Numerical Simulation of Fibre-Induced Drag Reduction in Turbulent Channel Flow
Numerical Simulation of Fibre-Induced Drag Reduction in Turbulent Channel Flow

PROEFSCHRIFT

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Preface

This thesis collects four years of research conducted at the Laboratory for Aero- and HydroDynamics at the Delft University of Technology. In these years I was privileged to meet many interesting people. Here I would like to thank those who in one way or another contributed in the preparation of this work.

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I close this list with the most important person in my life. Despite a distance you are with me in all I do. Therefore I dedicate this work to you Shivra.
Preface
Summary

Numerical Simulation of Fibre-Induced Drag Reduction in Turbulent Channel Flow
- J. J. J. Gillissen

Polymer-induced drag reduction is the phenomenon where the friction factor of a turbulent flow is reduced by the addition of small amounts of high-molecular-weight, linear polymers. Drag reduction has been studied extensively over the past 60 years but still there is no satisfactory theory to describe the phenomenon. In the last decade Direct Numerical Simulations (DNS) of turbulent drag reduction have become available. In DNS there is a perfect control of polymer properties such as concentration, molecular weight and flexibility. Moreover quantities like polymer orientation and extension can be monitored, which is extremely complicated to achieve experimentally.

Despite these advantages there are large drawbacks in using numerical tools to study drag reduction. Due to computer limitations, polymer dynamics in drag reducing solutions cannot be simulated after first principles, but require ad-hoc modeling assumptions. Present drag reduction simulations are based on highly idealized models, where flexible chains are modeled as two-point particles and interactions between different chains are neglected. Obviously the outcome of the simulations is questionable and can only be verified by a comparison to experimental data. To date quantitative comparisons between simulation and experiment have not been reported. In this thesis we aim at reducing the gap between simulation and laboratory by examining a special class of polymers which have a negligible level of flexibility, referred to as fibres. Compared to flexible polymers the modeling of fibres is less complex, allowing a better comparison to experimental data.

We use DNS to study drag reduction by fibres in turbulent channel flow. To account for the effect of the fibres on the fluid mechanics, the Navier-Stokes equations are supplemented by the divergence of the fibres stress tensor. The fibre stress is computed by the well-known constitutive equations, which are valid for solutions of non-interacting, rigid rods. Under drag reduction conditions the fibre stress cannot be computed directly using present computational resources. Similar as in Large Eddy Simulation this problem is dealt with by applying a filter to the governing equations. The filtering leads to unknown terms, which are modeled using closure approximations. We examine the performance of several closure schemes by comparing simulations of the filtered and the unfiltered equations. It is concluded that the closures do not introduce significant errors.

Instead of the closures, there are other, more fundamental shortcomings of the numerical model, such as neglecting interactions between the polymers. To determine the implication of this illegitimate assumption, simulations are compared to experimental data provided by the
literature. The comparison involves the friction factor dependence on Reynolds number and fibre concentration, as well as the profiles of the mean flow, the Reynolds stress and the turbulent kinetic energy. We see that there is good agreement in all observable trends at relatively small levels of drag reduction. This suggests that the constitutive equations describing solutions of non-interacting rods correctly reproduce the small drag reduction regime. At large drag reduction the simulations disagree with the experimental data. These discrepancies suggest that interactions between polymers, which are neglected in the numerical model, play a crucial part in large drag reduction.

In addition to model validation, we have studied the drag reduction mechanism. A simplified model for fibre stress is introduced as a viscous stress. The so-called fibre viscosity is defined in such a way that the resulting Reynolds averaged dissipation of the fluid kinetic energy matches the dissipation predicted by the full constitutive equations. Streamwise fibre orientation in the viscous sublayer results in negligible fibre viscosity in this region. Further away from the wall, fibres tend to align in directions corresponding to positive rates of strain. As an effect the fibre viscosity increases linearly with wall-distance. The fibre viscosity model predicts the correct amount of drag reduction and changes into turbulence statistics. This implies that fibre-induced drag reduction can be rationalized by an additional viscosity. The fact that the fibre viscosity roughly scales as $\phi r^2$, where $\phi$ is the polymer volume fraction and $r$ is the polymer length to diameter (aspect) ratio, explains that high aspect ratio particles can induce significant effects at very small volume fractions.

Finally we tackled the role of polymer flexibility on drag reduction. Simulations of constitutive equations describing solutions of flexible and rigid polymers predict almost the same amount of drag reduction when both are compared at equal $\phi r^2$, where $r$ for flexible polymers is based on the Reynolds average at the wall. These results indicate that viscosity is the key to understand drag reduction while elasticity plays a passive role.
Samenvatting

Numerieke Simulatie van Fiber-Geïnduceerde Weerstand-Vermindering in Turbulente Kanaal Stroming- J. J. J. Gillissen

Polymer-geïnduceerde weerstand-verminderen, een fenomeen waarbij de wrijvingscoëfficiënt van een turbulent stroming afneemt, middels het toedienen van kleine hoeveelheden, lineaire polymeren met een hoog moleculair gewicht. In de afgelopen 60 jaar is weerstandverminderen uitgebreid bestudeerd, maar een bevredigende theorie om het fenomeen te verklaaren is er niet. Sinds één decennium is het mogelijk om turbulente weerstand-verminderende te bestuderen met behulp van Directe Numerieke Simulatie (DNS). In een dergelijke, numerieke studie heeft men de volledige controle over de polymer-eigenschappen, zoals concentratie, moleculair gewicht en flexibiliteit. Tevens kunnen zaken als polymer-orienteering en polymeruitrekking bekeken worden, iets wat zeer gecompliceerd is om experimenteel te bewerkstelligen.

Naast deze voordelen zijn er grote nadelen verbonden aan het gebruik van numeriek gereedschap in de studie naar weerstand-verminderen. Met de huidige computer capaciteit is het onmogelijk om alle fysica in een weerstand-verminderende stromingen te simuleren.

In het hedendaagse, numerieke onderzoek naar weerstand-verminderen wordt gebruik gemaakt van zeer geidealiseerde modellen, waarbij flexibele ketens worden gereduceerd tot twee-punts deeltjes en waarbij de wisselwerking tussen de verschillende ketens wordt verwaarloosd. Hierdoor is de betrouwbaarheid van de resultaten onzeker en deze moeten geverifieerd worden door ze te vergelijken met experimenten. Tot heden waren er nog geen kwantitatieve vergelijkingen gerapporteerd in de literatuur. In dit proefschrift proberen we dit gat te dichten door naar polymeren met weinig flexibiliteit, welke we gemakshalve fibbers noemen. Het modelleren van fibbers is eenvoudiger dan voor flexibele polymeren. Dit maakt een betere vergelijking met experimenten mogelijk.

We gebruiken DNS om weerstand-verminderen door fibers te bestuderen in turbulente kanaal stroming. Om het effect van de fibers op de stroming te berekenen, voegen we de divergentie van de fiber-spanning-tensor toe aan de Navier-Stokes vergelijkingen. De fiber-spanning is berekend middels de welbekende vergelijkingen, die geldig zijn voor suspensies van stijve staven, welke niet met elkaar wisselwerken. Een directe berekening van de fiber-spanning onder weerstand-verminderde omstandigheden is onmogelijk met de huidige computer capaciteit. Zoals gebruikelijk in ‘Large Eddy Simulation’, wordt het probleem behandeld door de vergelijkingen te middelen. Het middelen leidt tot onbekende termen, welke gemodelleerd worden door sluitingshypothesen. We onderzoeken de prestatie van enkele sluitingsmodellen door simulaties te vergelijken van de gemiddelde en de on-gemiddelde vergelijkingen. Hieruit concluderen we dat de sluitingsmodellen geen significante fouten introduceren.
In plaats van de sluitingsmodellen zijn er andere, meer fundamentele tekortkomingen in het numerieke model, zoals de verwaarlozing van de wisselwerking tussen de polymeren. Om het effect van deze on-gelegitimeerde aanname te bepalen, vergelijken we de simulaties met experimenten uit de literatuur. De vergelijking heeft betrekking op de frictie factor afhankelijk van het Reynolds getal en de fiber concentratie, alsmede de profielen van de gemiddelde snelheid, de Reynolds spanning en de turbulente kinetische energie. We zien goede overeenstemming in alle trends, bij relatief weinig weerstand vermindering. Bij hoge weerstand-verminderings, wijken de simulaties af van de experimentele data. Deze discrepanties suggereren dat wisselwerking tussen polymeren, welke verwaarloosd zijn in het numerieke model, belangrijk zijn bij hoge weerstand-vermindering.

Behalve het valideren van het numerieke model, hebben we ook het weerstand-verminderingsmechanisme bestudeerd. Een versimpeld model is geïntroduceerd, waarbij de fiber-spanning is gemodelleerd als een viskeuze spanning. De zogenaamde fiber-viscositeit is zodanig gedefinieerd dat de resulterende Reynolds gemiddelde dissipatie van de kinetische energie van de vloeistof gelijk is aan de dissipatie, die voorspeld wordt door de volledige, constitutieve vergelijkingen. Stroomwaartse fiber-oriëntatie in de viskeuze onderlaag resulteert in een verwaarloosbare fiber-viscositeit in dit gebied. Verder van de wand af, neigen de fibers zich te orienteren in de richting waarin de vloeistof uittrekt. Hierdoor neemt de fiber-viscositeit lineair toe met de afstand tot de wand. Het fiber-viscositeit model voorspelt de juiste hoeveelheid weerstand-verminderings en veranderingen in de turbulentie. Dit impliceert dat fiber-geïnduceerde weerstand-verminderings begrepen kan worden middels een toegevoegde viscositeit. Het feit dat de fiber-viscositeit grofweg schaalt als $\phi r^2$, waarbij $\phi$ de fiber volume fractie is en $r$ de lengte tot diameter (aspect) verhouding van de fiber, verklaart dat fibers met een grote aspect verhouding, significante effecten kunnen veroorzaken bij extreem lage volume fracties.

Tenslotte bestuderen we het effect van polymer-flexibiliteit op weerstand-verminderings. Simulaties van oplossingen van flexibele en stijve polymeren voorspellen bijna dezelfde hoeveelheid weerstand-verminderings wanneer beide vergeleken worden bij een constante waarde van $\phi r^2$, waarbij $r$ voor de flexibele polymeren gebaseerd is op het Reynolds gemiddelde aan de wand. Dit resultaat laat zien dat viscositeit de belangrijkste factor is voor weerstand-verminderings, terwijl elasticiteit een passieve rol vervult.
Chapter 1

Introduction

1.1 Turbulent Pipe Flow

The flow through straight and round pipes is one of the most extensively studied problems in fluid mechanics. A fluid of mass density $\rho$ is driven by a constant pressure gradient $-d\Pi/dx$ through a pipe with a diameter $D$. Reynolds (1883) studied the conditions under which the flow is laminar or turbulent. By varying the pipe diameter, the fluid kinematic viscosity $\nu$ and the bulk fluid velocity $U$, he found that the problem can be described by a single dimensionless parameter, termed the Reynolds number.

$$Re = \frac{UD}{\nu}. \quad (1.1)$$

For $Re \lesssim 2000$ any disturbance in the flow is dissipated and the flow is laminar. For $Re \gtrsim 2000$ the flow can make a transition from laminar to turbulent.

This thesis deals with the amount of fluid that passes through the pipe for a given pressure gradient. The parameter of interest is the friction factor $f$ being the inverse square of the non-dimensional bulk velocity.

$$f = \left( \frac{U_T}{U} \right)^2. \quad (1.2)$$

Here $U_T = \sqrt{-\frac{d\Pi}{dx} \frac{D}{4\rho}}$ is the friction velocity. The friction factor is determined by the Reynolds number [Eq. (1.1)]. In the laminar regime the friction is completely due to viscosity and governed by Poiseuille’s law.

$$\frac{1}{\sqrt{f}} = \frac{Re \sqrt{f}}{8}. \quad (1.3)$$

In the turbulent regime, the velocity fluctuations induce additional momentum losses, reflected by a larger wall friction as compared to laminar flow, given by the Prandtl-Kármán law.

$$\frac{1}{\sqrt{f}} = 2.5 \log Re \sqrt{f} + 0.3. \quad (1.4)$$

From Eqs. (1.3) and (1.4) it is seen that turbulence puts severe limitations on the fluid transport at large Reynolds numbers. It is for this reason that many scientific efforts have been devoted towards understanding and controlling turbulent drag.
1.2 Turbulent Drag Reduction

1.2.1 Description

It is well-known that the addition of high-molecular-weight, linear polymers to a turbulent pipe flow can induce a reduction of the Reynolds-stress and consequently a reduction of the frictional drag. Obviously drag reduction is of high practical value, and the phenomenon is exploited to increase the transport capacity in a large number of applications, including the Trans-Alaska oil-pipe line (Burgers et al. 1980). An intriguing aspect is that significant drag reduction can be achieved using extremely small polymer concentrations \( c_m \). For instance, the addition of polyethyleneoxide with a molar mass of \( M_w \sim 10^6 \text{ g mol}^{-1} \) to an aqueous turbulent pipe flow can reduce the drag by a factor of four using \( c_m \) as low as a few parts per million (ppm) in weight (Virk 1971).

This seemingly controversial behavior can be understood by considering the additional volume averaged stress, due to the presence of the polymers \( \tau \). The contribution to \( \tau \) of a rigid elongated particle of length \( l \) is of the same order of magnitude as that of a sphere of diameter \( l \) (Batchelor 1970). Thus, polymers induce a relative increase in the volume averaged stress which is equal to \( \phi r^2 \), where \( \phi \) is the polymer volume concentration and \( r = l/d \) is the aspect ratio, with \( d \) the polymer diameter. Polymers used in drag reduction studies can have \( r \sim 10^4 \), meaning that significant effects can be observed at extremely small volume fractions \( c \sim 10^{-6} \).

Besides polymers, other additives have been used to reduce the drag, such as macroscopic slender particles (McComb and Chan 1985) surfactants (Ohlendorf et al. 1986) and micro-bubbles (Madavan et al. 1984). For an extensive overview the reader is referred to Gyr and Bewersdorff (1995).

Polymers which are effective in drag reduction consist of \( \gtrsim 10^5 \) monomers. Such large chains are usually highly flexible and are randomly coiled in solution at rest. The coiled polymer has no preferred orientation and, in a statistical sense, can be thought of as a spherical particle. In this configuration, the polymers do not exert substantial stresses to the fluid and therefore do not induce drag reduction. For a polymer to become an effective drag reducer it has to be unraveled to a stretched configuration. Polymer stretching can occur when the polymer is subjected to fluid deformation. In a deforming fluid velocity field, solvent molecules exchange momentum to the polymer in specific directions. When this momentum transfer exceeds the Brownian forces, the polymer coil unravels in the direction of extensional fluid deformation, corresponding to the greatest principle rate of extension. This process leads to an increase in polymer-stress with increasing strain rate, known as extensional thickening (Bird et al. 1977). For flexible polymers to become effective drag reducers, they must spend long enough time in flow regions, with sufficiently large strain rates. When vorticity is significant as compared to strain rate, polymers rotate away from the direction of elongational fluid deformation. In shear flow, there is an exact balance between vorticity and strain rate, such that polymers tend to align in the direction corresponding to zero strain rate. This results in a decrease in polymer-stress as a function of the shear rate, known as shear thinning (Bird et al. 1977). This explains that polymers have no effect in laminar pipe flow or in the viscous sublayer of turbulent pipe flow. Polymers produce large stresses in turbulent flow regions which are irrotational or extensional. In a turbulent boundary layer these regions occur between the near-wall vortices. As a result of large polymer stresses in the extensional inter-vortex regions, the near-wall vortices are dampened, which might explain the mechanism for drag reduction (Dubief et al. 2004, Paschkewitz, Dubief,
1.2. Turbulent Drag Reduction

Dimitropoulus, Shaqfeh and Moin 2004).

1.2.2 Gross Flow Measurements

![Graph showing friction factor versus Reynolds number in drag-reduced pipe flow using flexible polymers (Virk 1975b).]

Figure 1.1: Friction factor versus Reynolds number in drag-reduced pipe flow using flexible polymers (Virk 1975b). •, polyethyleneoxide \( M_w = 6.1 \text{ Mg mol}^{-1}, c_m = 450 \times 10^{-6}, D = 32.1 \times 10^{-3} \text{ m}; \circ, \) polyacrylamide \( M_w = 12.5 \text{ Mg mol}^{-1}, c_m = 110 \times 10^{-6}, D = 8.46 \times 10^{-3} \text{ m); The following regimes are indicated: (L), Newtonian laminar [Eq. (1.3)]; (T), Newtonian turbulent [Eq. (1.4)]; (M), maximum drag reduction [Eq. (1.7)], given below.]

Flexible Polymers

Drag reduction is best visualized by measuring the bulk flow \( U \) as a function of the applied pressure gradient \(-d\Pi/dx\). Fig. 1.1 shows experimental data for aqueous solutions of flexible polyethyleneoxide and polyacrylamide (Virk 1975b). The data are presented in Prandtl-Kármán (PK) coordinates (Tennekes and Lumley 1973). The vertical axis equals the bulk velocity normalized by the friction velocity \( 1/\sqrt{f} = U/U_\tau \), and the horizontal axis equals the frictional Reynolds number \( Re\sqrt{f} = U_\tau D/\nu \). For comparison we added the friction relations for laminar and turbulent flows, indicated with (L) and (T), respectively.

The polyethyleneoxide solution shows onset behavior; drag reduction only occurs above a critical Reynolds number \( Re_0 \). This so-called onset Reynolds number is related to the coil-stretch transition, which occurs when the strain rate in the flow \( U_\tau^2/\nu \) exceeds the inverse of the polymer relaxation time \( \lambda \). The relaxation time can be estimated using Flory’s relation \( \lambda \approx \mu R_G^3/(k_B T) \), where \( k_B \) is the Boltzmann constant, \( T \) is the temperature and \( R_G \) is the radius of gyration \( R_G \approx a N^\frac{2}{3} \), with \( N \) the polymerization index and \( a \) the size of a repeat unit.
Figure 1.2: Friction factor versus Reynolds number in drag-reduced pipe flow using rigid rod-like polymers (Sasaki 1991a). The polymer is xanthan, with molar mass $M_w = 1.4 \text{ Mg mol}^{-1}$. The pipe diameter $D = 6 \times 10^{-3} \text{ m}$. Different mass fraction $c_m$ are used. •, $c_m = 0$; □, $c_m = 10 \times 10^{-6}$; ■, $c_m = 25 \times 10^{-6}$; ▽, $c_m = 50 \times 10^{-6}$; ▼, $c_m = 100 \times 10^{-6}$; △, $c_m = 150 \times 10^{-6}$; ▲, $c_m = 200 \times 10^{-6}$. The following regimes are indicated: (L), Newtonian laminar [Eq. (1.3)]; (T), Newtonian turbulent [Eq. (1.4)]; (M), maximum drag reduction [Eq. (1.7)].

(Doi and Edwards 1986). For the polyacrylamide solution the coil-stretch transition occurs in the laminar regime. Since polymers are passive in laminar shear flow, this transition is not observed on the PK-plane. After onset the friction factor is related to the Reynolds number in a similar fashion as for Newtonian flow, i.e. $1/\sqrt{f}$ is proportional to $\log(Re\sqrt{f})$, but then with a slope larger than 2.5 (Virk 1971).

$$\frac{1}{\sqrt{f}} = (2.5 + \delta_1) \log Re\sqrt{f} + 0.3 - \delta_1 \log Re_0\sqrt{f}_0. \quad (1.5)$$

Here $f_0$ is the friction factor at $Re_0$ and $\delta_1$ is the slope increment. Virk (1971) proposed a correlation for $\delta_1$ in terms of the polymer number density $n$ and the polymer contour length $l = Na$.

$$\delta_1 = k (nl^3)^{\frac{1}{2}}. \quad (1.6)$$

For $k = (8 \pm 2) \times 10^{-3}$ Eq. (1.6) fits experimental data for a wide range of polymer-solvent pairs.

