymer modeling activity.

3. Polymer Models

Implementation of constitutive models with DNS has a complexity similar to the coupling of the DNS with optimal control theory.[27] DNS and optimal control theory involves Navier-Stokes equations and an equal number of adjoint Navier-Stokes equations combined with a simple optimality condition equation. This leads to a system of nine equations that can be solved for a limited number of applications because of the extreme computational cost. The cost may increase by a factor of 2-10 compared with the DNS cost alone. The DNS and polymer models have similar issues associated with increased complexity and computational cost combined with some model parameters that may be extremely difficult to correlate with experiments. In this section, Eulerian and Lagrangian approaches to modeling polymer flows are highlighted. Some of our preliminary results are also discussed where the primary focus here is the assessment of the cost of the models. Our ultimate goal is coupling the models with DNS to study the turbulent flat plate boundary layer drag reduction phenomena.

3.1 <u>Constitutive Models:</u>

Constitutive models for polymer/water solutions have been formulated using stress tensor transport equations to predict the impact of polymers on turbulence within an Eulerian construction (similar to the Navier-Stokes framework). For non-Newtonian fluid flows, the simplest relationship between the shear stress and strain rate is given by a power-law model, $\tau_{ij}^{P} = \kappa \dot{\gamma}_{ij}^{n}$. For a Newtonian fluid, $n=1$; for a pseudoplastic (e.g., polymer solution), $n<1$; and for a dilatant (e.g., corn starch and water solution), $n>1$. For the Newtonian flow, the slope of the curve simply becomes the viscosity $\kappa = \mu$. The impact of the nonlinear (non-Newtonian behavior) for a polymer solution is elevated viscosity near the wall and shear thinning.

Polymeric fluids are often referred to as viscoelastic fluids because such fluids are associated with nonlinear effects and time-dependent properties. Such fluids typically have memory effects. Hence, continuum polymeric fluid models should accommodate terms which retain past states. However, approaches which model dilute solutions of polymers in water may not require the retention of all terms (memory) of past states. In our research a host of models ranging from low to high fidelity, linear to nonlinear, and pseudo-steady to those retaining past states (memory) of the solution are being compared for use in simple steady to fully turbulent flows.

A breadth of models have been used to describe the polymer flows, primarily associated with viscoelastic steady or simple oscillatory flows which have numerous industrial applications.[28] The general classes of these models can be summarized as generalized Newtonian, linear viscoelastic, and kinetic.[6] Generalized Newtonian constitutive models are low-fidelity models that simply modify the shear stress in a nonlinear manner. These are valid for steady shear flows only, but have often been used for many different steady and unsteady flows. Slightly higher in fidelity, the linear viscoelastic models incorporate some measure of elastic effects on the flow. This is achieved by introducing a relaxation time t_1. The Maxwell model is probably the most famous of these constitutive equations. The model states that the stress at time t is related to the rate of strain at time t and all prior times, with a decay of the influence of all other past times. These models cannot describe the shear-rate dependence of viscosity, nonlinear normal stress phenomena, nor large-displacement small-strain phenomena. The models neglect past kinetic events. However, such models can give shear-rate dependent viscosity.

The Oldroyd 8-constant model[29] for the constitutive equation can be implemented to represent many models. The full form is

$$\begin{aligned}&\tau + \lambda_1 \tau_{(1)} + \frac{\lambda_3}{2}(\dot{\gamma}\cdot\tau + \tau\cdot\dot{\gamma}) + \frac{\lambda_5}{2} tr(\tau)\dot{\gamma} + \frac{\lambda_6}{2}(\tau : \dot{\gamma})\delta \\ &= -\eta_0\left(\dot{\gamma} + \lambda_2 \gamma_{(2)} + \lambda_4\{\dot{\gamma}\cdot\dot{\gamma}\} + \frac{\lambda_7}{2}\{\dot{\gamma} : \dot{\gamma}\}\delta\right)\end{aligned} \tag{4}$$

where λ_{1-7} are time constants and η_0 is the zero-shear-rate viscosity. For $\lambda_{1-7} = 0$, the Newtonian model is recovered; for $\lambda_{3-7} = 0$, the convected Jeffreys model (or Oldroyd-B) is obtained; for $\lambda_{2-7} = 0$, the convected Maxwell model is obtained. So, many different models may be explored through this one general 8-constant model.