Another important contribution by Virk (1971) is the identification of the so-called maximum drag reduction (MDR) asymptote. The transport efficiency $1/\sqrt{f}$ is bounded from above by an empirical function, independent of specific properties of the polymer solution.

$$\frac{1}{\sqrt{f}} = 11.7 \log Re\sqrt{f} - 41.8. \quad (1.7)$$
1.2. Turbulent Drag Reduction

Figure 1.3: Friction factor versus Reynolds number in drag-reduced pipe flow using macroscopic fibres (Hoving 2008). The nylon fibres used are displayed in Fig. 1.4. The pipe diameter $D = 50 \times 10^{-3}$ m. Different volume fractions $c$ are used. $\times$, $c = 0$; $\sigma$, $c = 8.5 \times 10^{-3}$; $\Box$, $c = 5.7 \times 10^{-3}$; $\Delta$, $c = 11.3 \times 10^{-3}$; $\nabla$, $c = 14.1 \times 10^{-3}$; $\blacktriangle$, $c = 16.9 \times 10^{-3}$; $\blacktriangledown$, $c = 19.7 \times 10^{-3}$; $\blacksquare$, $c = 22.4 \times 10^{-3}$; $\bullet$, $c = 25.2 \times 10^{-3}$. The Newtonian turbulent regime [Eq. (1.4)] is indicated with (T).

When the flow reaches this state, drag reduction cannot be further increased by adding more polymers to the fluid. The MDR curve is indicated in Fig. 1.1 with (M).

Rigid Polymers

Polyelectrolytes in de-ionized water or polymers with a helical backbone structure can have small flexibility and are extended in solutions at rest. These rigid polymers, referred to as fibres, also reduce drag. As shown in Fig. 1.2 drag reduction behavior in fibre solutions is different as that for flexible polymers. Since there is no coil-stretch transition, no onset phenomenon is observed. Instead the non-dimensional velocity $1/\sqrt{f}$ is displaced from the Newtonian curve by a magnitude $\delta_2$, independent of the Reynolds number.

$$\frac{1}{\sqrt{f}} = 2.5 \log \text{Re} \sqrt{f} + 0.3 + \delta_2.$$  \hspace{1cm} (1.8)

For small Reynolds numbers, when Eq. (1.8) exceeds Eq. (1.7), drag reduction is saturated and the fibre solutions follow the MDR curve.

A very intriguing aspect is that MDR does not depend on the polymer concentration or polymer properties, such as flexibility. This indicates that the drag reduction mechanisms are similar in flexible and rigid polymer solutions. This is surprising, considering that the polymer-solvent interaction is different for flexible and rigid polymers. Rigid polymers induce purely
dissipative, viscous stresses, while flexible polymers induce an additional elastic component. It might therefore be inferred that an additional viscosity is the key to understand drag reduction, while elasticity is an irrelevant side-effect.

**Macroscopic Fibres**

Drag reduction also occurs in suspensions of macroscopic fibres (McComb and Chan 1985). Compared to polymers, macroscopic fibres require larger concentrations to obtain the same level of drag reduction. However, they are more resistant to shear degradation, and can also operate in gases (Ljus et al. 2002), where polymers can be used in liquids only. As compared to polymers, the properties of macroscopic particles are better controllable, which provides advantages in the interpretation of drag reduction experiments. Fig. 1.3 shows the drag reduction behavior in suspensions of nylon fibres (Hoving 2008). A microscope image of the fibres is provided in Fig. 1.4. As apparent from Fig. 1.3, the drag reduction characteristics are more complicated as compared to those found for microscopic fibres, which were shown in Fig. 1.2. These complexities may be attributed to the large concentrations required to achieve significant drag reduction. At such large concentrations fibres are in mechanical contact with each other. As an effect clusters of entangled fibres are formed. The clusters induce larger resistance against fluid deformation as compared to fibres which are hydraulically individual. Another complexity might be related to the large length of the fibres. The fibres being larger than the near-wall vortical structures may explain the observed decrease in drag reduction at large Reynolds numbers. For a detailed interpretation of these experiments and additional results, see Hoving (2008).
1.2. Turbulent Drag Reduction

Figure 1.5: Velocity profiles in aqueous channel flow experiments for Newtonian flow and drag-reduced flow using flexible polymers (Warholic et al. 1999). The Reynolds number $Re = 2 \times 10^4$ and the channel height $D = 50.8 \times 10^{-3}$ m. The polymer used is a copolymer of polyacrylamide and sodium acrylamide. The polymer mass fraction $c_m = 0$ (circles), $c_m = 1.25 \times 10^{-6}$ (squares) and $c_m = 50 \times 10^{-6}$ (triangles).

1.2.3 LDA Measurements

Gross flow measurements provide limited insight into the drag reduction mechanisms. Obtaining a deeper understanding of the underlying physics, requires a more detailed characterization of the flow, such as the profiles of the mean velocity, turbulent stresses, etc. Laser Doppler Anemometry (LDA) is useful for this purpose. This technique measures one or two components of the instantaneous fluid velocity vector at a fixed point in space. Translating the measurement point in the wall-normal direction yields the mean velocity, and the components of the Reynolds stress tensor as functions of the wall-distance.

Mean Flow

Fig. 1.5 shows LDA measurements of the velocity profiles in a Newtonian fluid and two polymer solutions, corresponding to relatively small drag reduction (SDR) and maximum drag reduction (MDR) (Warholic et al. 1999). The variables are presented in wall-units, denoted with the superscript +. The velocity $\overline{u}^+ = \overline{u}/u_\tau$ and the wall-distance $y^+ = yu_\tau/\nu$ are made dimensionless with friction velocity $u_\tau$ and kinematic viscosity $\nu$.

The Newtonian velocity profile is linear for $y^+ \lesssim 12$ and logarithmic with a slope of approximately 2.5 for $y^+ \gtrsim 12$, referred to as the law of the wall (Tennekes and Lumley 1973). The linear and logarithmic regions are dominated by viscous stress and Reynolds stress and are referred to as the viscous layer and the inertial layer, respectively.
The drag-reduced flows have larger non-dimensional velocities, as compared to the Newtonian flow. The velocity profile is qualitatively different for SDR and MDR. At SDR the logarithmic velocity profile is parallel shifted upwards, while at MDR its slope is increased. Virk (1971) rationalized these trends by proposing a three-layer model for the velocity profile, as sketched in Fig. 1.6.

$$ u^+ = \begin{cases} y^+ & \text{if } 0 < y^+ < 11.6 \\ 11.7 \log(y^+) - 17 & \text{if } 11.6 < y^+ < 11.6 + \delta^+_E \\ 2.5 \log(y^+) + 9.2 \log(11.6 + \delta^+_E) - 17 & \text{if } 11.6 + \delta^+_E < y^+ < Re_\tau/2 \end{cases} \quad (1.9) $$

The non-dimensional pipe diameter is referred to as the frictional Reynolds number $Re_\tau = DU_\tau/\nu$. The elastic layer thickness $\delta^+_E$ describes the deviation from Newtonian flow and measures the amount of drag reduction. Without polymer additives ($\delta^+_E = 0$) Eq. (1.9) reduces to the law of the wall. With polymer additives ($\delta^+_E > 0$) the logarithmic profile shifts upwards, while its slope is kept constant. The shift is realized by the formation of the elastic layer in between the viscous and inertial layers. Similar as the inertial layer, the elastic layer is also logarithmic but then with a slope substantially larger that of the inertial layer. With increasing drag reduction the elastic layer extends. When it covers the complete pipe cross-section, the flow is at MDR. The larger slope of the logarithmic profile at MDR indicates a structurally different momentum transfer mechanism as compared to Newtonian flow.
1.2. Turbulent Drag Reduction

Figure 1.7: Reynolds shear stress $-\bar{u}'v'^+$ (open symbols) and polymer shear stress $\bar{\tau}_{xy}^+$ (filled symbols) in aqueous channel flow experiments for Newtonian flow and drag-reduced flow using flexible polymers (Warholic et al. 1999). The Reynolds number $Re = 2 \times 10^4$ and the channel height $D = 50.8 \times 10^{-3}$ m. The polymer used is a copolymer of polyacrylamide and sodium acrylamide. The polymer mass fraction $c_m = 0$ (circles), $c_m = 1.25 \times 10^{-6}$ (squares) and $c_m = 50 \times 10^{-6}$ (triangles).

Shear Stress

These changes can be studied in more detail by measuring the components of the shear stress balance. This balance is obtained by integrating the $x$-component of the Reynolds averaged Navier-Stokes equations over the $y$-direction.

$$1 - \frac{2y}{D} = \frac{d\bar{u}^+}{dy^+} - \bar{u}'v'^+ + \bar{\tau}_{xy}^+.$$  \hfill (1.10)

The equation describes the balance between the driving pressure gradient force and the dissipating forces due to viscous stress $d\bar{\tau}^+/dy^+$, Reynolds stress $-\bar{u}'v'^+$ and a contribution from the polymers, referred to as the polymer stress $\bar{\tau}_{xy}^+$. Drag reduction is realized by an increase in $d\bar{\tau}^+/dy^+$. This requires that the extra stress due to the polymers is overwhelmed by a reduction of the Reynolds stress.

The viscous stress and the Reynolds stress can be measured directly with LDA. Subsequently the polymer stress can be obtained by applying Eq. (1.10). Fig. 1.7 shows results of Warholic et al. (1999). These data indicate that at SDR the polymers have an effect only in the near-wall region, while in the outer region the polymer stress is close to zero. This implies that at SDR the physics in the inertial region is unaffected by the polymers. At MDR the picture is very different. Then the polymer stress dominates the momentum balance and the Reynolds stress is reduced to a marginal value over the whole domain.
Figure 1.8: Standard deviation of streamwise fluid velocity (open symbols) and wall-normal fluid velocity (filled symbols) in aqueous channel flow experiments for Newtonian flow and drag-reduced flow using flexible polymers (Warholic et al. 1999). The Reynolds number $Re = 2 \times 10^4$ and the channel height $D = 50.8 \times 10^{-3}$ m. The polymer used is a copolymer of polyacrylamide and sodium acrylamide. The polymer mass fraction $c_m = 0$ (circles), $c_m = 1.25 \times 10^{-6}$ (squares) and $c_m = 50 \times 10^{-6}$ (triangles).

Turbulent Kinetic Energy

A very interesting characteristic of drag reduction is the modifications of the turbulent kinetic energy (TKE), measured by the standard deviation of the fluid velocity vector. Fig. 1.8 shows LDA measurements of the profiles corresponding to the streamwise ($x$) and the wall-normal ($y$) velocity components (Warholic et al. 1999). For both Newtonain flow and drag-reduced flow most energy is contained in the streamwise velocity component. The anisotropy is largest near the wall, while in the center the TKE is evenly distributed over the different directions. The TKE peaks at $y^+ \approx 10$ and decreases thereafter towards the center. With increasing drag reduction, the peak-values shift away from the wall, indicating that the near-wall vortical structures, responsible for the friction factor, increase in size. At SDR there is a substantial increase of the TKE in the $x$-direction, while the TKE in the other directions are reduced. Larger TKE is surprising, considering that turbulent momentum losses are reduced. Similar as for the shear stress balance the changes are restricted to the near-wall region, whereas in the outer region the statistics are equivalent to those in Newtonian flow. At MDR on the other hand the statistics change over the whole domain, with a smaller TKE as compared to Newtonian flow. Still there is a substantial TKE contained in the streamwise component, while the contents in the other components are close to zero. A non-zero TKE points out that turbulence prevails at MDR. The turbulence properties of the MDR flow state however are very different as compared to classical Newtonian turbulence. Therefore the drag reduction
phenomenon offers the opportunity to study turbulence from a different perspective which could ultimately lead to a deeper understanding of the fundamentals of turbulence.

1.3 Objectives and Outline of the Thesis

Inspired by these intriguing aspects, many scientists have studied the problem of drag reduction from a fundamental point of view; to understand how minute amounts of microscopic polymers can induce substantial changes to the macroscopic scales of a turbulent flow. Despite numerous efforts conducted over the past sixty years, the problem of polymer-induced drag reduction is poorly understood. At present we have to satisfy ourselves with phenomenological models, like Eq. (1.9), which are fitted to experimental or numerical data, but the underlying physics are unclear.

Drag reduction originates from forces between the polymers and the solvent, referred to as polymer stresses. These stresses depend on the configuration of the polymers, such as orientation and extension. Therefore understanding drag reduction relies on the characterization of polymer configuration in turbulent flow. In simple, well-defined flow configurations, such as laminar shear, polymer configuration can be measured experimentally. In turbulent flow however this is a very complicated, if not impossible task.

Since experiments cannot provide the complete picture of the underlying physics, there is a need for drag reduction simulations. Simulations provide advantages which cannot be obtained experimentally, such as the complete control of polymer properties and knowledge of the full space- and time-dependencies of all dynamical variables. Despite these advantages there are large drawbacks involved in numerical simulations of drag reduction, due to the extreme complexity of the dynamics of entangled polymers in a turbulent flow. The complexity can be understood by considering that polymers which are effective in drag reduction consist of $\sim 10^5$ monomers. In solution these large chains are usually highly flexible and the configuration varies between randomly coiled and fully extended depending on the rate of strain of the solvent. In a drag-reduced flow the polymer concentration is large enough that interactions between different chains are important. In the turbulent deformation field, the chains twist around each other, forming clusters of entangled polymers. These dynamics are too complex to be simulated directly using present computation facilities.

At present only highly idealized models can be used in which flexible chains are modeled as two-point particles and the effects of entanglement and hydrodynamic interactions are neglected. Needless to say, these simulation have little scientific value without quantitative comparison to experimental data. The lack of such comparison in literature indicates failure of such attempts.

The main goal of this thesis is to quantitatively compare drag reduction simulations to experimental data. Our aim is to numerically reproduce and rationalize experimental data, as displayed in Fig. 1.2. We have decided to focus on fibres instead of more general flexible polymers, since fibres require less modeling. This reduces the complexity such that a more transparent comparison to experimental data can be made. However, even in the absence of flexibility, there are still several problems in the numerical modeling.

Some of the difficulties are related to the statistical description of the polymers. The polymer stress is expressed in terms of a probability distribution over the polymer orientation angles and position vectors. Due to computer restrictions the complete distribution function
cannot be solved under turbulent drag reduction conditions. Therefore the stress is obtained using an approximate method, involving the computation of low-order moments of the distribution function. This so-called moment approximation requires far less computational resources as compared to a direct computation of the distribution function. Unfortunately the reduced computational cost comes with a penalty. The equations governing the moments contain unknown terms, which require ad-hoc closure relations. In this thesis we assess the performance of several closure schemes under turbulent flow conditions by making a comparison to direct computations of the fibre distribution function.

In addition to the closures we also address the more fundamental shortcomings of the numerical model. Strictly speaking the constitutive equations are valid for dilute solutions, in which interactions between fibers play no role. However it can be shown that in principle drag reducing solutions are non-dilute. We determine the implication of neglecting interactions by making a comparison between the simulation and experimental data from the literature.

Besides model verification we aim to identify the crucial property of the polymer stress with respect to drag reduction. In general polymers generate viscoelastic stresses, meaning that polymers have the capacity to dissipate as well as to store fluid mechanical energy. Rigid polymers generate viscous stresses only while the more general flexible polymers generate additional elastic stresses. To elucidate the role of the elastic stresses on drag reduction we compare simulations of drag reduction, induced by rigid polymers and flexible polymers.

The outline of the remaining part of the thesis is as follows. In Chapters 2 and 3 we present and explain the equations governing fibre solution flow and the numerical methods used to solve these equations. These chapters do not provide original scientific knowledge, but serve to assist the reader interpreting the findings of our work, which are presented in the subsequent chapters.

In Chapter 4 we study the performance of the closure relations involved in the moment approximation. The approximate equations are used to simulate drag-reduced channel flow and the results are compared to simulations based on a direct computation of the complete fibre distribution function. Owing to CPU restrictions the ‘exact’ computation concerns fibres, which are severely subjected to Brownian motion. The diffusion, induced by Brownian motion smoothens the distribution function, allowing a direct computation with reasonable computational resources. The strongly preferred fibre orientations required for drag reduction are suppressed by Brownian motion. Therefore ‘exact’ simulations, needed to assess the performance of approximate methods, can only be performed for very small levels of drag reduction. Consequently the performance of the moment approximation at large levels of drag reduction remains an open question. This problem is partly resolved in Chapter 5, where we test closure accuracy for the case of non-Brownian fibres. Reynolds averaged fibre stresses are computed using an ‘exact’ method, based on tracking individual particles. Due to an inadequate number of particles the particle method does not provide instantaneous fibre stresses accurately. Therefore these stresses are not coupled back to the fluid equations of motion; the particles behave passively and there is no drag reduction. Despite this drawback, the study provides insight into certain shortcomings of the moment approximation. These insights have led to improvements in the numerical computation of the stress generated by non-Brownian fibres. In the same chapter we also examine the mechanism for fibre-induced drag reduction. A simplified, viscous model for the fibre stress is proposed. The model is shown to predict drag reduction and modifications in the turbulence statistics, which are in close agreement with those predicted by the full consti-
1.3. Objectives and Outline of the Thesis

Constitutive equations. Chapter 6 presents a parametric study on the friction factor in fibre solution channel flow. A relation is derived between the friction factor, the Reynolds number and the properties of the fibres, which applies to relatively small levels of drag reduction. The result is compared to experimental data from the literature. Subsequently Chapter 7 deals with the maximum drag reduction regime. Simulation results are compared qualitatively to experimental data from the literature, involving the profiles of first- and second-order fluid velocity statistics. In Chapter 8 we investigate the role of polymer flexibility on drag reduction by comparing simulations of constitutive equations describing solutions of rigid and flexible polymers. In Chapter 9 the thesis is closed with a summary of conclusions.

Chapters 4, 5, 6 and 8 have been published or submitted for publication in international scientific journals. Consequently, these chapters are self-contained and can be read individually. Each of these chapters present original knowledge as well as general considerations such as an introduction and a discussion on governing equations and numerical methods.
Chapter 1. Introduction
Chapter 2
Constitutive Equations

This chapter presents the mathematical formulation of turbulent, fibre solution, channel flow, which is the basis for the present numerical study. To account for the effect of the fibres on the fluid mechanics, the Navier-Stokes equations are supplemented by the fibre stress tensor. The equations for the fibre stress are based on several simplifying assumptions. The assumed conditions are discussed and compared to experimental drag reduction conditions from the literature.

The fibre stress tensor depends on a distribution function $\Psi$ of the fibre position and orientation vectors. Due to computer restrictions $\Psi$ cannot be computed in turbulent flows. To approximate the fibre stress we compute the second-order moments of $\Psi$. Equations for the moments are derived by applying an averaging operator to the transport equation for $\Psi$. The averaged equations contain unknown terms. Models for these terms are discussed.

2.1 Channel Flow

In this work Direct Numerical Simulation (DNS) is used to study turbulent fibre solution channel flow. In particular we are interested in the reduction of the friction factor due to the addition of the fibres.

In channel flow, a fluid of mass density $\rho$ and kinematic viscosity $\nu$ is driven by means of a constant pressure gradient $-d\Pi/dx$ between two parallel, no-slip walls separated by a distance $D$. Periodic boundary conditions are assumed in the wall-parallel directions. The choice of the channel geometry instead of the more practical pipe geometry is motivated by the fact that the dynamics in the near-wall layer, responsible for the friction factor, are similar in pipe and channel flow (Tennekes and Lumley 1973), while the problems related to the singularity in the cylindrical coordinate system do not have to be addressed in Cartesian calculations. It is known that the near-wall vortical structures increase in size with increasing drag reduction (Li et al. 2006). Therefore, findings from channel flow studies can only be extrapolated to pipe flow, for relatively small levels of drag reduction.

The simulations are based on the incompressible, Navier-Stokes equations, supplemented by the divergence of the fibre stress tensor.

\[
\rho \frac{Du}{Dt} = \nabla \cdot (-\Pi \delta + 2 \mu S + \tau),
\]

(2.1a)

\[
\nabla \cdot u = 0.
\]

(2.1b)
Here $\mathbf{u}$ is the fluid velocity vector, $t$ is time, $\nabla$ is the nabla operator, $\delta$ is the unit tensor, $D/Dt = \partial / \partial t + \mathbf{u} \cdot \nabla$ is the material derivative, $\mathbf{S} = \frac{1}{2} (\nabla \mathbf{u}^T + \nabla \mathbf{u})$ is the rate of strain tensor, $\Pi$ is the pressure, $\mu = \nu \rho$ is the solvent dynamic viscosity and $\mathbf{\tau}$ is the fibre stress tensor, for which additional equations have to be solved.

The most important parameter describing this flow is the effective, frictional Reynolds number.

$$Re_\tau = \frac{U_\tau D}{\nu_{\text{eff}}}.$$  
(2.2)

Here

$$U_\tau = \sqrt{\frac{d\Pi D}{dx \ 2 \rho}},$$  
(2.3)

is the friction velocity and

$$\nu_{\text{eff}} = \nu + \frac{\tau_{xy}}{\rho \frac{dx}{dy}} \biggr|_{\text{wall}},$$  
(2.4)

is the effective viscosity at the wall, consisting of the Newtonian viscosity and an additional contribution due to the presence of the fibres.

### 2.2 Fibre Motion and Stress

#### 2.2.1 Fibre Motion

We assume a homogeneous suspension of cylindrical rods of length $l$ and diameter $d$, with aspect ratio $r = l/d \gg 1$. The volume concentration of the rods is $c$, defined as the total volume of the rods, per unit volume of the solution. For example we consider the rigid polymers used in the drag reduction studies of (Sasaki 1991b): $l \approx 5 \times 10^{-6}$ m, $d \approx 10^{-9}$ m, $r \approx 10^4$ and $c \approx 10^{-5}$.

The fibres are smaller than the Kolmogorov length scale $l_K$, which is estimated as $l_K \approx DR e^{-3/4}$. Using the parameters of (Sasaki 1991b): $Re_\tau \sim 10^3$ and $D = 6 \times 10^{-3}$ m, we find $l/l_K \approx 0.17$. The condition $l < l_K$ implies that fibre motion is unaffected by inertial effects and that the fluid flow surrounding an individual fibre can be described by the Stokes equations.

Under these conditions, a fibre translates as a material point and rotates as a material line, while being subjected to Brownian motion. Ignoring effects of a finite aspect ratio, fibre translation and rotation can be written as (Doi and Edwards 1986):

$$\dot{\mathbf{x}} = \mathbf{u} - \kappa_\rho \nabla \ln \Psi,$$  
(2.5a)

$$\dot{\mathbf{p}} = (\nabla \mathbf{u})^T \cdot \mathbf{p} - (\nabla \mathbf{u})^T: \mathbf{p} \mathbf{p} \mathbf{p} - \kappa_\rho \nabla \mathbf{p} \ln \Psi.$$  
(2.5b)

Here $\mathbf{x}$ is the fibre position vector and $\mathbf{p}$ is its orientation unit vector. The fluid velocity and velocity gradient at position $\mathbf{x}$ are denoted $\mathbf{u}$ and $\nabla \mathbf{u} = \sum_{ij} \partial u_i / \partial x_j \mathbf{e}_i \mathbf{e}_j$ where the $\mathbf{e}_i$'s are the Cartesian unit vectors. The over-dot represents time differentiation, $\nabla$ is the nabla operator and $\nabla \mathbf{p}$ is the nabla operator projected on the unit sphere.

The tendency of Brownian motion to homogenize the particle distribution is equivalent to an external force acting on the particles, which is given by the gradient of $k_B T \ln \Psi$. Here $\Psi(\mathbf{p}, \mathbf{x}, t)$ is the probability distribution of finding a fibre with orientation $\mathbf{p}$ at position $\mathbf{x}$ and time $t$, $k_B$ is the Boltzmann constant and $T$ is the temperature. The diffusion takes place in
2.2. Fibre Motion and Stress

physical as well as orientational space. The corresponding spatial diffusivity $\kappa_s$ and orientational
diffusivity $\kappa_r$ are given by:

$$\kappa_s \approx \frac{10k_BT}{\mu l},$$ (2.6a)

$$\kappa_r \approx \frac{10k_BT}{\mu l^3},$$ (2.6b)

where we have neglected the logarithmic dependence of the numerical factor 10 on the fibre
aspect ratio.

To estimate the role of Brownian motion in drag-reducing polymer solutions, we compare
the rotary diffusion time-scale $t_B = \kappa_r^{-1}$ to a characteristic time scale of the flow. For the above
mentioned experimental parameters, it is found that $t_B$ is two orders of magnitude larger than
the large eddy turn-over time $t_L \approx (D^2/\nu)Re_r^{-1}$, which is the largest time scale in the flow.
Apparently Brownian motion does not play an important part and is therefore neglected in
most of this work.

2.2.2 Fibre Stress

The macroscopic effect on the fluid mechanics due to the presence of the fibres is given by a
stress tensor $\tau$, obtained by averaging the forces between the fibres and the fluid. The averaging
volume is small compared to the spatial variations of the fluid velocity field and large enough
to contain a statistical sample of fibres.

Provided that interactions between fibres can be neglected, the fibre stress can be derived
rigorously, by summing the contributions generated by hydrodynamically individual fibres (Doi
and Edwards 1986).

$$\tau = 2\alpha \mu \left[ S : \langle pppp \rangle + 3\kappa_r \left( \langle pp \rangle - \frac{1}{3} \delta \right) \right].$$ (2.7a)

Here $\alpha$ is the fibre concentration parameter, the fractional increase in the volume averaged stress
due to the presence of the fibres.

$$\alpha \approx 0.1cr^2,$$ (2.7b)

where we have ignored the logarithmic dependence of the numerical factor 0.1 on the fibre aspect
ratio. For the experimental conditions described in Sec. 2.2.1 we find $\alpha \approx 44$. The scaling of $\alpha$
with $cr^2$ means that a fibre of length $l$ makes a contribution to the stress, which is of the same
order of magnitude as that of a sphere with diameter $l$. This explains that significant effects are
observed using very small volume fractions, provided that the aspect ratio is large.

Eqs. (2.7) are strictly valid when the solution is dilute, in the sense that the fibres are
hydrodynamically independent. This condition is satisfied when the spacing $s$ between a fibre
and its nearest neighbor $s \geq l$, i.e. when $cr^2 \leq 1$. Since in this regime $\alpha \lesssim 1$, the fibres do
not generate a notable effect and there is no drag reduction. Drag reduction requires the spacing
between the fibres $s \lesssim l$ but $s \gtrsim d$. In this semi-dilute regime, $cr^2 \gtrsim 1 \gtrsim cr$, hydrodynamic
interactions are important while mechanical contacts are rare. These restrictions are satisfied
under the aforementioned, experimental conditions, for which we estimate $cr^2 \approx 4 \times 10^2$ and
$cr \approx 7 \times 10^{-2}$. When the concentration is further increased to $cr \gtrsim 1$, the spacing becomes
$s \lesssim d$. This means that the fibres are in constant mechanical contact with each other, which
induces a drag increase rather than a drag reduction.
We stress once more that drag-reducing solutions are non-dilute which is outside the range of the validity of the constitutive equations (2.5) and (2.7). In Chapters 6 and 7 we determine the implications of this inconsistency, by making a detailed comparison of our simulation results to experimental data from the literature.

The fibre stress involves averaging \( \langle \cdots \rangle \) over a statistical ensemble of fibres, contained in a volume \( V \), centered at the point where the stress is to be determined. By definition \( V \) is smaller than the Kolmogorov length-scale. The averaging can be expressed as an integral over \( p \)-space and \( V \) weighted with \( \Psi \).

\[
\langle \cdots \rangle = \frac{1}{V} \int_V dV \int_p d\Psi \cdots .
\]

(2.7c)

The effect of Brownian motion on the fibre stress is given by the rotary Peclet number \( Pe_r \) defined as the ratio of the characteristic shear \( \gamma \) and the rotary diffusivity \( \kappa_r \).

\[
Pe_r = \frac{U^2}{\kappa_r \nu_{eff}}
\]

Here we have chosen \( \gamma \) as the mean shear rate at the wall \( U^2/\nu_{eff} \). For \( Pe_r \ll 1 \), fibre rotation is dominated by Brownian motion. As a result \( \langle pp \rangle = \delta/3 \) and the fibre stress attains the form of a Newtonian stress: \( \tau = (2\mu_\alpha/3)S \). The resulting flow is equivalent to a Newtonian flow with an increased viscosity. Obviously there is no drag reduction, but rather a drag increase. However when variables are scaled with effective viscosity [Eq. (2.4)] and drag reduction is evaluated at constant effective, frictional Reynolds number [Eq. (2.2)], the \( Pe_r \ll 1 \) case is equivalent to the Newtonian case without drag reduction. When \( Pe_r \gg 1 \), fibres orient in preferred directions. This introduces a non-Newtonian character to the fibre stress, effectively resulting in drag reduction.

2.2.3 Fibre Transport Equation

Fibre stress is a macroscopic fluid property, obtained by volume-averaging the fluid properties on the micro-scale. As given by Eq. (2.7c) the averaging can be expressed in terms of the fibre distribution function \( \Psi \). The evolution equation of \( \Psi \) describes a redistribution of probability due to fibre translation and rotation (Doi and Edwards 1986).

\[
\frac{\partial \Psi}{\partial t} + \nabla \cdot (x\Psi) + \nabla_p \cdot (p\Psi) = 0.
\]

(2.9)

Due to the homogeneity of Eq. (2.9) an additional constraint is required to determine \( \Psi \). Since in fully developed turbulent channel flow the spatial distribution of material points is homogeneous we impose

\[
\int_p d\Psi = 1,
\]

(2.10)

which is referred to as the normalization condition.

Inserting Eqs. (2.5) into Eq. (2.9) yields:

\[
\frac{\partial \Psi}{\partial t} + \nabla \cdot (u\Psi) + \nabla_p \cdot \left[ \left( (\nabla u)^T \cdot p - (\nabla u)^T : pp \right) \Psi \right] - \kappa_s \nabla^2 \Psi - \kappa_r \nabla^2_p \Psi = 0.
\]

(2.11)

This equation is referred to as the Fokker-Planck equation.
2.2. Fibre Motion and Stress

2.2.4 Simple Flows

Figure 2.1: The orientation of a fibre in the principal coordinate system of a 2D rate of strain tensor is parameterized with the spherical coordinates $\theta$ and $\phi$.

Figure 2.2: Three limiting cases of a homogeneous 2D velocity gradient field. (a) pure strain ($Q=-1$), (b) pure shear ($Q=0$), (c) pure rotation ($Q=1$).

To provide insight in the constitutive equations (2.7) and (2.11), we present analytical solutions for simple, yet instructive flows. We consider the special case of non-Brownian fibres, subjected to a homogeneous, stationary and 2D fluid velocity gradient. The solutions of $\Psi$ are constructed in the coordinate system spanned by the eigenvectors of the rate of strain tensor $S$, denoted as $e_1$, $e_2$ and $e_3$. In this frame the 2D velocity gradient is written as:

$$\nabla u^T = \begin{pmatrix} S & 0 & \Omega \\ 0 & 0 & 0 \\ -\Omega & 0 & -S \end{pmatrix},$$

(2.12)

where $S^2 = \frac{1}{2} (S : S)$ and $\Omega^2 = -\frac{1}{2} (\Omega : \Omega)$ are the second invariants of the strain tensor $S = \frac{1}{2} (\nabla u^T + \nabla u)$ and the vorticity tensor $\Omega = \frac{1}{2} (\nabla u^T - \nabla u)$. Fibre orientation is parameterized
with the spherical coordinates $\theta$ and $\phi$, as sketched in Fig. 2.1.

$$p = \sin \theta \cos \phi e_1 + \cos \theta e_2 + \sin \theta \sin \phi e_3. \quad (2.13)$$

Fibre rotation in the $\theta$- and $\phi$-direction is equal to the $\theta$- and $\phi$-component of $\nabla u^T \cdot p$. With Eqs. (2.12) and (2.13) these are written as:

$$\begin{align*}
\dot{p}_\theta &= \frac{1}{2} S \sin 2\theta \cos 2\phi, \quad (2.14a) \\
\dot{p}_\phi &= \sin \theta (\Omega + S \sin 2\phi). \quad (2.14b)
\end{align*}$$

The fibres orient in the plane $\theta = \pi/2$, being the stable zero of Eq. (2.14a). The distribution over the angle $\phi$ is governed by Eq. (2.9). Without the temporal and spatial derivatives and using Eq. (2.14b) and $\theta = \pi/2$, this equation reduces to:

$$\frac{\partial}{\partial \phi} \left[ \Psi (S \sin 2\phi + \Omega) \right] = 0. \quad (2.15)$$

Together with the normalization condition:

$$\int_0^{2\pi} d\phi \Psi = 1, \quad (2.16)$$

the problem can be solved, yielding the following distribution function.

$$\Psi = \begin{cases} 
\delta (\phi - \phi_s) & \text{if } \left( \frac{\Omega}{S} \right)^2 < 1 \\
\frac{\sqrt{1 - (\Omega/S)^2}}{2\pi (1 + \pi \sin 2\phi)} & \text{if } \left( \frac{\Omega}{S} \right)^2 > 1
\end{cases} \quad (2.17)$$

The solution is interpreted as follows. If $(\Omega/S)^2 < 1$ all fibres have the same orientation angle $\phi_s$, being the stable zero of $\dot{p}_\phi$, given by $\Omega + S \sin 2\phi_s = 0$ and $(\partial/\partial \phi) (\Omega + S \sin 2\phi) \mid_{\phi=\phi_s} < 0$. If

Figure 2.3: Fibre-strain alignment as a function of the second invariant of the normalized 2D velocity gradient tensor.
2.3. Moment Approximation

\((\Omega/S)^2 > 1\), \(\dot{p}_\phi\) has no zeros and \(d\phi\psi(\phi)\) is interpreted as the relative time spent by the rotating fibres in the interval \((\phi, \phi + d\phi)\).

To quantify the effect of the fibres on the flow we consider here the dissipation of fluid kinetic energy due to the fibre stress \(\epsilon_F = S : \tau = 2\alpha\mu S : \langle pppp \rangle : S\) relative to the dissipation due to the Newtonian stress \(\epsilon = 2\mu S : S\). When normalized with the fibre concentration parameter \(\alpha\) this ratio expresses the alignment of the fibres w.r.t. the axes of fluid deformation. It is therefore referred to as fibre-strain alignment.

\[
\xi = \frac{\epsilon_F}{\epsilon alpha} = \frac{S : \langle pppp \rangle : S}{S : S}. \tag{2.18}
\]

By combining Eqs. (2.12), (2.13), (2.17) and (2.18), we find for \(\xi\):

\[
\xi = \begin{cases} 
\frac{1}{2}\sqrt{1 - \left(\frac{\Omega}{S}\right)^2} & \text{if } \left(\frac{\Omega}{S}\right)^2 < 1 \\
\frac{1}{2}\sqrt{\left(\frac{\Omega}{S}\right)^2 - 1} - \left(\frac{\Omega}{S} - \sqrt{\left(\frac{\Omega}{S}\right)^2 - 1}\right) & \text{if } \left(\frac{\Omega}{S}\right)^2 > 1
\end{cases} \tag{2.19}
\]

Fig. 2.3, shows \(\xi\) as a function of the second invariant of the normalized velocity gradient tensor \(Q\).

\[Q = (\Omega^2 - S^2)/(\Omega^2 + S^2). \tag{2.20}\]

Parameter \(Q\) determines the flow topology as explained in Fig. 2.2. In straining flow \((Q = -1)\) fibres orient in the positive strain direction, giving large \(\xi\). In shearing \((Q = 0)\) fibres orient in the zero strain direction, giving zero \(\xi\). In rotational flow \((Q = 1)\) \(\Psi\) is isotropic, giving intermediate \(\xi\). This result nicely illustrates that fibres have negligible effect in regions dominated by shear, while being highly dissipative in regions dominated by strain.

2.3 Moment Approximation

2.3.1 Moment Evolution Equation

Under drag reduction conditions, the diffusivities in Eq. (2.11) are of such small magnitude that \(\Psi\) contains small scales in physical as well as orientational coordinates, analogous to the case of a passive scalar at small diffusivity (Batchelor 1959). As an effect Eq. (2.11) cannot be solved numerically and approximations are needed. Fortunately, the computation of the fibre stress [Eq. (2.7a)] requires only low-order moments of \(\Psi\), defined as averages of even-order dyads of the fibre orientation vector. The second and fourth-order moments are given by:

\[
\langle pp \rangle = \frac{1}{V} \int_V dV \int_p dp \Psi pp, \quad \langle pppp \rangle = \frac{1}{V} \int_V dV \int_p dp \Psi pppp. \tag{2.21}
\]

The transport equations of \(\langle pp \rangle\) is derived by multiplying the Fokker-Planck equation (2.11) by \(pp\) and subsequently applying the averaging operator [Eq. (2.7c)] (Doi and Edwards 1986).

\[
\frac{D\langle pp \rangle}{Dt} - \nabla u^T \cdot \langle pp \rangle - \langle pp \rangle \cdot \nabla u - \kappa_s \nabla^2 \langle pp \rangle - 6\kappa_r \left(\frac{1}{3} \delta - \langle pp \rangle\right) = -2\nabla u : \langle pppp \rangle + s. \tag{2.22}
\]
Without the diffusive terms, this equation states that the fibres rotate as material lines, while being advected as material points. The term $2\nabla u : \langle pppp \rangle$ ensures that the fibres maintain a constant length, which would have been absent if the fibres could stretch freely, like material lines.

Equation (2.22) contains two unknown terms, which have to be modeled: the fourth-order moment $\langle pppp \rangle$ and the sub-grid-term $s$. The fourth-order moment and the sub-grid-term contain unknown information regarding variations of $\Psi$ in orientational space and physical space, respectively.

### 2.3.2 Fourth-Order Moment Closure

The unknown fourth moment $\langle pppp \rangle$ appears in the equation of change for the second moment $\langle pp \rangle$. It is possible to derive an equation for $\langle pppp \rangle$ in a similar way as for $\langle pp \rangle$. However this equation contains the unknown sixth-order moment $\langle pppppp \rangle$. In fact all moment equations contain higher-order moments and the system of moment equations can never be closed. This is a consequence of the nonlinear dependence of fibre rotation on fibre orientation [Eq. (2.5b)]. Obtaining a closed set of moment equations requires an ad-hoc relation, expressing a higher-order moment in terms of a lower-order moment. In this work we approximate the stress by solving the equation of change for the second moment (2.22) and apply a closure to express the fourth moment in terms of the second moment.

The purpose of the fourth-order moment closure is to model information, regarding orientational variations of $\Psi$. To quantify the amount of unknown information we expand the orientational part of $\Psi$ in a series of spherical harmonics.

$$
\Psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_l^m \Phi_l^m. \tag{2.23}
$$

Here $A_l^m$ are the expansion coefficients and $\Phi_l^m$ are the spherical harmonics of degree $l$ and order $m$ (Abramowitz and Stegun 1965). Each expansion coefficient is one scalar of information. The normalization condition (Eq. 2.10) requires $A_0^0 = 1$ and point symmetry $\Psi(-p) = \Psi(p)$ requires $A_l^m = 0$ for odd $l$. It can be shown that the coefficients of the $n$th-order moment of $\Psi$ are linearly related to the $A_l^m$ up to degree $n$. Therefore the purpose of the fourth-order moment closure is to relate the $A_4^1$ to the $A_2^2$. Since in the $\langle pp \rangle$-principal frame there are three non-zero $A_l^m$ and two non-zero $A_l^m$, $\langle pppp \rangle$ is related to $\langle pp \rangle$ by three scalar functions depending on two scalar arguments (Cintra and Tucker 1995).

In this work we use the EBOF (Eigenvalue-Based Optimal Fitted) closure proposed by Cintra and Tucker (1995). It is an expression in terms of the principal values of $\langle pppp \rangle$ and $\langle pp \rangle$ fitted to solutions of the Fokker-Planck equation for simple flows. The IBOF (Invariant-Based Optimal Fitted) closure, used for the turbulent flow calculations in Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin (2004), is similar to EBOF, except that it is formulated in terms of the tensor invariants. Both methods are proved to be of equal accuracy and are probably the best schemes available at present (Chung and Kwon 2002). In Appendix A the details of the EBOF closure are explained and in Chapter 4 we study the performance of this closure in turbulent channel flow.
2.3. Sub-Grid Closure

The smallest length-scale of $\Psi$ is referred to as the Batchelor scale $l_B$ which is related to the Kolmogorov scale $l_K$ by: $l_B = l_K Sc^{-1/2}$ (Batchelor 1959). The Schmidt number $Sc$ is defined as the ratio of the momentum diffusivity $\nu_{eff}$ and the fibre mass diffusivity $\kappa_s$.

$$Sc = \frac{\nu_{eff}}{\kappa_s} = \left( \frac{D}{T} \right)^2 \frac{Pe_{r}}{Re_{r}^2}.$$  

(2.24)

Using the experimental parameters given in Sec. 2.2.1, we find $Sc \approx 2 \times 10^5$. This means that under realistic drag reduction conditions $l_B$ is orders of magnitude smaller than $l_K$. In our simulations we do not resolve scales smaller than $l_K$. Instead we apply an averaging operator [Eq. (2.7c)] to the fibre transport equation [Eq. (2.11)], with a filter length of the order of $l_K$, such that the resulting solution is smooth on the scales which are numerically being solved. The filtering leads to an unknown sub-grid term in Eq. (2.22), which is modeled as diffusion:

$$s = \kappa \nabla^2 (pp),$$  

(2.25)

with an artificial diffusivity $\kappa$ of the order of $\nu_{eff}$. Essentially this means that we put the Schmidt number artificially to unity. The exact value of $\kappa$ is chosen in order to provide a numerically stable and smooth solution depending on the details of the velocity field and on the size of the grid-cells. A detailed description of the sub-grid term and an examination of the performance of the sub-grid model (2.25) are given in Chapter 5.
Chapter 2. Constitutive Equations
Chapter 3

Numerical Methods

This chapter presents the numerical methods used for solving the equations, governing turbulent fibre solution channel flow. The methods are adopted and modified from Ptaszynski et al. (2003). Spatial derivatives are computed with a Fourier-basis for the homogeneous directions and a second-order, central, finite-differences scheme for the wall-normal direction. Time integration is achieved with the second-order, explicit Adams-Bashforth scheme. Conservation of mass is ensured using a projection method. The computer code is written in FORTRAN and parallelized using the Message Passing Interface (MPI).