The turbulent flow of interest is time-dependent, extremely dynamic, and non-homogeneous. The extrapolation and enhancements of the various non-Newtonian models to predict and understand the drag reduction associated with polymer solutions is our goal. Previous work with the power-law class of models (a viscous anisotropic model) relying on elongated polymers aligned always parallel to the velocity field, showed drag reduction and turbulent statistics that were in qualitative agreement with the pipe flow experiments.[11] For a Maxwell class of models, a viscoelastic anisotropic model showed drag reduction and turbulent statistics in qualitative agreement with experiments for pipe flow, except the peak of the rms velocities moved toward the wall; the simpler viscous anisotropic model was in better agreement with experiments.[11] The comparison between the various models and complex issues associated with numerical stability and boundary/initial conditions will be left to a future paper; however, in section 3.3, a brief discussion is given concerning the cost of these models linked with DNS.

3.2 Kinetic Models:

For polymer-induced turbulent drag reduction, the kinetic models track the macromolecule polymer dynamics through a Lagrangian framework coupled with the Eulerian DNS. Because this is a coupled problem, the flow transports and stretches/deforms the polymers, and the polymers in turn affect the viscosity, shear, and turbulence production phenomena. Because the polymers can have different scales than the turbulence, multiple time and spatial scales exist for the coupled polymer-turbulent flow. Typically the spatial scales for polymers are orders of magnitude smaller than the turbulent flow scales. Although the time-evolution process for polymer motion may be much smaller than turbulence, there appears to be an overlap region that is important to realize drag reduction.

An important parameter in characterizing macromolecule-type drag reduction is related to the polymer relaxation time t_l. Experiments[30] using laser-light scattering suggest that the polymers stretch out in the turbulent flow when sufficient stress (due to high strain rate) is encountered in the flow. A significant drag reduction is observed when this stretching process occurs. It has been suggested that a polymer-eddy interaction occurs when the relaxation time of the polymer is comparable to the small-scale eddy turnover time. The relaxation time is related to the molecular weight of the polymer. For low concentrations this interaction of polymer and turbulence leads to drag reduction and for high concentrations drag reduction primarily results from the viscous effects of polymer solutions. However, only small concentrations are required for drag reduction and, to minimize system penalties, small concentrations are clearly the goal. For non-Newtonian fluids (viscoelastic), the Deborah number[31,32] (De) becomes important and is defined as the ratio of elastic to viscous time scales. The Deborah number is defined as $De = t_1/T = \dot{\varepsilon}t_1$ where t_1 is the largest time constant for the slowest molecular motion (relaxation time), T is the time constant of the flow system, or solution, and $\dot{\varepsilon}$ is the elongation rate. For $De \to 0$, the flow system behaves as a Newtonian fluid, and for $De \to \infty$ the fluid behaves like a Hookean-elastic solid. Typically for polymer solutions, $t_1 \approx 10^{-3}s$ for dilute solutions and $t_1 \approx 10^{3}s$ for concentrated solutions. For the turbulent boundary layer, the characteristic time scale of the flow is approximately $\mathrm{T} = \delta/U_\infty$ (boundary layer thickness/free-stream velocity). Rheological measurements have clearly shown that the elongation rate $\dot{\varepsilon}$ is a very useful parameter in examining the viscoelastic behavior of polymer solutions. Essentially, when $\dot{\varepsilon}$ increases and reaches a critical value $\dot{\varepsilon}_c$, the properties of the polymer dramatically change in that the polymers experience a "fully-stretched chain state." Experiments with simple flows suggest this to occur near $De \approx 1$. The dependence of this critical elongation rate has been shown to relate to the monomer chain length N and molecular weight M as

$\dot{\varepsilon}_c \propto N^a \propto M^a$. For good solvents, a=-1.8 has been suggested and a=-2.3 has been found using Monte Carlo simulation techniques.