3.1 Governing Equations

In this work we use Direct Numerical Simulation (DNS) to compute turbulent fibre suspension channel flow. The channel geometry is sketched in Fig 3.1. A fluid is driven by means of a constant pressure gradient $-d\Pi/dx$ between two parallel, no-slip walls, separated by a distance $D$, in the $y$-direction. The wall-parallel directions are referred to as stream-wise ($x$) and span-wise ($z$). The velocity components in the stream-wise, wall-normal and span-wise directions, are denoted $u$, $v$ and $w$. Furthermore subscripts $x$, $y$ and $z$ or 1, 2 and 3 denote components of vectors and tensors. The dimensions of the channel are $DL_x$ and $DL_z$ in the $x$- and $z$-directions. The fluid consists of fibres, homogeneously dissolved into a solvent with kinematic viscosity $\nu$ and mass density $\rho$. The fibre length is $l$ and the ratio of the fibre length and the fibre diameter $d$ is referred to as the aspect ratio $r = l/d$.

In the computer code the variables are non-dimensionalized with fluid mass density $\rho$, friction velocity $U_r = \left[-(d\Pi/dx)(D/\rho)(1/2)\right]^{1/2}$ and channel height $D$. For clarity we summarize the governing equations in this non-dimensional form. The fluid equations of motion are the Navier-Stokes equations:

\[
\frac{D\mathbf{u}}{Dt} = -\nabla \Pi + \frac{1}{Re_r} \nabla^2 \mathbf{u} + \nabla \cdot \mathbf{\tau}, \quad (3.1a)
\]

and the continuity equation:

\[
\nabla \cdot \mathbf{u} = 0. \quad (3.1b)
\]

Here $\mathbf{u}$ is the fluid velocity vector, $t$ is time, $\nabla$ is the nabla operator, $\delta$ is the unit tensor, $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the material derivative, $\Pi$ is the pressure and $Re_r$ is the frictional
Chapter 3. Numerical Methods

Figure 3.1: The channel geometry. The coordinate axes are referred to as streamwise $x$, wall normal $y$ and spanwise $z$. The velocity components in $x$, $y$ and $z$ are denoted $u$, $v$ and $w$.

Reynolds number:

$$Re = \frac{U_D}{\nu}.$$  

The effect of the fibres on the fluid mechanics is given by the fibre stress tensor $\tau$.

$$\tau = \frac{2\alpha}{Re} \left[ \nabla u : \langle pppp \rangle + \frac{3}{Pe_r} \left( \langle pp \rangle - \frac{1}{3} \delta \right) \right].$$  

(3.1c)

Here $\langle pp \rangle$ and $\langle pppp \rangle$ are the second and fourth-order moments of the fibre distribution function and $\alpha$ is the fibre concentration parameter, which depends on the fibre volume fraction $c$ and the fibre aspect ratio $r$ as:

$$\alpha \approx 0.1cr^2.$$  

Furthermore $Pe_r$ is the rotary Peclet number, defined as the inverse product of the large-eddy-turn-over time $t_L = D/U_\tau$ and the rotary diffusivity $\kappa_r \approx 10k_BT/(\mu l^3)$, where $k_B$ is the Boltzmann constant and $T$ is the temperature.

$$Pe_r = \frac{U_\tau}{\kappa_r D}.$$
3.2 Spatial Derivatives

Equation (3.1) is discretized on a three dimensional Cartesian grid. The number of grid-points in the x-, y- and z-directions is \( N_x \), \( N_y \) and \( N_z \), respectively. The grid is non-uniform and staggered in the y-direction, as sketched in Fig. 3.2. The velocity components \( u \) and \( w \), the pressure and the components of \( \langle pp \rangle \) and \( \langle pppp \rangle \) are defined in the cell centers, and the velocity component \( v \) is defined on the cell faces. The y-positions of the cell-faces are denoted \( y_{F_k} \), where \( k = 0 \cdots N_y \) and \( y_{F_0} = 0 \) and \( y_{F_{N_y}} = 1 \). The grid is non-uniform, such that the grid-spacing \( \Delta y_k = y_{F_k} - y_{F_{k-1}} \) smoothly increases away from both walls. The y-positions of the cell-centers are given by \( y_{C_k} = (y_{F_k} + y_{F_{k-1}})/2 \), for \( k = 1 \cdots N_y \).

### 3.2.1 Homogeneous Directions

Spatial derivatives in the homogeneous directions (x and z) are computed with the Fourier basis functions (Canuto et al. 1988). A variable is transformed to Fourier space, using Fast Fourier Transformation. Then each Fourier component is multiplied by its wavenumber and subsequently the Fourier sequence is transformed back to physical space, using inverse Fast Fourier Transformation. For example we consider the 1D problem where a variable \( u \) is discretized on a
domain with length $L_x$, using $N_x$ grid-points, located at position $x_j = jL_x/N_x$, with $j$ an integer between 1 and $N_x$. The first and second-order derivatives at the $j$th grid-point are given by:

$$\frac{du}{dx}(x_j) = \frac{1}{N_x} \sum_{k=-N_x/2+1}^{N_x/2-1} \sum_{l=1}^{N_x} \frac{2\pi ik}{L_x} u(x_l) \exp\left(\frac{2\pi ik(j-l)}{N_x}\right),$$  \hspace{1cm} (3.2a)

$$\frac{d^2u}{dx^2}(x_j) = \frac{1}{N_x} \sum_{k=-N_x/2+1}^{N_x/2-1} \sum_{l=1}^{N_x} -\left(\frac{2\pi k}{L_x}\right)^2 u(x_l) \exp\left(\frac{2\pi ik(j-l)}{N_x}\right),$$  \hspace{1cm} (3.2b)

where $i$ is the imaginary unit and $k$ and $l$ are integers.

### 3.2.2 Wall-Normal Direction

Wall-normal derivatives are computed using the second-order, central finite-difference scheme (Hirsch 1988). For non-uniform meshes this scheme is strictly first-order accurate. The scheme is chosen for robustness and efficiency reasons. The derivative of a cell-centered quantity is defined in the cell faces. Again we explain this by considering the 1D problem where a function $u$ is discretized on a domain with length $L_y$ on $N_y$ cell-centered grid-points $y^C_j$. The derivative of this function at position $y^F_j$ is approximated by:

$$\frac{du}{dy}(y^F_j) = \frac{u(y^C_{j+1}) - u(y^C_j)}{y^C_{j+1} - y^C_j}. \hspace{1cm} (3.3a)$$

Equivalently the derivative of a cell-faced quantity, is defined at the cell centers and is approximated by:

$$\frac{du}{dy}(y^C_j) = \frac{u(y^F_j) - u(y^F_{j-1})}{y^F_j - y^F_{j-1}}. \hspace{1cm} (3.3b)$$

Second-order derivatives are obtained by successive application of Eqs. (3.3a) and (3.3b).

$$\frac{d^2u}{dy^2}(y^F_j) = \frac{u(y^C_{j+1}) - u(y^C_j)}{y^C_{j+1} - y^C_j} - \frac{u(y^C_j) - u(y^C_{j-1})}{y^C_j - y^C_{j-1}}, \hspace{1cm} (3.3c)$$

$$\frac{d^2u}{dy^2}(y^C_j) = \frac{u(y^F_{j+1}) - u(y^F_j)}{y^F_{j+1} - y^F_j} - \frac{u(y^F_j) - u(y^F_{j-1})}{y^F_j - y^F_{j-1}}. \hspace{1cm} (3.3d)$$

Whenever a cell-centered quantity is needed at the cell faces, or vise versa, the following interpolation schemes are used.

$$u(y^F_j) = \frac{u(y^C_{j+1}) + u(y^C_j)}{2}, \hspace{1cm} (3.3e)$$

$$u(y^C_j) = \frac{u(y^F_{j+1}) + u(y^F_{j-1})}{2}. \hspace{1cm} (3.3f)$$
3.3 Boundary Conditions

To implement boundary conditions for cell-centered variables, two extra virtual grid-points are defined: $y^C_0 = -y^C_1$ (see Fig. 3.2) and $y^C_{N_y+1} = 2 - y^C_{N_y}$. To ensure value zero at the walls of a cell-centered variable $u$ we use:

$$u(y^C_0) = -u(y^C_1), \quad u(y^C_{N_y+1}) = -u(y^C_{N_y}). \quad (3.4a)$$

To ensure a zero wall-normal derivative at the walls of a cell-centered variable $u$ we use:

$$u(y^C_0) = u(y^C_1), \quad u(y^C_{N_y+1}) = u(y^C_{N_y}). \quad (3.4b)$$

3.3 Boundary Conditions

For all variables, periodic boundary conditions are employed in the wall-parallel directions $x$ and $z$. On the walls ($y = 0$ and $y = 1$) we use no-slip conditions for the velocity:

$$u \big|_{walls} = 0. \quad (3.5a)$$

The boundary conditions for $\langle pp \rangle$ are chosen differently in the different chapters. In Chapters 4 and 5 we use the conventional method for polymer momentum equations (Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin 2004, Ptasinski et al. 2003).

$$\frac{\partial}{\partial y} \langle pp \rangle \big|_{walls} = 0. \quad (3.5b)$$

In Chapter 5 we demonstrate that these conditions result in large fibre stress errors in the viscous layer. To improve the results we have decided to use different conditions for the simulations presented in Chapters 6, 7 and 8.

$$\frac{\partial}{\partial y} \langle p_i p_j \rangle \big|_{walls} = 0 \quad \text{if } i \neq 2 \text{ and } j \neq 2$$

$$\langle p_i p_j \rangle \big|_{walls} = 0 \quad \text{if } i = 2 \text{ or } j = 2 \quad (3.5c)$$

3.4 Spatial and Temporal Resolutions

Here we consider the resolution required to fully resolve turbulent fibre solution channel flow. Turbulent flows can be thought of as a superposition of eddies of different length- and time-scales. The required spatial resolution is determined by the smallest length-scales of the fluid velocity field and the fibre orientation field, referred to as Kolmogorov scale $l_K$ and Batchelor scale $l_B$, respectively. Under realistic drag reduction conditions $l_B \ll l_K$. As an effect a fully resolved computation of the fibre orientation field demands huge computational resources, which is outside the scope of the present work. Instead we use an approximate method which ensures
that \( l_B \sim l_K \), as explained in 2.3.3. Therefore the required grid-resolution is fully determined by \( l_K \).

Since \( l_K \approx DRe_\tau^{-3/4} \) a computational domain with a volume of \( \sim D^3 \) requires \( \sim Re_\tau^{9/4} \) grid-points. The required time resolution is determined by the Kolmogorov time-scale \( t_K \approx (D/U_\tau)Re_\tau^{-1/2} \). This suggests that the time integration over a single large-eddy-turn-over time \( t_L \approx D/U_\tau \) requires \( \sim Re_\tau^{1/2} \) computational steps. Actually, for numerical stability reasons, more time steps are needed. A stable numerical solution requires \( \Delta t \lesssim \Delta x/u \). Here \( \Delta x \) is the grid-spacing, which is \( \sim l_K \) in a fully resolved simulation and \( u \) is the fluid velocity, reaching a maximum in the center of the channel of approximately \( u \approx U_\tau/\sqrt{T} \approx 10U_\tau \). Therefore simulating over one \( t_L \) requires \( \sim 10Re_\tau^{3/4} \) time steps. All together we find that the computational cost of a DNS of turbulent channel flow over one \( t_L \) scales as \( Re_\tau^3 \). It is for this reason that DNS of turbulent channel flow is limited to relatively small \( Re_\tau \).

## 3.5 Time Stepping

### 3.5.1 Navier-Stokes Equations

The equations of fluid motion (3.1a) and (3.1b) are advanced in time using a pressure correction method (van Kan 1986). For this purpose Eq. (3.1a) is split into the following predictor step:

\[
\frac{u^* - u(t - \Delta t)}{\Delta t} = 2\delta_x + \frac{3}{2} f(t - \Delta t) - \frac{1}{2} f(t - 2\Delta t),
\]

and corrector step:

\[
\frac{u(t) - u^*}{\Delta t} = -\nabla \Phi.
\]

Here \( t \) is the new time level, \( \Delta t \) is the constant time step and \( \Phi \) is a scalar introduced to ensure continuity [Eq. (3.1b)]. Furthermore \( 2\delta_x \) is the non-dimensional mean pressure gradient and \( f \) is the sum of the advection, fibre stress and viscous terms:

\[
f = \nabla \cdot (-uu + \tau) + \frac{1}{Re_\tau} \nabla^2 u.
\]

As described by Eq. (3.6a) term \( f \) is treated with the second-order, explicit Adams-Bashforth scheme. By taking the divergence of Eq. (3.6b) and imposing \( \nabla \cdot u(t) = 0 \), a Poisson equation for \( \Phi \) is obtained:

\[
\nabla \cdot u^* = \Delta t \nabla^2 \Phi.
\]

This equation is transformed to Fourier-space in the directions \( x \) and \( z \). This gives the following, ordinary, differential equation.

\[
iki_x u^* + ik_z \hat{u}^* + \frac{\partial \hat{u}^*}{\partial y} = \Delta t \left( -k_x^2 - k_z^2 + \frac{\partial^2}{\partial y^2} \right) \hat{\Phi}.
\]

Here a variable with a hat is the Fourier transform of the corresponding variable without a hat and \( k_x \) and \( k_z \) are wave-numbers in \( x \)- and \( z \)-direction. According to Eqs. (3.6) the following
3.6. Parallelization

condition holds at the walls:

\[ \left. \frac{\partial \Phi}{\partial y} \right|_{\text{walls}} = \left. \frac{\partial^*}{\Delta t} \right|_{\text{walls}} = \left[ \frac{3}{2} \left( \frac{1}{Re} \frac{\partial^2 \hat{v}}{\partial y^2} + ik_x \tau_{xy} + ik_z \tau_{yz} + \frac{\partial \hat{p}_w}{\partial y} \right) (t - \Delta t) - \frac{1}{2} \left( \frac{1}{Re} \frac{\partial^2 \hat{v}}{\partial y^2} + ik_x \tau_{xy} + ik_z \tau_{yz} + \frac{\partial \hat{p}_w}{\partial y} \right) (t - 2\Delta t) \right]_{\text{walls}}. \]

This condition cannot be applied since in the present discretization scheme \( \partial^2 \hat{v}/\partial y^2 \) is unknown at the walls. Instead the following conditions are used.

\[ \left. \frac{\partial \hat{\Phi}}{\partial y} \right|_{\text{walls}} = \left. \frac{\partial^*}{\Delta t} \right|_{\text{walls}} = 0. \] (3.7b)

Consequently quantity \( \Phi \) is not exactly equal to the ‘real’ pressure \( \Pi \). It can be shown however, that with this method the velocity field is computed correctly. Since we are not interested in details of the pressure field, we do not pay extra effort to precisely compute this quantity. Using the discretized forms of the wall-normal derivatives [Eqs. (3.3)] in Eqs. (3.7) leaves a system of linear equations for \( \hat{\Phi} \). For each \( k_x \) and \( k_z \) the system is put in tri-diagonal matrix form and solved using Gaussian elimination. After transforming \( \hat{\Phi} \) to \( \Phi \) the correction step [Eq. (3.6)b] is carried out, providing the velocity field at the new time level.

3.5.2 Moment Equations

The moment evolution equation (3.1d) is advanced in time using the second-order, explicit Adams-Bashforth scheme.

\[ \frac{\langle \mathbf{p}\mathbf{p} \rangle(t) - \langle \mathbf{p}\mathbf{p} \rangle(t - \Delta t)}{\Delta t} = \frac{3}{2} g(t - \Delta t) - \frac{1}{2} g(t - 2\Delta t). \] (3.8a)

Here \( g \) equals:

\[ g = -\nabla \cdot u \langle \mathbf{p}\mathbf{p} \rangle + \nabla u^T \cdot \langle \mathbf{p}\mathbf{p} \rangle + \langle \mathbf{p}\mathbf{p} \rangle \cdot \nabla u - 2\nabla u : \langle \mathbf{p}\mathbf{p}\mathbf{p}\mathbf{p} \rangle - \frac{6}{Pe_e} \left( \langle \mathbf{p}\mathbf{p} \rangle - \frac{1}{3} \delta \right) + \frac{1}{Pe_s} \nabla^2 \langle \mathbf{p}\mathbf{p} \rangle. \] (3.8b)

The unknown fourth-order moment \( \langle \mathbf{p}\mathbf{p}\mathbf{p}\mathbf{p} \rangle \) is expressed in terms of \( \langle \mathbf{p}\mathbf{p} \rangle \) by means of a closure, which is discussed in Appendix A.

3.6 Parallelization

The FORTRAN computer code is parallelized using the Message Passing Interface (MPI). The computational domain is divided into slices in the wall-normal direction (see Fig. 3.3(a)). On each processor Eqs. (3.1) are solved in one of these slices. In order to compute wall-normal derivatives, the variables in the grid-points in the top and bottom layers of each slice are communicated to the adjacent slices. Furthermore for solving the Fourier transformed Poisson equation (3.7), the data are transposed into slices in the stream-wise direction (see Fig. 3.3(b)). After the matrix equations are solved, the pressure data are transposed back to the original slice-configuration.
3.7 CPU-Requirements

Finally we comment on the CPU-requirements for a typical run. A time integration over 20 time units of a non-Newtonian flow with $Re_\tau = 360$ and $\alpha = 25$ using $L_x = 4.5$, $L_z = 2.25$ and $\Delta t = 10^{-4}$ on $96^3$ grid-points requires a total of $2 \times 10^6$ time steps, taking 30 days on a single AMD Opteron 2.0 GHz processor.
Chapter 4

On the Performance of the Moment Approximation for the Numerical Computation of Fibre Stress in Turbulent Channel Flow

Fibre-induced drag reduction can be studied in great detail by means of Direct Numerical Simulation (DNS) (Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin 2004). To account for the effect of the fibres, the Navier-Stokes equations are supplemented by the fibre stress tensor, which depends on the distribution function of fibre orientation angles. We have computed this function in turbulent channel flow, by solving the Fokker-Planck equation numerically. The results are used to validate an approximate method for calculating fibre stress, in which the second moment of the orientation distribution is solved. Since the moment evolution equations contain higher order moments, a closure relation is required to obtain as many equations as unknowns. We investigate the performance of the Eigenvalue-Based Optimal Fitted (EBOF) closure scheme (Cintra and Tucker 1995). The closure predicted stress and flow statistics in two-way coupled simulations are within 10% of the ‘exact’ Fokker-Planck solution.

4.1 Introduction

It is well known that the addition of a small amount of long-chained flexible polymers to a turbulent pipe flow can induce changes in the turbulent structures, leading to a reduction of the drag (Ptasinski et al. 2003). Similar but less profound effects have also been observed using stiff polymers (Paschkewitz et al. 2005), and macroscopic slender particles (McComb and Chan 1985). An extensive overview w.r.t. drag reduction can be found in Gyr and Bewersdorff (1995).

It is a generally accepted assumption that the key properties of a polymeric liquid are elasticity and viscous anisotropy. Elasticity originates from the ability of polymers to stretch and

A slightly different version of this chapter is published as an article in Physics of Fluids (Gillissen et al. 2007a)
recoil, introducing a mechanism of energy transfer between the polymers and the fluid. Viscous anisotropy, or a directional dependent viscosity, is the result of the anisotropic distribution of polymer orientation angles.

The physical mechanisms underlying polymer-induced drag reduction are not well understood and numerical tools have widely been used to gain deeper insight. Most numerical work on polymer-induced drag reduction is based on computing the additional stress generated by the polymers, which is added to the Navier-Stokes equations. Commonly, the constitutive models for the stress tensor are expressions in moments of the statistical distribution of polymer configuration. Due to the nonlinear nature of polymer motion, moment evolution equations suffer from a closure problem. In this paper we study the closure problem, involved in the computation of the stress in a suspension of rigid rod-like polymers, referred to as fibres.