As the strain rate reaches a second critical point, the stretched out chain ruptures. This rupture process has been shown to be a function of molecular weight in steady shear flow[33] (and will most likely be related to the specific polymer as well). Computationally, a rupture analysis may be investigated by either varying the maximum distance of the beads prior to a “rupture” and/or analyzing the local strain rate versus molecular weight versus peak forces for the polymers.
A widely used model in the Lagrangian framework is referred to as the “dumbbell model.” The kinetic force balance equations are in general represented by multiple beads (mass foci) connected by springs (resistive force). A promising yet simple bead-spring model is the FENE (finite-extensible nonlinear elastic) model (or variation thereof). The transport equation for this model operates in a Lagrangian reference frame, and hydrodynamic force corrections are added. So, all macromolecules must be tracked in the simulation.

Here, we use the rigid-mass and elastic dumbbell models to assess the relative importance of the elongation/stretching process for the polymer macromolecules. These models are sufficiently complex to capture the decrease in viscosity with strain rate, which will be important for the turbulent boundary layer flow. Although the polymer may be modeled with a number of beads, a two-bead dumbbell model would have masses (m_1, m_2) with radii (a_1, a_2) located by position vectors (r_1, r_2) relative to the origin of the laboratory reference frame. The dynamic state of a dumbbell can be instantaneously specified with the position vectors and the velocities of the bead.

Instead of developing constitutive models, the Lagrangian approach tracks individual macromolecule polymers, assessing the two-way coupling effects of flow on polymer and polymer on flow. An equation of motion for each bead of the macromolecule can be given as

$$\begin{aligned} &\frac{\partial r}{\partial t} = u_p, \qquad m\frac{\partial u_p}{\partial t} = -\zeta(u_p - u) - k_b T\frac{\partial}{\partial r}(\ln\Psi) + F \\ &\frac{\partial \Psi}{\partial t} = -(R\cdot\nabla u)\cdot\frac{\partial \Psi}{\partial R} + \frac{2k_bT}{\zeta}\frac{\partial}{\partial R}\cdot\frac{\partial \Psi}{\partial R} + \frac{2}{\zeta}\frac{\partial}{\partial R}\cdot F\Psi \end{aligned} \tag{5}$$

where k_b is the Boltzman constant, T is the temperature, R is the configuration vector between two adjacent beads, and ζ is the friction coefficient for a single bead. Following Stoke's law, this becomes $\zeta = 6\pi\mu a$. The scalar distribution function ψ is a sum of contributions from the hydrodynamic force, the Brownian motion force, the force through the internal resistance, and force due to collisions.[34] Initially, we will take the internal behavior of the macromolecule as governed by the finite extendable nonlinear elastic (FENE) dumbbell model.[7] The force law relationship for the flexible macromolecule is

$$F = \frac{KR}{1-(R/R_0)^2} \tag{6}$$

where R_o is the maximum distance the beads can displace (or elongate), and $K=k_bT/N^{6/5}a^2$ is the spring constant as a function of temperature T and number of monomers N. Alternate internal force law relationships will be investigated in a future paper.

After solving equations (5-6), the non-Newtonian stress contribution can be determined from

$$\tau^P = -n\langle RF\rangle + nk_bT\delta \quad \text{with} \quad \langle RF\rangle = \int_V RF\Psi \tag{7}$$

where n is the number density of dumbbells and $\langle RF\rangle$ is the volume-average value of the dynamical quantity RF. The terms on the right are from tension in the connectors and bead motion, respectively. The forces acting on the macromolecule act within the distribution function equation as well.

Using the FENE construct, a constitutive model has been developed and evaluated for turbulent channel flow.[35,36] The model qualitatively agreed with experiments, indicating that extensional viscosity plays a role in drag reduction. Key results of the model included an increase in the streamwise rms velocity and decrease in the wall-normal and spanwise rms velocities, in addition to a decrease in the streamwise vorticity fluctuations. The model also predicted an increase in the size of the mean streamwise vortex structure consistent with the experiments. These non-Newtonian computations within the constitutive approach can require 15 times the computational cost of turbulent simulations alone.[35] In a different study using a Lagrangian-particle tracking approach, turbulent channel flow simulation results with the FENE model indicated that the polymer chain unravels to about 87% of the fully extended length and is oriented at about 7° to the flow direction.[13] This later result will be useful in the validation of our investigations.