In contrast to flexible polymers, numerical simulations of turbulent fibre suspensions are rare. To the authors’ knowledge only the Stanford group has published on so-called two-way coupled turbulent flow simulations, in which the fibre dynamics are solved as well as the interaction between the fibres and the fluid (Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin 2004). Their method is based on a moment equation derived using a closure. They find that Brownian motion has an adverse effect on drag reduction. Contributions of the different stress components to the momentum and energy equations are studied in detail. Drag reduction is found to originate from the damping of the near wall vortices by cross-stream fibre alignment in the bi-extensional inter-vortex regions.

In stead of solving fibre moments, a more direct approach is to solve the complete distribution function, which is governed by the Fokker-Planck equation. This method is ‘exact’, since it does not require a closure relation. On the other hand it requires much more computational resources as compared to the moment approximation. Numerical solutions of the distribution function can be obtained by computing the trajectories and orientations of individual particles. Manhart (2003) adopted such a method, and studied the influence of particle aspect ratio and Brownian motion on fibre stress. He finds that the rheological properties deviate from Newtonian with increasing aspect ratio \( r \), and for very large aspect ratio \( r > 100 \) the properties remain unchanged. Furthermore with increasing Brownian diffusion, the mean of the stress increases and the standard deviation of the stress decreases.

In this study the spatial and orientational operators in the Fokker-Planck equation are discretized to obtain the fibre distribution function in turbulent channel flow. These solutions are used to investigate the performance of the EBOF closure (Cintra and Tucker 1995), used in the evolution equation for the second moment of this function. To fully study the effect of the closure on the fluid mechanics, two-way coupled simulations are performed. A brief comparison in Newtonian turbulent channel flow has been reported earlier in Paschkewitz, Dimitropoulus, Hou, Somandepalli, Mungal, Shaqfeh and Moin (2004). The closure predicted mean stress was found to differ up to 30% from the Fokker-Planck solutions taken from Manhart (2003).

The paper is organized as follows. In Sec. 4.2 the theory for the stress in a fibre suspension is explained. Sec. 4.3 deals with the numerical procedure for calculating the fibre distribution function. Then in Sec. 4.4 the moment approximation and the involved closure problem are discussed. In Sec. 4.5 the numerical details for solving the turbulent fibre suspension channel flow are given. Results from the moment approximation and the Fokker-Planck equation are compared in Sec. 4.6. Conclusions are given in Sec. 4.7. In Appendix A the EBOF closure is explained.
4.2 Constitutive Equations

An extensive treatment of the theory given in this section can be found in Doi and Edwards (1986). We consider Brownian rigid rods which are homogeneously suspended in a Newtonian solvent. The fibre volume fraction is \( c \) and the solvent viscosity is \( \mu \). The fibres are monodispersed, inertia-free, neutrally buoyant, non-interacting and much smaller than the length scale over which the fluid velocity gradient changes. The flow around an individual fibre is governed by Stokes equations. Under these assumptions the fibre center of mass \( \mathbf{x} \) and the fibre orientation unit vector \( \mathbf{p} \) evolve according to:

\[
\dot{\mathbf{x}} = \mathbf{u} - \kappa_s \nabla \ln \Psi, \quad \dot{\mathbf{p}} = \nabla \mathbf{u}^T \cdot \mathbf{p} - \nabla \mathbf{u}^T : \mathbf{ppp} - \kappa_r \nabla \ln \Psi, \tag{4.1}
\]

where the effect of finite \( r \) has been neglected. We only consider the behavior in the limit of infinite \( r \). Here \( \mathbf{u} \) is the local fluid velocity, \( \nabla \) is the gradient operator in physical space, \( \nabla_p \) is the gradient operator on the unit sphere, \( \kappa_s \) is the spatial diffusion rate and \( \kappa_r \) is the rotational diffusion rate.

The distribution function \( \Psi(\mathbf{p}, \mathbf{x}, t) \) gives the probability of finding a fibre with orientation \( \mathbf{p} \) at position \( \mathbf{x} \) and time \( t \). Since the fibres are homogeneously suspended, the sum of the orientation probabilities is independent of position and time and set to one:

\[
\int d\mathbf{p} \Psi = 1. \tag{4.2}
\]

The evolution of \( \Psi \) is described by the Fokker-Planck equation:

\[
\frac{\partial \Psi}{\partial t} + \nabla \cdot (\dot{\mathbf{x}} \Psi) + \mathbf{u} \cdot (\dot{\mathbf{p}} \Psi) = 0. \tag{4.3}
\]

Together with the equations of fibre motion (4.1) the Fokker-Planck equation reads:

\[
\frac{\partial \Psi}{\partial t} + \nabla \cdot (\mathbf{u} \Psi) + \nabla_p \cdot \left( [\nabla \mathbf{u}^T \cdot \mathbf{p} - \nabla \mathbf{u}^T : \mathbf{ppp}] \Psi \right) - \kappa_s \nabla^2 \Psi - \kappa_r \nabla^2_p \Psi = 0. \tag{4.4}
\]

Function \( \Psi \) determines the additional stress \( \boldsymbol{\tau} \) in the suspension generated by the fibres. In the limit of \( r \to \infty \):

\[
\boldsymbol{\tau} = \alpha \mu \left[ 2 \nabla \mathbf{u} \cdot \langle \mathbf{ppp} \rangle + 6 \kappa_r \left( \langle \mathbf{pp} \rangle - \frac{1}{3} \delta \right) \right]. \tag{4.5}
\]

where \( \langle \cdots \rangle \) signifies the orientational average over \( \Psi \):

\[
\langle \cdots \rangle = \int d\mathbf{p} \Psi \cdots, \tag{4.6}
\]

\( \alpha \) is the concentration parameter:

\[
\alpha \approx 0.1cr^2, \tag{4.7}
\]

and \( \delta \) is the unit tensor. Two stress contributions can be distinguished in Eq. (4.5). The viscous stress \( \alpha \mu 2 \nabla \mathbf{u} \cdot \langle \mathbf{ppp} \rangle \) equals the projection of the Newtonian viscous stress on to the fibre directional vectors. The elastic stress \( 6 \alpha \mu \kappa_r \left( \langle \mathbf{pp} \rangle - \frac{1}{3} \delta \right) \) originates from the Brownian tendencies to move the distribution towards isotropy.
4.3 Numerical Method for the Fokker-Planck Equation

4.3.1 Galerkin’s Method

Our numerical solution procedure for the orientation part of the Fokker Planck equation (4.4) utilizes Galerkin’s principle with the spherical harmonics as the trial functions. The technique has been used for the case of simple shear in Stewart and Sorensen (1972). For simplicity we use a short notation for the rotational advection operator in Eq. (4.4):

\[
\partial_t \Psi + \sum_{i,j} \nabla u_{ij}^T M_{ij} \Psi - \kappa_r \nabla_p^2 \Psi = 0.
\]  

(4.8)

In general function \( \Psi \) is not only a function of time and orientation but it is also a function of position. However, since we are concerned here with the numerical method for solving the orientation dependence of \( \Psi \), the dependence upon the position is suppressed. The methods used to solve the spatial dependence are discussed in Sec. 4.5. The orientational part of function \( \Psi \) is expanded in spherical harmonics up to degree \( N \):

\[
\Psi^N = \sum_{l=0}^{N} \sum_{m=-l}^{l} A_l^m \Phi_l^m, \tag{4.9}
\]

with \( A_l^m \) the expansion coefficients and \( \Phi_l^m \) the spherical harmonics of degree \( l \) and order \( m \) (Abramowitz and Stegun 1965). The series expansion is inserted into Eq. (4.8), giving:

\[
\frac{\partial}{\partial t} \sum_{l,m} A_l^m \Phi_l^m + \sum_{i,j} (\nabla u)^T_{ij} M_{ij} \sum_{l,m} A_l^m \Phi_l^m + \kappa_r \sum_{l,m} l(l+1) A_l^m \Phi_l^m = R^N. \tag{4.10}
\]

Here we have used that \( \nabla_p^2 \Phi_l^m = -l(l+1) \Phi_l^m \). Due to the finite truncation the r.h.s. of Eq. (4.10) is not zero but equal to the residual function \( R^N \). The \( A_l^m \) are obtained using Galerkin’s method by setting the residual function orthogonal to all basisfunctions \( \Phi_l^m \) up to degree \( N \). Using the orthogonality property of the spherical harmonics, this yields:

\[
\frac{\partial}{\partial t} A_l^m + \sum_{i,j} (\nabla u)^T_{ij} \sum_{l,m} (\Phi_l^m | M_{ij} \Phi_l^m) A_l^m + \kappa_r p(p+1) A_p^m = 0, \tag{4.11}
\]

where the inner product is defined as \( (a | b) = \int dp ab \). The coefficients \( (\Phi_l^m | M_{ij} \Phi_l^m) \) are computed numerically using Gauss-Legendre integration (Schwarztrauber 2002). The normalization condition (Eq. 4.2) requires \( A_0^0 = 1 \) and point symmetry \( \Psi(-p) = \Psi(p) \) requires \( A_l^m = 0 \) for odd \( l \).

4.3.2 Accuracy

Here we study the accuracy of the method outlined above for the case of simple shear:

\[
\nabla u^T = \begin{pmatrix} 0 & \gamma & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{4.12}
\]
4.3. Numerical Method for the Fokker-Planck Equation

with $\gamma$ the shear rate. The stationary solution to Eqs. (4.11) and (4.12), obtained using a LU-solver, depends on two parameters: the order of truncation $N$ and the rotary Peclet number $Pe_r$. This number is defined as the ratio of the characteristic shear and the rotary diffusion coefficient:

$$Pe_r = \frac{\sqrt{\frac{1}{2} (\nabla u + \nabla u^T)^2}}{\kappa_r}. \quad (4.13)$$

When suspended in shear flow fibres tend to align in the streamwise direction. The level of fibre alignment is controlled by Brownian motion, which smears out the distribution function. With increasing $Pe_r$ (diminishing rotary diffusion), $\Psi$ evolves from isotropic to localized in the streamwise direction. Since in that direction there is no strain, an increase in alignment results in a decrease in shear stress. This so-called shear thinning phenomenon is illustrated in Fig. 4.1, showing the shear viscosity $\eta_{xy}$ as a function of $Pe_r$.

$$\eta_{xy} = \frac{\tau_{xy}}{\alpha \mu \gamma}. \quad (4.14)$$

In Fig. 4.1 we also show the truncation error $e^N$, which is defined as:

$$e^N = \sqrt{\frac{\int dp (\Psi^N - \Psi)^2}{\int dp \Psi^2}}. \quad (4.15)$$

Here we approximated the exact solution $\Psi$ with $\Psi^{48}$, which for this case gave almost identical results as with $\Psi^{64}$. With increasing $Pe_r$, the peak width of $\Psi$ decreases and more modes are needed to accurately approximate this shape. Accordingly, the value of $N$ required
for an accurate solution increases with \( Pe_r \). This dependence is used in choosing the values for \( Pe_r \) and \( N \) in the turbulent channel flow simulations described in Sec. 4.5.

4.4 Moment Approximation

4.4.1 Moment Evolution Equations

The distribution of fibre orientation depends both on spatial and orientation coordinates (Eq. 4.4). As a consequence numerical computations are very expensive. However, the fibre stress depends solely on its second and fourth order moments \( \langle pp \rangle \) and \( \langle pppp \rangle \). A direct computation of these moments by solving the corresponding transport equations reduces computational costs considerably. The moment transport equations are derived by multiplying the Fokker-Planck equation (4.4) by \( pp \) (or \( pppp \) or etc.) and subsequently integrating over the orientation angles. By this procedure the evolution equation for the second moment is found to be (Doi and Edwards 1986):

\[
\frac{\partial \langle pp \rangle}{\partial t} + u \cdot \nabla \langle pp \rangle - \nabla u^T \cdot \langle pp \rangle - \langle pp \rangle \cdot \nabla u + 2 \nabla \cdot (ppp) - \kappa_s \nabla^2 \langle pp \rangle - 6 \epsilon_r \left( \frac{1}{3} \delta - \langle pp \rangle \right) = 0.
\]

The unknown fourth moment \( \langle pppp \rangle \) appears in the equation of change for the second moment. In fact all moment evolution equations contain higher order moments and the system of moment evolution equations can never be closed. This is a consequence of the nonlinear dependence of fibre rotation on fibre orientation (Eq. 4.1). To obtain a closed set of moment equations an ad hoc relation must be adopted to express a higher order moment in terms of a lower moment. The error introduced by this so-called closure relation is the subject of the present study.

4.4.2 Closure

In terms of the expansion (Eq. 4.9) the closure relates \( A^m_4 \) to \( A^m_2 \). Since in the \( \langle pp \rangle \)-principal frame there are three non-zero \( A^m_4 \) and two non-zero \( A^m_2 \), \( \langle pppp \rangle \) is related to \( \langle pp \rangle \) through three scalar functions depending on two scalar arguments (Cintra and Tucker 1995). These relations can be constructed by parameterizing the distribution function (Chaubal and Leal 1997) or by fitting ‘exact’ solutions of the Fokker-Planck equation (Cintra and Tucker 1995, Chung and Kwon 2002). In this work, we study the EBOF (Eigenvalue-Based Optimal Fitted) closure proposed by Cintra and Tucker (1995). It is an expression in principal values of \( \langle pppp \rangle \) and \( \langle pp \rangle \) fitted to solutions of the Fokker-Planck equation for simple flows. The IBOF (Invariant-Based Optimal Fitted) closure, used for the turbulent flow calculations in Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin (2004), is similar to EBOF, except that it is formulated in terms of the tensor invariants. Both methods are proved to be of equal accuracy and are probably the best schemes available at present (Chung and Kwon 2002).

We have constructed three EBOF schemes, fitting solutions of the Fokker-Planck equation at three different rotary Peclet numbers \( Pe_r = 50, 200 \) and 800. The details and results of this procedure are given in Appendix A. We refer to these schemes as EBOF50, EBOF200 and EBOF800. In Fig. 4.1 we show the performance of these closures in predicting the shear viscosity (Eq. 4.14) as a function of \( Pe_r \). The solid line shows the ‘exact’ solution computed
with the Fokker-Planck equation. In the weak flow regime $Pe_r < 10$ the closures produce the correct result $\eta_{xy} = 1/3$. For larger $Pe_r$ the closures produce a power law $\eta_{xy} \sim Pe_r^n$ with a smaller exponent $n \approx -0.45$ than the exact value of $-1/3$. Eventually at even larger $Pe_r$ the closures produce qualitatively wrong results, $\eta_{xy}$ deviates from the power law and approaches a constant.

It is likely that the EBOF closure performs best for flow problems in which $Pe_r$ matches $Pe_r$ used in the fit solutions. With increasing $Pe_r$ these solutions become increasingly expensive with the spherical harmonics method. Therefore, for relatively large $Pe_r$ a particle method like Manhart (2003) would be more suitable.

The subject of this paper is the performance of the EBOF closure in two-way coupled turbulent fibre suspension channel flow. With increasing $Pe_r$ the convergence of the expansion (Eq. 4.9) decreases, effectively increasing the importance of the $l = 4$ modes and the closure. Therefore the simulations are carried out at $Pe_r$ as large as numerically feasible. A difficulty in turbulent flow is the wide variety of Peclet numbers, making the choice of $Pe_r$ used in the fit data an important issue. The effect of this choice is studied in Sec. 4.6.1.

4.5 Numerical Method for the Turbulent Channel Flow

4.5.1 Eulerian Method

We numerically solve the incompressible Navier-Stokes equations complemented by the divergence of the fibre stress (Eq. 4.5) in the channel geometry (Fig. 3.1):

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla \Pi + \nu \nabla^2 \mathbf{u} + \frac{1}{\rho} \nabla \cdot \tau, \quad \nabla \cdot \mathbf{u} = 0. \tag{4.17}$$

Here $\Pi$ is the pressure, $\rho$ is the mass density and $\nu = \mu/\rho$ is the kinematic viscosity. The fibre stress is computed using two methods: the Fokker-Planck equation (4.4) and the moment equation (4.16) closed with EBOF200 (Appendix A). The flow is driven between two parallel no-slip walls by means of a constant pressure gradient $-\partial \Pi/\partial x$. Periodic boundary conditions are imposed in the homogeneous directions $x$ and $z$. Wall normal derivatives of $\Psi$ and its moments are zero at the walls.

We use a pseudo-spectral flow solver, which is similar to the one used by Ptasinski et al. (2003). Spatial derivatives are computed with a Fourier-basis for the homogeneous directions and a second order central finite differences scheme for the wall normal direction. Time integration is achieved with the second order explicit Adams Bashforth scheme. Conservation of mass is ensured using a standard projection method. Poisson’s equation is transformed to Fourier space in the homogeneous directions and a tri-diagonal solver is used for the resulting three band matrices. The variables are discretized on a non-equidistant staggered mesh. Fibre orientation, pressure and the velocity components in the homogeneous directions are defined in the cell centers. The wall normal velocity component is defined on the cell faces.

The concentration parameter $\alpha = 10$ (Eq. 4.7). This implies $n l^3 \sim 100$, with $l$ the fibre length and $n$ the number of fibres per unit volume. This parameter value corresponds to a semi-dilute suspension, meaning that fibre-fibre interactions are important (Doi and Edwards 1986).
For simplicity we don’t take these effects into account. Our main focus is the fourth order moment closure. The Reynolds number

$$Re_{r} = \frac{U_{r}D}{\nu} = 449,$$  \hspace{1cm} (4.18)

where $U_{r}$ is the friction velocity $U_{r} = [-\overline{(d\Pi/dx)(D/\rho)(1/2)})^{1/2}$ and $D$ is the full channel height. The effective Reynolds number

$$Re_{eff} = \frac{U_{r}D}{\nu_{eff}},$$  \hspace{1cm} (4.19)

is based on the effective viscosity at the wall $\nu_{eff}$:

$$\nu_{eff} = \frac{\nu}{\overline{|\tau_{xy}|}} + \frac{1}{\rho} \left| \overline{\tau_{xy}} \right| \bigg|_{walls},$$  \hspace{1cm} (4.20)

where $\tau_{xy}$ is the fibre shear stress and the bar signifies averaged. The effective Reynolds number is around 250 being somewhat different for the Fokker-Planck simulation and the moment simulation. We use this relatively low value for $Re_{eff}$ due to two computational restrictions. First, the number of spatial grid points, necessary to resolve all the scales in the turbulent flow increases as $Re_{eff}^{9/4}$. To solve the Fokker-Planck equation an orientation resolution is required on top of the spatial resolution. Secondly, the time step needed to ensure a stable simulation of the Fokker-Planck equation is inversely proportional to the maximum shear rate in the channel, which in turn is proportional to the Reynolds number.

As argued in Sec. 4.4.2 we aim at testing the closure at $Pe_{r}$ as large as possible. With increasing $Pe_{r}$ the gradients in the orientational part of $\Psi$ become steeper, and more spherical basis functions are required to accurately describe $\Psi$. We decided that for $N = 12$ (91 orthogonal modes) the computation is still tractable. Allowing a maximum truncation error of $1\%$, it follows from Fig. 4.1 that we can use a maximum value of $Pe_{r} = 50$. Since the largest shear rates occur at the wall, this Peclet number is based on the mean shear rate at the wall:

$$Pe_{r} = \frac{U_{r}^{2}}{\nu_{eff} \kappa_{r}}.$$  \hspace{1cm} (4.21)

Note that this is a global definition. The local the Peclet number (Eq. 4.13) varies over space and time. The spatial Peclet number is defined as:

$$Pe_{s} = \frac{U_{r}D}{\kappa_{s}}.$$  \hspace{1cm} (4.22)

Since $Pe_{s}/Pe_{r} \sim (D/l)^2/Re_{eff}$ (Doi and Edwards 1986), realistic $Pe_{s}$-values are relatively large. The characteristic scales of the spatial variation of $\Psi$ decrease with $Pe_{s}$, analogous to that of passive scalars (Batchelor 1959). This causes $\Psi$ to be very detailed spatially, requiring an unfeasible number of grid points. Since under-resolving results in numerical instabilities, we have to use an artificial small value for $Pe_{s}$. Tests have shown that our numerical solution is stable and well-behaved up to $Pe_{s} = 125$, which is the value used. This value is comparable to that used in other numerical studies on polymer moment equations (see for instance Ptasinski et al. (2003)). The effect of a relatively large artificial diffusivity on the solution of the Fokker-Planck equation will be investigated in depth in a subsequent work. Here we note that these
4.6. Results

effects are most likely to be similar to those observed in polymer moment equations, where it is generally found that the numerical solution does not change significantly for values larger than $Pe_s \sim Re_{eff} \Delta v_{eff} / \Delta x^2$. Here $\Delta x$ is the typical mesh dimension and $\Delta t$ the time step. So-called local artificial diffusion schemes have been developed to minimize the diffusion influence (Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin 2004). This technique could not be used here since it yields local $\text{det}(pp) < 0$, causing instabilities in the Fokker-Planck solution.

The channel dimensions and number of grid points are $5D \times D \times 2.5D$ and $96 \times 96 \times 96$ in the streamwise $x$, wall normal $y$ and spanwise $z$ direction. The grid is non-uniform in $y$ with a 4% increase in cell-volume per cell away from the wall. The grid-cell size in $\nu_{eff}/U_r$-units (wall-units) at the wall and in the channel center are $13.0 \times 1.2 \times 6.5$ and $13.0 \times 4.7 \times 6.5$ in the $x$, $y$ and $z$ direction. Except in the wall-normal direction close to the wall, the grid-cell size matches the one used by (Kim et al. 1987), which is generally accepted as resolving all relevant turbulent scales. A time step of $\Delta t = 5 \times 10^{-5} D/U_r$ is used. After the simulation is statistically converged, 200 samples are collected during the time interval of $t = 5D/U_r$. A Newtonian reference case is computed using the same parameters except for $\alpha = 0$ and $Re_r = Re_{eff} = 250$.

The MPI-parallelized FORTRAN computer codes were run on AMD Opteron 2.0 GHz processors. For the Fokker-Planck simulation 7 processors were used. Together they took 300 seconds per time step. The moment simulation was run on a single processor, taking 30 seconds per time step.

4.5.2 Lagrangian Method

In Appendix A three different EBOF schemes are derived at three different $Pe_r$. We determined the relative performance of the different EBOF schemes. These preliminary tests were done at low costs by performing one-way coupled Lagrangian simulations, eliminating the computation of the spatial derivatives in the Fokker-Planck equation. The reduced cost allows a larger $Pe_r$ so that the influence of this parameter on closure performance can be studied. Therefore, two rotary Peclet numbers are considered $Pe_r = 50$ and $Pe_r = 200$. The Reynolds number is $Re_r = 360$.

To solve the Fokker-Planck equation and moment equation along the trajectories of fluid particles, fluid velocity and velocity gradient values at the position of the fluid particles are interpolated. The interpolation scheme uses the Fourier-basis in the homogeneous directions and a third order polynomial fit in wall normal direction. The position of the fluid particles is advanced in time using the second order Adams Bashforth scheme. We use $N = 32$ corresponding to 561 orthogonal basisfunctions. The domain size and number of grid points are $3D \times D \times 1.5D$ and $96 \times 96 \times 96$ in the $x$, $y$ and $z$-direction. The grid in wall normal direction is stretched as described in Sec. 4.5.1. The grid-cell size in wall units at the wall and in the channel center are $11.3 \times 1.8 \times 5.7$ and $11.3 \times 6.7 \times 5.7$. The integration is carried out over 1000 fluid trajectories over a time interval of $t = 10D/U_r$ using a time step of $\Delta t = 1.5 \times 10^{-5} D/U_r$. Statistics are computed over 1000 samples per trajectory.
4.6 Results

4.6.1 Lagrangian One-Way Coupled Simulations

Stresses computed with the Lagrangian method are given in Fig. 4.2. Only the streamwise normal stress component is considered, since the closure error in this component is largest. The stress is computed using \( \alpha = 1 \) (Eq. 4.5) and scaled with wall shear stress \( \rho U_2^2 \). Note that the stress shown in this figure is not coupled back to the equations of fluid motion, i.e. these simulations are one-way coupled. We use \( \bar{\cdots} \), \( \langle \cdots \rangle \) and \( \langle \cdots \rangle_{\text{rms}} \) to denote mean part, fluctuating part and standard deviation. Wall distance is presented in wall units, where 250 wall units correspond to the full channel height.

With increasing \( P_e_r \), the stress decreases, which is most pronounced in the viscous sublayer \( (y^+ < 10) \). This effect, also observed by (Manhart 2003), is due to shear thinning discussed
4.6. Results

Figure 4.3: Mean (Left) and standard deviation (Right) of fourth order components of $\Psi$. Comparison between Fokker-Planck equation (—) and moment equation closed with EBOF200 (—-).

in Sec. 4.3.2. It is found that the performance of the different closures depend on $Pe_r$ and wall distance. At $Pe_r = 50$ EBOF50 produces the best results for $y^+ > 10$ in both the mean and the standard deviation. For $y^+ < 10$ the mean is best captured by EBOF200, while EBOF800 produces the best standard deviation. Since the overall error for EBOF200 is smallest, this scheme is used for the two-way coupled simulations. Increasing $Pe_r$ from 50 to 200, the closure error in the stress standard deviation increases slightly. At $Pe_r = 200$, EBOF800 produces the best results for both the mean and the standard deviation.

4.6.2 Eulerian Two-Way Coupled Simulations

Figures 4.3 and 4.4 show fibre orientation and fibre stress in the two-way coupled turbulent channel flow simulation. In the viscous sublayer the flow is dominated by shear and particles are strongly orientated in the streamwise direction. Here the moments of $\Psi$ are highly anisotropic and deviate relatively little from their mean values. Further away from the wall turbulent fluctuations enhance the rms values and move the mean values towards isotropy. The moment equation closed with EBOF200 (see Appendix A) is compared to the direct computation of $\Psi$. The agreement is good. The streamwise component of $p$ is slightly overestimated and the fluctuations in $p$ are somewhat underestimated. Errors in stress are $\sim 10\%$ for both the mean and the standard deviation.

Flow statistics scaled with $U_r$, $\rho$ and $\nu_{eff}$ are presented in Figures 4.5 - 4.7, comparing Newtonian flow and non-Newtonian flow computed with the Fokker-Planck equation and the moment equation. The effective Reynolds numbers (Eq. 4.19) are $Re_{eff} = 255$ for the Fokker-Planck simulation and $Re_{eff} = 271$ for the moment simulation. This difference is because the closure predicts a lower fibre shear stress as compared to the ‘exact’ Fokker-Planck result (see Fig. 4.1). It is noted that fibre statistics differ due to the slight difference in $Re_{eff}$. Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin (2004) investigated this issue and found the difference to be quite modest at low $Re_{eff}$ values.
Before discussing closure performance in more detail, we first compare the fibre suspension flow to the Newtonian flow. Figure 4.5 reveals that the fibres reduce the drag by 5%, defined as the relative decrease in drag coefficient $f$:

$$f = \left( \frac{U'}{U} \right)^2,$$

where the bulk velocity $U$ equals the streamwise velocity averaged over the channel. Note that this reduced friction is realized when $Re_{eff}$ is kept constant. When $Re_{eff}$ would have been kept constant, we would observe a drag increase. There are modest changes in the turbulent structures, typical for a ‘drag reduced’ flow. The turbulent velocity intensity $u_{rms}$ is increased in $x$ and reduced in $y$ and $z$. The turbulent vorticity intensity $\omega_{rms}$ is increased in $z$, and reduced in $x$ and $y$. The Reynolds shear stress $-\overline{u'v'}$ (Eq. 4.24) and the production due to mean shear $P$ (Eq. 4.25) are reduced.

The comparison between the Fokker-Planck equation and the moment equation reveals the following. The mean velocity and the turbulent velocity and vorticity intensities differ less than 5%. Also the terms in the averaged momentum equation:

$$\frac{\nu}{\nu_{eff}} \frac{\partial \overline{u}}{\partial y} - \overline{u'v'} + \overline{\tau_{xy}} = 1 - 2 \frac{y}{Re_{eff}},$$

and the terms in the averaged turbulent kinetic energy equation (Tennekes and Lumley 1973):

$$-2\overline{u'v'}\frac{\partial u'}{\partial x} - \frac{\partial}{\partial x} \overline{u'v'} + \left( \frac{u'u' + 2u'^2}{\rho} \right) + \frac{\nu}{\nu_{eff}} \frac{\partial^2 u'}{\partial x^2} u' + 2\frac{\nu_{eff}}{\partial x} \frac{\partial u'}{\partial x} \frac{\partial u'}{\partial x} + 2\frac{\partial}{\partial x} \frac{\partial^2 u'}{\partial x^2} u' + 2\frac{\partial}{\partial x} \frac{\partial u'}{\partial x} + 2\frac{\partial u'}{\partial x} \frac{\partial u'}{\partial x} = 0,$$

agree very well. A relatively large error is observed for $y^+ < 5$, where the closure predicted dissipation due to fibre stress $\epsilon^f$ and the diffusion due to fibre stress $D^f$ are 10% too small. These errors are related to the error in shear-viscosity, as discussed in Sec. 4.4.2. The lower $\epsilon^f$ near the wall is linked with the lower peak value of $P$ at $y^+ \approx 15$. 
4.7 Conclusions

Two-way coupled turbulent fibre suspension flow simulations using the Fokker-Planck equation and the EBOF closure are compared at low rotary Peclet number $Pe_r = 50$, being the ratio of wall shear and rotary diffusion. The EBOF predicted fibre stress, momentum budgets and kinetic energy budgets are within 10% of the Fokker-Planck solution. A one-way coupled simulation at $Pe_r = 200$ shows a slight increase in closure error, which indicates that the error grows with $Pe_r$. Since significant drag reduction occurs for $Pe_r > 10^3$, closure performance in drag reduced flow is still an open issue.

It is possible to construct an EBOF closure which is asymptotically correct for simple shear in the limit $Pe_r \rightarrow \infty$ by imposing extra constraints on the parametric form (Eq. (A.1) in Appendix A). This would require an extension of the number of fit-parameters. Although we have not done this here, we think that this will improve results in turbulent shear flows at large $Pe_r$.

Figure 4.5: Mean (Left) and standard deviation (Right) of the fluid velocity. Comparison between Fokker-Planck equation (---), moment equation closed with EBOF200 (---) and Newtonian (---).
Figure 4.6: Left: standard deviation of vorticity. Right: Contributions to the averaged momentum equation (Eq. 4.24). Comparison between Fokker-Planck equation (—), moment equation closed with EBOF200 (--) and Newtonian (- -).

Figure 4.7: Contributions to the averaged turbulent kinetic energy equation (Eq. 4.25). Comparison between Fokker-Planck equation (—), moment equation closed with EBOF200 (--) and Newtonian (- -).
Chapter 5
The Stress Generated by non-Brownian Fibres in Turbulent Channel Flow Simulations

Turbulent fibre suspension channel flow is studied using direct numerical simulation (DNS). The effect of the fibres on the fluid mechanics is governed by a stress tensor, involving the distribution of fibre position and orientation. Properties of this function in channel flow are studied by computing the trajectories and orientations of individual particles, referred to as particle method. It is shown that, owing to computer restrictions, the instantaneous stress, needed in channel flow simulations, cannot be solved directly with the particle method.

To approximate the stress we compute the second-order moment of the fibre distribution function. This method involves an unknown sub-grid term, which is modeled as diffusion. The accuracy of the moment approximation is studied by comparing Reynolds averaged fibre stresses to results obtained from the particle method. It is observed that the errors are $\sim 1\%$ for $y^+ \gtrsim 20$, and $\sim 20\%$ for $y^+ \lesssim 20$. The model is improved by applying a wall damping function to the diffusivity.

The moment approximation is used to simulate drag-reduced channel flow. A simplified model for fibre stress is introduced as fibre viscosity times rate of strain, where fibre viscosity is defined as the ratio of Reynolds averaged dissipation due to fibre stress and Reynolds averaged dissipation due to Newtonian stress. Fluid velocity statistics predicted by the simple model compare very well to those obtained from the moment approximation. This means that the effect of fibres on turbulent channel flow is equivalent to an additional Reynolds averaged viscosity.

5.1 Introduction

Suspended linear polymers, with a large length to diameter ratio, can induce significant changes in the flow properties of the carrier fluid at volume concentrations as low as $10^{-5}$. Most striking is the reduction of the drag coefficient in turbulent pipe flow (Toms 1948).

\footnote{A slightly different version of this chapter is published as an article in *Physics of Fluids* (Gillissen et al. 2007b)}
A distinction can be made between rigid and flexible polymers. Rigid polymers (fibres) affect the carrier fluid through viscous effects only, whereas flexible polymers induce both viscous as well as elastic effects (Doi and Edwards 1986). Numerical research points out that elasticity has an adverse effect on drag reduction (Den Toonder et al. 1997, Min et al. 2003), which implies that polymer-induced drag reduction is most likely due to viscous effects. Attributing drag reduction to viscous effects is further confirmed by simulations showing that rigid polymers (Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin 2004) and flexible polymers (Ptasinski et al. 2003) induce very similar changes in the turbulent structures.

A qualitative explanation of drag reduction based on viscosity arguments was provided by Lumley (1973). It is based on the shear thinning property (Doi and Edwards 1986), causing polymer viscosity to be approximately zero in the viscous sublayer. Outside this layer turbulence induces non-zero polymer viscosity which in turn dampens the turbulence. This effect induces a thickening of the viscous sublayer and consequently a reduction of the drag. More recent studies confirmed that drag reduction can be predicted by assuming an additional viscosity which is zero in the viscous sublayer and increases with wall-distance (Benzi, Ching, Lo, L’vov and Procaccia 2005, De Angelis et al. 2004).

The problem of drag reduction is of extreme complexity since it involves the combination of polymer dynamics and turbulence. It is for this reason that a quantitative theory is still lacking, despite numerous experimental, numerical and theoretical works, conducted over the past 50 years. This paper deals with Direct Numerical Simulation (DNS) of fibre suspension channel flow. The aim is to provide a simplified picture of the fibre stress tensor, which accounts for the effect of the fibres on the fluid mechanics. Sec. 5.2 deals with numerical details of the channel flow simulation and the mathematical description of fibre stress. This stress is governed by a constitutive equation, involving the statistical distribution of fibre position and orientation. Properties of this function are derived using a particle method, i.e. by computing the trajectories and orientations of individual particles. From the analysis it follows that a direct computation of fibre stress is unfeasible. We investigate an approximate method to compute fibre stress in Sec. 5.3. The method consists of solving the second-order moments of the distribution function, referred to as moment approximation. The accuracy of this method is determined by making a comparison to the ‘exact’ particle method. In Sec. 5.4 the moment approximation is used to simulate drag-reduced channel flow. A simplified model for fibre stress is introduced as an additional viscosity. This so-called fibre viscosity is defined in such a way that the additional dissipation equals the dissipation due to the ‘exact’ fibre stress. The model is verified by a comparison to the simulation using the moment approximation. Conclusions are given in Sec. 5.5.

5.2 Governing Equations and Numerical Details

5.2.1 Channel Flow

Fibre suspension flow is governed by the incompressible Navier-Stokes equations, supplemented by the divergence of the fibre stress tensor $\tau$ (Doi and Edwards 1986).

$$\frac{D\mathbf{u}}{Dt} = \nabla \cdot \left( -\Pi\delta + 2\mu S + \tau \right), \quad \nabla \cdot \mathbf{u} = 0. \quad (5.1)$$
5.2. Governing Equations and Numerical Details

Figure 5.1: Comparison of mean (a) and standard deviation (b) of fluid velocity as a function of wall distance. Kim et al. (1987) (circles), our code on a $1.5D \times D \times 0.75D$ channel (dashed lines), our code on a $6D \times D \times 3D$ channel (solid lines).

Here $u$ is the fluid velocity vector, $t$ is time, $\nabla$ is the nabla operator, $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$ is the material derivative, $\delta$ is the unit tensor, $S = \frac{1}{2} (\nabla \mathbf{u}^T + \nabla \mathbf{u})$ is the rate of strain tensor, $\Pi$ is the pressure, $\rho$ is the solvent mass density, $\mu$ is the solvent dynamic viscosity and $\nu = \mu/\rho$ is the solvent kinematic viscosity.

Eq. (5.1) is integrated numerically in the channel geometry. The simulations discussed in Sec. 5.2 and 5.3 are one-way coupled, meaning that fibre dynamics are influenced by the flow, but not vice versa, i.e. $\tau = 0$ in Eq. (5.1). The flow is driven by means of a constant pressure gradient between two parallel no-slip walls separated a distance $D$ in $y$-direction. Periodic boundary conditions are imposed in the homogeneous directions $x$ and $z$. We use a pseudo-spectral flow solver. Spatial derivatives are computed with a Fourier-basis for the homogeneous directions and a second-order central finite differences scheme for the wall normal direction. Time integration is achieved with the second-order explicit Adams Bashforth scheme. Conservation of mass is ensured using a projection method. Poisson’s equation is transformed to Fourier space in the homogeneous directions and a tri-diagonal solver is used for the resulting tri-diagonal matrices. The variables are discretized on a non-equidistant staggered mesh. Pressure and the velocity components in the homogeneous directions are defined in the cell centers. The wall normal velocity component is defined on the cell faces.

The Reynolds number $Re_{\tau} = \rho U_{\tau}D/\mu = 360$ is based on the friction velocity $U_{\tau} = [(1/2)(-d\Pi/dx)(D/\rho)]^{1/2}$. The over-bar denotes Reynolds averaging. The channel dimensions and resolutions in $x$ (stream-wise), $y$ (wall-normal) and $z$ (span-wise) are $1.5D \times D \times 0.75D$ and $48 \times 192 \times 48$, which are similar to Jiménez and Pinelli (1999). We have chosen to use this small domain, since it allows performing simulations, using relatively little computer resources. The small domain influences the numerical solution quantitatively, while qualitatively the solution resembles the solution on large domains (Jiménez and Pinelli 1999). In the present study quantitative details are of less importance, since the aim is to compare different fibre stress models. The grid is non-uniform in $y$-direction such that $y$ of the $ith$ grid-point is given by:
Chapter 5. The Stress Generated by non-Brownian Fibres

0.5(1 + \arctan(3(i/192 - 0.5))/\arctan(1.5)). The grid-spacing in \nu/U_\tau-units at the wall and in the channel center are 11 \times 0.88 \times 5.6 and 11 \times 2.9 \times 5.6 in the \(x, y\) and \(z\) direction. This resolution resembles the one used in Kim et al. (1987), which is generally regarded as sufficient resolving the small scales of the turbulent flow. The time step is \(\Delta t = 3.6 \times 10^{-2} \nu/U_\tau^2\). According to Reynolds decomposition \(\overrightarrow{u}, (\cdots)'\) and \(\langle \cdots \rangle_{\text{rms}}\) denote mean part, fluctuating part and standard deviation. A variable with superscript \(+\) is scaled with \(\mu, \rho\) and \(U_\tau\).

In Fig. 5.1 fluid velocity statistics are compared to the data of Kim et al. (1987), who also performed DNS of turbulent channel flow at \(Re_\tau = 360\). The differences are due to different channel dimensions, which is supported by the results of a simulation performed on a larger domain with dimensions \(6D \times D \times 3D\). In Fig. 5.1 it is shown that the corresponding results agree very well with Kim et al. (1987), which verifies our simulation code.

5.2.2 Fibres

We assume a suspension of buoyantly-free, cylindrical rods of length \(l\) and diameter \(d\), with aspect ratio \(r = l/d \gg 1\). The effects of a finite \(r\) and Brownian motion are ignored. Furthermore it is assumed that the fibres are non-interacting, massless and substantially smaller than the Kolmogorov length-scale.

Under these conditions the fibres translate as material points and rotate as material lines (Doi and Edwards 1986).

\[
\dot{x} = u, \quad \dot{p} = \nabla u^T \cdot p \cdot (\delta - pp). \tag{5.2}
\]

Here \(x\) is the particle position vector, \(p\) is the particle orientation unit vector and the overdot represents time differentiation. The particle volume fraction \(c\) is homogeneous, since the distribution of material points in incompressible turbulent channel flow evolves towards homogeneity, independent of the initial distribution (Tennekes and Lumley 1973). In the following the restrictions of the above mentioned assumptions are discussed.

The effects of finite \(r\) on rotary motion (Jeffery 1922):

\[
\dot{p} = \frac{r^2 - 1}{r^2 + 1} \nabla u^T \cdot p \cdot (\delta - pp) + \frac{2}{r^2 + 1} \Omega \cdot p, \tag{5.3}
\]

are of order \(r^{-2}\) and can therefore be ignored for \(r \gtrsim 100\). Here \(\Omega = \frac{1}{2} (\nabla u^T - \nabla u)\) is the vorticity tensor.