3.3 Costs Polymer Model:

In this section, preliminary cost estimates are provided for both the constitutive model and macromolecule. For this paper, extra stress tensor transport equations are implemented and cost estimates are provided for the Giesekus, FENE-P, and convective Jeffreys models. Table 1 shows the cost of the non-Newtonian models normalized by the DNS cost for a 32x32x32 grid on a 500MHz Beowolf single processor. Because the non-Newtonian models add six additional equations, the cost increases to slightly more than a factor of two over the DNS computational cost. The difference in the cost of various models results from any simplifications that may arise in equation (4).

Table 1. Normalized computational cost of constitutive equations (courtesy of Nathan Grube).

non-Newtonian model	**Cost**
DNS/Giesekus	2.28
DNS/FENE-P	2.35
DNS/Convected Jeffreys	3.23

For the Lagrangian evolution equations (5-6), Table 2 displays the time required for tracking the macromolecule evolution in a stationary fluid using a 333 MHz processor. For a given number of monomers, there is a one-to-one cost increase with the increase in the number of polymers after 100 polymers are modeled. These initial results for a simplified force model (internal forces and sinusoidal imposed force) yields some insights into the cost with number of polymers and monomers compared with the fully coupled system. The diffusion equation implementation has increased the cost of computation three-fold over model problem cost (Table 2). Note, that no optimization of the code has been attempted at this point.

The true cost of the macromolecule model coupled with the DNS approach for the turbulent boundary layer flow problem will depend on the molecular weight, number of monomers in the model, the flow Reynolds number, concentration of polymers, etc. We can get a preliminary estimate of the polymer requirements for this problem by selecting an initial test case. Choose a Reynolds number based on displacement thickness (δ^*) of 1000. The domain has $100\delta^*$, $20\delta^*$, and $20\delta^*$ for the streamwise, wall-normal, and spanwise directions. Assuming the polymer has a molecular weight of 1 million, a density of 2 g/cm^3, a concentration of 1%, the simulation must track approximately 1 million polymers. Although more complete information on the polymer properties is needed to refine this estimate, this simple analysis combined with the computational cost estimate below indicates that it should be feasible to solve this complex Eulerian/Lagrangian system.

Table 2: Computation time for polymer systems (courtesy of Scott Austin).

# Polymer Masses	# Polymers	Computation Time (sec)
2	10^0	0.371E-03
	10^1	0.117E-02
	10^2	0.998E-02
	10^3	0.953E-01
	10^4	0.953E+00
	10^5	0.956E+01
3	10^0	0.398E-03
	10^1	0.155E-02
	10^2	0.134E-01
	10^3	0.133E+00
	10^4	0.135E+01
	10^5	0.174E+02
5	10^0	0.430E-03
	10^1	0.221E-02
	10^2	0.206E-01
	10^3	0.199E+00
	10^4	0.204E+01
	10^5	0.203E+02

4. Conclusions

This paper has summarized the experimental observations associated polymer-induced drag reduction in turbulent pipe, channel, and flat plate flows. With drag reduction, the 'interactive" (or buffer) region increases in extent and moves away from the wall, the streamwise rms velocity increases, the wall-normal (radial) rms velocity decreases and the Reynolds stress decreases. Furthermore, the large-scale structures increase in size.

The discussion has focused on coupling DNS and polymer models toward understanding, modeling, and controlling turbulent boundary layer flows for drag reduction. Preliminary estimates suggest that a factor of 2 or more time is required to compute the non-Newtonian problem.

Acknowledgement

This material is based upon work supported by the DARPA under Contract No. MDA972-01-C-001, Dr. Parney Albright, Program Manager. This research is being conducted jointly with Dr. Thomas S. Chyczewski, Mr. Nathan Grube, and Mr. Scott Austin at PSU/ARL.

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