Brownian motion induces diffusion on fibre position and orientation. Adding diffusion to fibre rotation gives:

\[
\dot{p} = \nabla u^T \cdot p \cdot (\delta - pp) - \kappa_r \nabla p \ln \Psi, \tag{5.4}
\]

where \(\Psi(p, x, t)\) is the probability of finding a fibre with orientation \(p\) at position \(x\) at time \(t\). The rotary diffusivity \(\kappa_r = 1/t_B\), where \(t_B\) is a diffusion time scale (Doi and Edwards 1986):

\[
t_B \approx \frac{\mu l^3}{10 k_B T}, \tag{5.5}
\]

with \(k_B \approx 1.4 \times 10^{-23} \text{ m}^2 \text{ kg} \text{ s}^{-2} \text{ K}^{-1}\) the Boltzmann constant and \(T\) the temperature. For simplicity we have ignored the logarithmic dependence of the numerical factor 10 on the fibre
aspect ratio in Eq. (5.5). Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin (2004) simulated fibre suspension channel flow at $Re_e \approx 700$, $c = 7.5 \times 10^{-3}$, $r = 100$ and $t_B/t_L \approx 25$, with $t_L$ the large eddy turn-over time $t_L \approx (D^2/v)Re_e^{-1}$. The drag coefficient was 18.5% smaller than the corresponding value in Newtonian flow. Increasing $t_B/t_L$ from 25 to $\infty$ induced a further marginal change of 0.6% to the drag coefficient. This means that in the study of drag reduction Brownian motion can be neglected for $t_B/t_L \gtrsim 100$. We can recast this condition into a minimum fibre length. If we assume: $Re_e = 360$, $r = 100$, $T = 3 \times 10^2$ K, $\nu = 1 \times 10^{-6}$ m$^2$s$^{-1}$, $\rho = 10^3$ kg m$^{-3}$ and $D = 5 \times 10^{-2}$ m then $l \gtrsim 3 \times 10^{-8}$ m, in order for the neglect of Brownian motion to be justified. This constraint is met by commercially available rigid-rod like polymers. 

For instance the xanthan polysaccharide and the schizophyllum polysaccharide used in drag reduction experiments have a length of $l \approx 1 \times 10^{-6}$ m (Sasaki 1991a).

The assumption that the particle length $l$ is smaller than the Kolmogorov length scale $l_K \approx D Re_e^{-3/4}$ (Tennekes and Lumley 1973) is valid when $l/D \ll Re_e^{-3/4}$. Assuming fibre length to be smaller than one tenth of the Kolmogorov length scale at $Re_e = 360$ and $D = 5 \times 10^{-2}$ m gives $l \lesssim 6.0 \times 10^{-5}$ m.

Fibres being smaller than $l_K$ implies that inertial effects of the fibres can be neglected and that the surrounding fluid flow is governed by the Stokes equations. It further implies that the undisturbed velocity field in the vicinity of the fibres can be considered a linear function of space.

When considering interactions, it is convenient to distinguish between different regimes of concentration (Doi and Edwards 1986). In the dilute regime $cr^2 \lesssim 1$, the distance $s$ between a fibre and its nearest neighbor $s \gtrsim l$ and interactions can be neglected. In the semi-dilute regime $cr^2 \gtrsim 1 \gtrsim cr$, the spacing between the fibres is $s \lesssim l$ but $s \gtrsim d$. Although physical contacts are rare, the fibres are affected by hydrodynamic interactions. In the concentrated regime $cr \gtrsim 1$, the spacing is $s \lesssim d$ and fibres are in constant physical contact with each other. Drag reducing suspensions fall within the semi-dilute regime. Folgar and Tucker (1984) measured fibre orientation in laminar shear flow of semi-dilute suspensions with $r = 83$ and $cr^2$ ranging between $(3 - 40)$. They interpreted the effect of interactions as a rotary diffusivity $\kappa_r$ proportional to the characteristic shear rate $\gamma$.

$$\kappa_r = C_I \gamma.$$ (5.6)

The proportionality constant $C_I$ defines the relative importance of hydrodynamic interactions on fibre motion. This parameter was found to range between $(3 - 4) \times 10^{-3}$. These rather low values suggest that neglecting interactions does not introduce too large errors.

### 5.2.3 Fibre Distribution Function

The probability $\Psi(p, x, t)$ of finding a fibre with orientation $p$ at position $x$ at time $t$ is governed by (Doi and Edwards 1986):

$$\frac{\partial \Psi}{\partial t} + \nabla \cdot (\dot{x} \Psi) + \nabla_p \cdot (\dot{p} \Psi) = 0, \quad \int \Psi d\Omega = 1,$$ (5.7)

where $\nabla_p$ is the nabla operator on the unit sphere $\Omega$ and $\dot{x}$ and $\dot{p}$ are given by Eq. (5.2). The first equality in Eq. (5.7) is referred to as the Fokker-Planck equation. It describes the advection of probability in fibre position and orientation space. The second equality in Eq. (5.7)
Figure 5.2: (a) Development of the first and third eigenvalues $a_{11}$ and $a_{33}$ of $\mathbf{pp}$ along a fluid path. (b) The two-point correlation $\Gamma$ of $\mathbf{qq}$, with $\mathbf{q}$ defined in Eq. (5.8). (c) Absolute value of Fourier-transform of $\Gamma$ (dots).

is needed due to homogeneity of the Fokker-Planck equation. It expresses that the spatial fibre distribution is homogeneous.

A particle method is used to identify properties of $\Psi$ in turbulent Newtonian channel flow. The simulations are one-way coupled. The method is similar to the one used by Manhart (2003) and involves computing fibre trajectories in position and orientation space, governed by Eqs. (5.1) and (5.2). Fluid velocity and velocity gradient values at the position of the particles are interpolated. The interpolation scheme uses the Fourier-basis in the streamwise direction and a third order polynomial fit in spanwise and wall-normal directions. We use expensive Fourier interpolation rather than polynomial interpolation in the streamwise direction, since the latter induces large wiggles with period $\Delta_x/u_x$ in the time signal of particle velocity. Here $\Delta_x$ is the grid-spacing in streamwise direction. The position and orientation of the fibres is advanced in time with the second-order Adams Bashforth scheme.

First, we study the $p$-dependence of $\Psi$, by computing $p(t)$ of $10^4$ fibres which follow the
same material point \( x(t) \). The initial conditions for the orientation of the fibres are random. Fig. 5.2(a) shows the development of the eigenvalues \( a_{ii} \) of \( \langle pp \rangle \). Here the average \( \langle \cdots \rangle \) is taken over the particles which follow the same material point. By definition: \( a_{11} + a_{22} + a_{33} = 1 \) and \( a_{11} \geq a_{22} \geq a_{33} \geq 0 \). It appears that \( \Psi \) develops from the isotropic initial distribution \((a_{11} = 1/3)\) via a planar distribution \((a_{33} = 0)\) into a uni-directional distribution \((a_{11} = 1)\). This demonstrates that after a finite time interval, of approximately \( 10^3 \nu / U_r^2 \), the orientation of a fibre does not depend on its initial conditions. This effect is related to the tendency of the fibres to align parallel to the direction of the greatest principal rate of extension. Fibre orientation being independent of initial conditions implies that each point in the space-time domain corresponds to one unique fibre orientation. Thus we can write for the distribution function:

\[
\Psi(p, x, t) = \delta(p - q(x, t)) ,
\]

with \( \delta(\cdots) \) the Dirac-delta function and \( q(x, t) \) the direction of a fibre at position \( x \) at time \( t \). It is noted that the same behavior occurs (not shown) when the effects of a finite aspect ratio are taken into account in the description of fibre rotation, i.e. when rotation is given by Eq. (5.3).

Next the \( x \)-dependence of \( \Psi \) is studied. For this purpose a simulation is carried out of Eqs. (5.1) and (5.2) for \( 10^6 \) particles with initial random \( x \) and \( p \). After \( 10^3 \nu / U_r^2 \) time units, fibre orientation is assumed independent of initial conditions. To study how the fibres
are orientated with respect to each other we consider a correlation function $\Gamma$. This function expresses the relative orientation of two fibres, which are separated in space but not in time, as a function of the spatial separation $|dx|$ between the two fibres. The correlation $\Gamma(|dx|)$ is defined as the squared inner product $(q_1 \cdot q_2)^2 = \cos(\theta)^2$ averaged over fibre pairs. Here $\theta$ is the angle between the orientation vectors $q_1$ and $q_2$ of a fibre pair as sketched in Fig. 5.3. Fully correlated and uncorrelated orientations correspond to $\Gamma = 1$ and $\Gamma = 1/3$, respectively. The statistical errors, related to the finite sample size, restrict the range for which $\Gamma$ is accurately determined to $|dx|^+ \geq 0.05$. It means that the number of particle pairs, which are separated a distance $\leq 0.05$ from each other, is inadequate to obtain an accurate prediction for $\Gamma(|dx|)$. The result in Fig. 5.2(b) shows that $\Gamma(|dx|^+ = 0.05) = 0.88$. This indicates that there are significant variations of fibre orientation over a length-scale much smaller than the Kolmogorov length-scale. To show that this behavior is closely related to that of turbulent advection of a passive scalar, we show in Fig. 5.2(c) the power spectrum of $qq$, defined as the Fourier-transform of $\Gamma$. For wavenumber $k > 2\pi/l_K$, the spectrum decays as $k^{-1}$, similar to the energy spectrum of a passive scalar in turbulent flow at small diffusivity (Batchelor 1959). Here $l_K$ is the Kolmogorov length scale, which is estimated as $2\pi/l_K^+ \approx 2\pi Re^{-1/4} \approx 1.4$.

### 5.2.4 Fibre Stress

The fibre stress $\mathbf{\tau}$ in Eq. (5.1) equals the rate of strain projected on the fibre directional vectors by means of a double contraction with the fourth-order moment of the fibre distribution function (Doi and Edwards 1986):

$$\mathbf{\tau} = 2\alpha \mu S : \langle pppp \rangle, \quad \alpha \approx 0.1cr^2. \quad (5.9)$$

In the expression for the fibre concentration parameter $\alpha$, we have ignored the logarithmic dependence of the numerical factor 0.1 on the aspect ratio.
5.3. Moment Approximation

Eq. (5.9) involves averaging $\langle \cdots \rangle$ over fibres contained in a volume $V$, surrounding the point at which the stress is to be determined. The average can be expressed as an integral over the unit sphere $\Omega$ and $V$, weighted with $\Psi$.

$$
\langle \cdots \rangle(x, t) = \frac{1}{V} \int_V dV \int_\Omega d\Omega \Psi(p, y, t) \cdots ,
$$

(5.10)

By definition the dimensions of $V$ are smaller than the smallest length-scales of $\nabla u$, such that $\nabla u$ may be considered constant in $V$. The number of particles needed to accurately compute stress in turbulent channel flow is estimated by assuming that $\nabla u$ does not change appreciably over $10 \nu/U_\tau$-units, being the grid spacing in streamwise direction in well-resolved simulations (Kim et al. 1987). Fig. 5.2(b) shows that $1 - \Gamma(|dx|^2 = 10) \approx 0.45$ indicating that fibre orientation within a grid-cell is distributed with standard deviation $\sim 1$. Assuming fully uncorrelated fibre orientations within one grid-cell, we estimate the standard deviation of the sum of these orientations as $\sim 1/\sqrt{N}$, where $N$ is the number of fibres per grid-cell. Thus for a $10\%$ accuracy in stress $\sim 10^2$ particles per grid-cell are necessary. A direct numerical simulation of channel flow at low $Re_\tau$ requires $\sim 10^6$ grid-cells and thus a total of $\sim 10^8$ particles. Due to the need for a spectral interpolation scheme, as explained in Sec. 5.2.3, simulating such large numbers of particles is an extremely demanding task.

Due to the inadequate number of particles, instantaneous stress cannot be computed from our particle simulation. Reynolds averaged stresses however, can be computed and are plotted in Fig. 5.4(a), using $\alpha = 1$. To compute these averages it is assumed that $\langle \cdots \rangle = \overline{\cdots}$. It is noted that these stresses are not coupled to the fluid equations of motion. An interesting feature is that at the wall all stress components are zero, i.e. fibres orient in directions of zero strain rate. This is related to the fact that at the wall $S = S_{xy}(e_x e_y + e_y e_x) + S_{yz}(e_y e_z + e_z e_y)$ and the observation that at the wall $p_y = 0$, as shown in Fig 5.4(b). Here $e_i$ are the Cartesian unit vectors.

5.3 Moment Approximation

5.3.1 Moment Evolution Equation

As pointed out in the previous section, instantaneous fibre stress cannot be computed using a particle method. A statistical method based on Eq. (5.7) can be used. Owing to its small-scale variations, $\Psi$ cannot be solved directly and approximations are needed. In this work the so-called moment approximation is investigated.

The transport equation for the second moment of $\Psi$ is derived by multiplying Eq. (5.7) by $pp$ and applying the averaging operator [Eq. (5.10)] to the result.

$$
\frac{1}{V} \int_V dV \int_\Omega d\Omega \left( pp \left[ \frac{\partial \Psi}{\partial t} + \nabla \cdot (u \Psi) + \nabla_p \cdot (\nabla u^T \cdot p \cdot (\delta - pp) \Psi) \right] \right) = 0.
$$

(5.11)

Applying Eq. (5.8) and integrating over $\Omega$ yields:

$$
\frac{1}{V} \int_V dV \left[ \frac{\partial qq}{\partial t} + \nabla \cdot (uqq) - \nabla u^T \cdot qq - qq \cdot \nabla u + 2 \nabla u : qqqq \right] = 0.
$$

(5.12)
Applying Eq. (5.10) and assuming $\nabla u$ to be constant in $V$ yields:

$$\frac{D\langle pp \rangle}{Dt} - \nabla u^T \cdot \langle pp \rangle - \langle pp \rangle \cdot \nabla u + 2\nabla \cdot (\langle pppp \rangle - s) = 0,$$

with

$$s = -\frac{1}{V} \int_V dV \nabla \cdot [(u(y) - u(x)) \cdot qq] = -\frac{1}{V} \int_V dV \nabla \cdot \left[ \nabla u(x) \cdot (y - x) qq \right].$$

Here $y$ is a position vector varying over $V$, $x$ is the position of the center of $V$, $\nabla u(x)$ is the velocity gradient at $x$ and $\langle pp \rangle$ and $\langle pppp \rangle$ are the second and fourth-order moments of $\Psi$. Equation (5.13) cannot be solved directly. Two unknowns have to be modeled: the fourth-order moment and the sub-grid-term $s$.

The fourth moment appears in the equation of change for the second moment owing to the nonlinear dependence of fibre rotation on fibre orientation [Eq (5.2)]. To obtain a closed set of equations a model must be adopted to express $\langle pppp \rangle$ in terms of $\langle pp \rangle$. Accurate models have been developed by parameterizing the distribution function (Chaubal and Leal 1997) and by fitting ‘exact’ solutions of the Fokker-Planck equation (Cintra and Tucker 1995, Chung and Kwon 2002). In this work, we use the closure developed by Wetzel (1999), who extended the method introduced by Cintra and Tucker (1995). The closure expresses the principal values of $\langle pppp \rangle$ as functions of the principal values of $\langle pp \rangle$ by means of a fit to numerical solutions to Eq. (5.7) for simple flows. The fit coefficients are constrained to produce correct $\langle pppp \rangle$ for the three limiting cases of isotropic, bi-axial and uni-axial distribution functions.

The sub-grid term $s$ represents the effects of the unresolved variations of $qq$ on $\langle pp \rangle$. The length-scales of these variations are smaller than the linear dimensions of $V$. We use diffusion to model this term:

$$s = \kappa \nabla^2 \langle pp \rangle,$$

where $\kappa$ is referred to as the artificial diffusivity. This is the conventional approach used in numerical simulations of polymer moment equations (Paschkewitz, Dubief, Dimitropoulus, Shaqfeh and Moin 2004, Ptasinski et al. 2003) since it ensures stable and smooth numerical solutions (Sureshkumar and Beris 1995).

### 5.3.2 Performance

The accuracy of the moment approximation [Eqs. (5.1), (5.9), (5.13) and (5.15)] is investigated by comparing Reynolds averaged stress to the ‘exact’ values obtained from the particle simulation.

The accuracy is determined by two factors: the fourth-order moment closure and the sub-grid model. In a previous work, we studied the accuracy of the fourth-order moment closure separately (Gillissen et al. 2007a). Very accurate results in turbulent channel flow were obtained using the closure scheme developed by Cintra and Tucker (1995), which is believed to be less accurate than the scheme used here (Wetzel 1999). Therefore we assume that errors introduced by the moment approximation are mainly due to the inadequacy of the sub-grid model.

The numerical methods to solve Eqs. (5.13) and (5.15) are similar to the methods used for Eq. (5.1) as described in Sec 2.1. The moment and stress components are defined in the cell-centers and zero wall-normal derivatives at the walls are used as boundary conditions for
5.3. Moment Approximation

Figure 5.5: Mean stress components using $\alpha = 1$ in Newtonian flow, computed with particle method (solid lines), moment approximation using sub-grid model Eq. (5.15) (dashed lines) and moment approximation using sub-grid model Eq. (5.16) (dash-dotted lines).

These variables. Simulations are carried out for different values of the artificial diffusivity $\kappa$. This parametric study revealed that the error in mean stress decreases with decreasing $\kappa$. However, for $\kappa \lesssim \nu$, the solution $\langle pp \rangle$ exhibits spurious wiggles. In Fig. 5.5 the stress for $\kappa = \nu$ is compared to the ‘exact’ stress. The moment approximation predicts accurate stress for $y^+ > 20$, while it overestimates stress for $y^+ < 20$. The moment approximation does not predict zero stress at the wall, in contrast to the ‘exact’ result. In Fig 5.5 it is demonstrated that by damping the diffusivity in the near-wall region ($y^+ < 30$):

$$ s = \kappa \nabla \cdot f_w \nabla \langle pp \rangle, \quad f_w = \begin{cases} \sin^2(\pi y^+/60) & \text{if } y^+ < 30 \\ 1 & \text{if } y^+ > 30 \end{cases} $$

(5.16)

the moment approximation is improved to predict zero stress at the wall, as well as a qualitatively correct behavior in the near-wall region.

It is therefore concluded that the artificial diffusivity causes incorrect fibre stress at the
5.4 Drag-Reduced Flow

5.4.1 Comparison to Newtonian Flow

![Graphs showing velocity profiles](image)

Figure 5.6: Mean (a) and standard deviation (b) of the fluid velocity. Comparison between drag-reduced flow computed with full constitutive equation (solid lines), drag-reduced flow computed with simplified constitutive equation (circles) and Newtonian flow (dashed lines).

The moment approximation [Eqs. (5.1), (5.9), (5.13) and (5.16)] is used to simulate non-Newtonian fibre suspension channel flow. The simulations are two-way coupled, i.e. the fluid affects the fibres and vice versa. Parameters are $\alpha = 10$, $\kappa = \nu$ and $Re_{\tau} = 360$. Further simulation details are given in Sec. 5.2.1. In Figs. 5.6(a) and 5.6(b) fluid velocity statistics in fibre suspension flow and Newtonian flow are compared. The larger mean velocity in the fibre suspension implies that the fibres reduce the drag coefficient $f = (U_\tau/U)^2$. Here the bulk velocity is defined as $U = (1/D) \int_0^D \tau dy$. The outward shift of the intercept of the linear profile ($y^+ < 10$) and the logarithmic profile ($40 < y^+ < 100$) indicates a thickening of the viscous and buffer layers. The parallel upward shift of the mean velocity profile in the logarithmic layer ($40 < y^+ < 100$) indicates that the flow is in the ‘small drag reduction’ (SDR) regime, whereas in the ‘large drag reduction’ regime the slope increases (Warholic et al. 1999). Typical for SDR-flow, the turbulent velocity intensity $u_{rms}$ is increased in $x$ and reduced in $y$ and $z$. These results are consistent with findings of previous numerical research (Paschkewitz, Dubief, Dimitropoulos, Shaqfeh and Moin 2004).
5.4. Drag-Reduced Flow

Figure 5.7: (a) Normalized fibre viscosity $\mu_f/(\alpha \mu)$ as a function of wall distance in drag-reduced flow (solid line) and Newtonian flow (dashed line). (b) Newtonian dissipation $\tau^+$ (lines) and normalized fibre dissipation $\tau_f^+/\alpha$ (circles) in Newtonian flow (solid line and filled circles) and drag-reduced flow (dashed line and open circles).

5.4.2 Simplified model

The aim of the present work is to provide a simplified, yet accurate, description of the effect of fibres on fluid mechanics. The reduced model is based on arguments provided by Lumley (1973), who explains drag reduction by an additional viscosity, i.e. by modeling fibre stress as:

$$\tau = 2\mu_f S. \quad (5.17)$$

Lumley argues that the fibre viscosity $\mu_f$ is induced by turbulence. As an effect turbulence is dampened, which results in a thickening of the viscous sublayer and consequently a reduction of the drag. To explore this idea we begin by defining $\mu_f$ based on the integral energy balance, which in non-dimensional form reads:

$$2U^+ = \int_0^{Re} \left( \tau^+ + \tau_f^+ \right) dy^+. \quad (5.18)$$

Here $\tau_f = S : \tau = 2\alpha \mu S : \langle pppp \rangle : S$ is dissipation of kinetic energy due to fibre stress and $\tau = 2\mu S : S$ is dissipation due to Newtonian stress.

Since the drag coefficient $f = 1/U^+2$ is directly related to the fibre dissipation $\tau_f$, we define $\mu_f$ in such a way that the dissipation predicted by Eq. (5.17): $\tau_f = 2\mu_f S : S$ equals the ‘real’ dissipation.

$$\mu_f = \frac{\mu_f \tau^+}{\tau} = \mu_0 \frac{\langle pppp \rangle : S}{S : S}. \quad (5.19)$$

Fig. 5.7(a) shows $\mu_f/(\alpha \mu)$ as a function of wall-distance in Newtonian and drag-reduced flow. The normalized fibre viscosity $\mu_f/(\alpha \mu)$ is smaller in drag-reduced flow as compared to Newtonian
flow. Fig. 5.7(b) shows that this is linked to a decrease of $\tau_f/\alpha$, while $\tau$ is remarkably similar in both flows.

A simulation is carried out of Eqs. (5.1) and (5.17) with $\mu_f(y)$ taken from the drag-reduced channel flow simulation, given in Fig. 5.7(a). Resulting non-Newtonian flow statistics are compared to the simulation of the full constitutive equations in Figs. 5.6(a) and 5.6(b). The striking agreement implies that fibre-induced drag reduction can be regarded as an effect due to an additional Reynolds averaged viscosity. This means that characteristic directions of the fibre stress tensor, are not of key importance for drag reduction. Also its fluctuations in time and space are not relevant.

5.5 Conclusions

It is demonstrated that a direct computation of the stress generated by non-Brownian fibres in turbulent channel flow is computationally unfeasible. We have approximated the stress by computing the second-order order moment of the fibre distribution function. The method involves a sub-grid term, which is modeled as diffusion. It is shown that the accuracy of the method is improved by applying a wall-damping to the diffusivity.

Non-Newtonian fibre suspension channel flow is simulated and compared to Newtonian flow. The fibres induce a reduction of the drag coefficient. A simplified constitutive model as a viscous stress is studied. The proposed fibre viscosity $\mu_f$ is defined in such a way that the resulting Reynolds averaged dissipation equals the dissipation induced by the ‘exact’ fibre stress. The simplified model induces changes in the flow which are nearly identical to those predicted by the full constitutive equations. It is therefore concluded that the characteristic directions of the fibre stress tensor, as well as its fluctuations in time and space can be ignored in the study of drag reduction. Instead the effect of the fibres can be considered as a Reynolds averaged isotropic viscosity, which reduces the complexity of the problem considerably. This result validates important assumptions made in the theory of drag reduction by (Benzi, De Angelis, L’vov and Procaccia 2005).
Chapter 6

Fibre-Induced Drag Reduction

We use direct numerical simulation to study turbulent drag reduction by rigid polymer additives, referred to as fibres. The simulations agree with experimental data from the literature in terms of friction factor dependence on Reynolds number and fibre concentration. An expression for drag reduction is derived by adopting the concept of the elastic layer.

6.1 Introduction

The addition of long-chain, linear polymers to turbulent pipe flows induces a reduction of the friction drag. Similar effects have also been observed for other additives, such as surfactants, macroscopic slender particles and gas bubbles. For an overview see Gyr and Bewersdorff (1995). The drag reduction phenomenon is exploited in a number of application, including the Trans Alaska Pipeline (Burgers et al. 1980). Besides economical motivations, many studies on drag reduction have been performed to gain understanding of wall-bounded turbulence and rheology of polymeric liquids, such as Virk (1971), Lumley (1973), Ryskin (1987), Sreenivasan and White (2000) and Benzi, De Angelis, L’vov and Procaccia (2005).

Virk (1971) found that friction data in polymer solution pipe flow can be rationalized by assuming the following parameterization for the velocity profile:

\[
\bar{u}^+ = \begin{cases} 
  y^+ & \text{if } 0 < y^+ < 11.6 \\
  11.7 \log y^+ - 17 & \text{if } 11.6 < y^+ < 11.6 + \delta_E^+
  \\
  2.5 \log y^+ + 9.2 \log \left( 11.6 + \delta_E^+ \right) - 17 & \text{if } 11.6 + \delta_E^+ < y^+ < \text{Re}_r/2
\end{cases}
\]  

(6.1)

Variables with superscript + are given in wall-units, i.e. the velocity \( \bar{u}^+ = \bar{u}/U_r \) and distance to the wall \( y^+ = yU_r/\nu \) are scaled with solvent kinematic viscosity \( \nu \) and friction velocity \( U_r = \left[ -(d\Pi/dx)(D/\rho)(1/4) \right]^{1/2} \), where \( -d\Pi/dx \) is the pressure gradient which drives the flow, \( D \) is the pipe diameter and \( \rho \) is the fluid mass density. The non-dimensional pipe diameter is referred to as the frictional Reynolds number \( \text{Re}_r = U_r D/\nu \), which is related to the bulk Reynolds number \( \text{Re} = U D/\nu \) and the friction factor \( f = U_r^2/\nu \) by

\[
\text{Re}_r = \sqrt{f} \text{Re}.
\]  

(6.2)

\[\text{A slightly different version of this chapter has been published as an article in Journal of Fluid Mechanics (Gillissen et al. 2008a)\]
Figure 6.1: (a) Friction factor versus Reynolds number in drag-reduced pipe flow. Lines, model [Eqs. (6.1) and (6.3)]; symbols, measurements using Xanthan solutions with different mass fraction $c_m$ (Sasaki 1991a). •, $c_m = 0$; □, $c_m = 10 \times 10^{-6}$; ■, $c_m = 25 \times 10^{-6}$; ▽, $c_m = 50 \times 10^{-6}$; △, $c_m = 100 \times 10^{-6}$. (b) Friction factor versus Reynolds number in drag-reduced channel flow. Lines, model [Eqs. (6.1) and (6.6)]; symbols, simulations with parameters listed in Table 6.1, below.

From the pipe wall ($y^+ = 0$) to the pipe centerline ($y^+ = Re_\tau/2$), Eq. (6.1) describes three parts, referred to as the viscous layer with thickness $11.6$, the elastic layer with thickness $\delta_E^+$ and the inertial layer, respectively. Without polymer additives $\delta_E^+ = 0$, Eq. (6.1) reduces to the Newtonian law of the wall (Tennekes and Lumley 1973). With polymer additives $\delta_E^+ > 0$ and the profile in the inertial layer is parallel shifted upward compared to the Newtonian profile. The friction factor $f$ is related to the non-dimensional velocity, averaged over the pipe cross-sectional area:

$$\frac{1}{\sqrt{f}} = \frac{8}{Re_\tau^2} \int_0^{Re_\tau/2} (Re_\tau/2 - y^+) \, dy^+. \quad (6.3)$$

A parameterization for $f$ in terms of $Re_\tau$ and $\delta_E^+$ is obtained by inserting Eq. (6.1) into Eq. (6.3). Fig. 6.1(a) shows this relation for fixed values of $\delta_E^+$ in Prandtl-Kármán (PK) coordinates (Tennekes and Lumley 1973). For $Re_\tau \to \infty$, the drag reduction curves ($\delta_E^+ > 0$) are parallel shifted upward compared to the Newtonian curve ($\delta_E^+ = 0$).

An important polymer property is flexibility, describing its ability to coil and stretch. In this context polymers can be categorized into flexible and rigid, each having very different drag reduction characteristics (Virk 1975a). In contrast to flexible polymers, for which an experimentally based parameterization has been formulated (Virk 1971), rigid ones, which we refer to as fibres, have been studied far less extensively and an equivalent parameterization is lacking.

The present work aims at providing a basis for such parameterization by means of direct numerical simulation (DNS). Before turning to the simulations, we first review the experimentally established knowledge. Fig. 6.1(a) shows experimental data in PK-coordinates (Sasaki 1991a). Results are shown for different fibre mass fractions $c_m$, defined as the mass of the fibres per unit mass of the solution. For sufficiently large $Re_\tau$ the data for each $c_m$ follow lines of constant $\delta_E^+$. The friction data appears to be parameterized with Eqs. (6.1) and (6.3),
6.1. Introduction

and $\delta_E^+$ therein is independent of $Re_\tau$. In the limit $Re_\tau \to \infty$ we can write the following relation between friction factor and Reynolds number:

$$\frac{1}{\sqrt{f}} = 2.5 \log Re \sqrt{f} + 9.2 \log (1 + 0.086\delta_E^+)\,.$$ (6.4)

This typical behavior of constant $\delta_E^+$ as a function of $Re_\tau$ distinguishes fibres from flexible polymers. The configuration of a flexible polymer varies from randomly coiled to fully stretched with increasing fluid deformation, introducing a rather complex Reynolds number dependence in their drag reduction efficiency (Virk 1971).

A complete description of the friction factor in fibre solutions requires a relation between $\delta_E^+$ and properties of the fibres. Here we consider the dependence on the fibre mass fraction $c_m$. Fig. 6.2(a) shows $\delta_E^+$ as a function of $c_m$ for various fibre solutions in log-log coordinates. Each $\delta_E^+$-value is obtained by fitting Eq. (6.4) to a set of measured data points on the PK-plane. There is an approximately linear dependence of $\delta_E^+$ on $c_m$, demonstrated by the dashed lines which are drawn with slope 1. There seems to be a very simple empirical law, that the drag reduction parameter $\delta_E^+$ is proportional to the number of fibres in the flow. As can be seen from Fig. (6.2a), the different solutions yield different values for $\delta_E^+/c_m$, indicating a further dependence of $\delta_E^+$ on the hydraulic properties of the fibres. To date, this dependence remains unknown.

This work is aimed at closing this problem, by means of DNS. In contrast to experiments, all conditions in simulations are known, which is of key importance for interpreting polymeric turbulent flows. However, owing to computer restrictions a limited level of physical detail can be taken into account. Therefore we take care to determine the physical significance of the simulations by comparing them to the available experimental data. To our knowledge this study is the first to quantitatively compare DNS of drag reduction to experiments. The limited detail,
on the other hand, also has advantages. The reduced equations contain only the most important parameters and so a parametric study can yield a relation for drag reduction in terms of the Reynolds number and fibre properties. This would have been more difficult or even impossible when irrelevant side-effects were taken into account.

6.2 Mathematical Model

6.2.1 Assumptions

We use DNS to study the friction factor in turbulent fibre-solution channel flow. The choice of the channel geometry instead of pipe is motivated by the fact that the dynamics in the near-wall layer responsible for the friction factor are similar in pipe and channel flow (Tennekes and Lumley 1973), but the problems related to the singularity in the cylindrical coordinate system do not have to be addressed in Cartesian calculations.

The effect of the fibres on the fluid mechanics is modeled by adding the fibre stress to the fluid equations of motion. The equations governing this stress are based on simplifying assumptions. Here we will compare these assumptions to the experimental conditions of Sasaki (1991b). The fluid used in these experiments consists of Na-polyacrylate with molecular weight $M_w = 1.7 \text{ Mg mol}^{-1}$ dissolved in distilled water at room temperature $T = 3 \times 10^2 \text{K}$, $\rho = 10^3 \text{ kg m}^{-3}$ and $\nu = 10^{-6} \text{ m}^2 \text{s}^{-1}$. This polymer can be regarded a neutrally buoyant, rigid particle of length $l = 5 \times 10^{-6} \text{ m}$ and diameter $d = 10^{-9} \text{ m}$. The fibre aspect-ratio $r = l/d \sim 10^4$ is large enough that the effects of a finite aspect-ratio can be ignored (Manhart 2003). Other relevant experimental parameters are the frictional Reynolds number $Re_f \sim 10^3$, the pipe diameter $D = 6 \times 10^{-3} \text{ m}$ and the mass fraction $c_m \sim 10^{-5}$. Brownian motion can be neglected since the rotary diffusion time scale $t_B \approx \rho \nu l^3/(10k_B T) = 3 \text{ s}$ (Doi and Edwards 1986) is much larger than the large-eddy-turn-over time $t_L \approx (D^2/\nu)Re_f^{-1} = 4 \times 10^{-2} \text{ s}$ (Tennekes and Lumley 1973). Here $k_B$ is the Boltzmann constant. The flow field around an individual fibre can be assumed a linear function of space since fibre length $l \approx 5 \times 10^{-6} \text{ m}$ is smaller than the Kolmogorov length scale $l_K \approx DRe_f^{-3/4} = 3 \times 10^{-5} \text{ m}$ (Tennekes and Lumley 1973). This further implies that fibre inertia is negligible and that the flow around an individual fibre can be described by the Stokes equations.

Because of computer restrictions, we ignore hydrodynamic and physical interactions between fibres: an individual fibre moves and interacts with the flow as if the solution were dilute (Doi and Edwards 1986). Ignoring these events allows a statistical description, which is numerically tractable. Since in principle drag reduction does not occur in dilute solutions, this assumption is not satisfied under realistic conditions. Consequently, the physical significance of our numerical model is questionable and will therefore be determined by a comparison to experimental data from the literature.

6.2.2 Governing Equations

Under the above-mentioned assumptions, the flow is governed by the incompressible Navier-Stokes equations, supplemented by the divergence of the fibre stress tensor $\mathbf{\tau}$ (Doi and Edwards...
6.2. Mathematical Model

\[ D \frac{Du}{Dt} = \nabla \cdot (-\Pi \delta + 2\mu S + \tau), \]  
(6.5a)

\[ \nabla \cdot u = 0, \]  
(6.5b)

\[ \tau = 2\alpha \mu S : \langle pppp \rangle. \]  
(6.5c)

Here \( u \) is the fluid velocity vector, \( t \) is time, \( \nabla \) is the nabla operator, \( \delta \) is the unit tensor, \( D = \frac{\partial}{\partial t} + u \cdot \nabla \) is the material derivative, \( S = \frac{1}{2}(\nabla u^T + \nabla u) \) is the rate-of-strain tensor, \( \Pi \) is the pressure, \( \mu = \nu \rho \) is the solvent dynamic viscosity and \( p \) is the fibre orientation unit vector. The concentration parameter \( \alpha \) is related to the fibre number density \( n \) and fibre length \( l \) as:

\[ \alpha \approx 0.1nl^3. \]  
(6.5d)

For simplicity we have neglected the logarithmic dependence of the numerical factor 0.1 on the fibre aspect ratio. Parameter \( \alpha \) equals the ratio of the scalar magnitude of the fibres stress and the Newtonian stress, and measures therefore the non-Newtonian character of the flow. To estimate a realistic value for \( \alpha \) we use \( n = c_m \rho \mathcal{N}_A/M_w \), where \( \mathcal{N}_A \) is the Avogadro number. For the experimental conditions described in Sec. 6.2.1 we find \( \alpha \approx 44 \).

The fibre stress involves averaging \( \langle \cdots \rangle \) over a statistical ensemble of fibres, contained in a (small) volume, centered at the point where the stress is to be determined. The fibre stress \( \tau \) can be interpreted as a viscous stress, with viscosity depending on the orientation of the fibres relative to the axes of fluid deformation. The required information regarding fibre orientation is contained in \( \langle pppp \rangle \), which is referred to as the fourth-order moment of the fibre orientation distribution function. This quantity is approximated by solving the equation of change for the second-order moment \( \langle pp \rangle \):

\[ \frac{D\langle pp \rangle}{Dt} - \nabla u^T \cdot \langle pp \rangle - \langle pp \rangle \cdot \nabla u + 2\nabla u : \langle pppp \rangle = s, \]  
(6.5e)

and applying a closure relation to express \( \langle pppp \rangle \) in terms of \( \langle pp \rangle \). Equation (6.5e) states that the fibres rotate as material lines, while being advected by the fluid velocity field. The term \( 2\nabla u : \langle pppp \rangle \) ensures that the fibres maintain a constant length, and would have been absent if the fibres could stretch freely, like material lines. Owing to viscosity, there is a no-slip condition on the fibre surface. This induces a resistance against the deformation of the surrounding fluid, which is expressed by the fibre stress tensor [Eq. (6.5c)].

We express \( \langle pppp \rangle \) in terms of \( \langle pp \rangle \) by using the scheme developed by Wetzel (1999). This model relates the principal values of \( \langle pppp \rangle \) to the principal values of \( \langle pp \rangle \) by means of a fit to exact solutions. The fit coefficients are constrained to reproduce correct \( \langle pppp \rangle \) for the three limiting cases of isotropic, bi-axial and uni-axial distribution functions. The sub-grid term \( s \) is due to the unresolved spatial variations (Gillissen et al. 2007b). This term is modeled as diffusion:

\[ s = \kappa \nabla^2 \langle pp \rangle, \]  
(6.5f)

where \( \kappa \) is referred to as artificial diffusivity. The errors in fibre stress in turbulent channel flow due to the sub-grid model and the fourth-order moment closure have been shown to be small (Gillissen et al. 2007a, Gillissen et al. 2007b).

It is noted that these constitutive equations are valid in the dilute regime \( nl^3 \ll 1 \) (Doi and Edwards 1986). In this limit, fibre stress is negligible compared to Newtonian stress, i.e. the
solution behaves as Newtonian and drag reduction does not occur. Significant drag reduction requires $n_0^3 \gg 1$, which is outside the range of the validity of the model. It will be shown that despite this inconsistency the equations are capable of correctly reproducing experimental drag reduction data.

6.3 Numerical Method

6.3.1 Channel Flow

We simulate turbulent fibre solution channel flow [Eqs. (6.5)]. The flow is driven by means of a constant pressure gradient between two parallel no-slip walls separated by a distance $D$. Periodic boundary conditions are imposed in the homogeneous directions $x$ and $z$. We use a pseudo-spectral flow solver. Spatial derivatives are computed with a Fourier-basis for the homogeneous directions and a second-order, central, finite-differences scheme for the wall-normal direction $y$. Time integration is achieved with the second-order, explicit Adams-Bashforth scheme. Conservation of mass is ensured by using a projection method. The Poisson equation is transformed to Fourier space in the homogeneous directions and a tri-diagonal solver is used for the resulting matrix equations. The variables are discretized on a non-equidistant, staggered mesh. Fibre stress, pressure and the velocity components in the homogeneous directions are defined at the cell-centers. The wall-normal velocity component is defined at the cell-faces.

The usual boundary conditions applied to polymer moment equations are zero wall-normal derivatives at the walls:

$$\frac{\partial}{\partial y} \langle pp \rangle |_{y=0} = 0.$$

Gillissen et al. (2007b) showed that with these conditions Eqs. (6.5e) and (6.5f) yield $p_y(y = 0) \neq 0$, resulting in large stress errors in the viscous layer. To obtain $p_y(y = 0) = 0$ the following boundary conditions are employed:

$$\frac{\partial}{\partial y} (p_ip_j)|_{y=0} = 0 \quad \text{if } i \neq 2 \text{ and } j \neq 2$$

$$\langle p_ip_j \rangle |_{y=0} = 0 \quad \text{if } i = 2 \text{ or } j = 2$$

For these conditions the sub-grid term $\kappa \nabla^2 \langle pp \rangle$ [Eq. (6.5f)] may induce a particle flux through the walls. To conserve the number of fibres we force $\text{tr} \langle pp \rangle = 1$ on each grid-point and at each time step.

6.3.2 Parameters

The flow is characterized by two dimensionless parameters, the frictional Reynolds number $Re_\tau$ [Eq. (6.2)] and the concentration parameter $\alpha$ [Eq. (6.5d)]. To determine the friction factor dependence on these parameters, nine runs were carried out using different $Re_\tau$ and $\alpha$. Details are given in Table 6.1. The frictional Reynolds number is based on the friction velocity $U_\tau$, which in channel flow is given by:

$$U_\tau = \left[-\frac{\partial \Pi}{\partial x}(D/\rho)(1/2)\right]^{1/2}.$$

The channel dimensions and resolutions in $x$ (stream-wise), $y$ (wall-normal) and $z$ (span-wise) are $D(L_x \times 1 \times L_z)$ and $96 \times N_y \times 96$. For the Newtonian flows (runs 1 and 5), the streamwise and spanwise dimensions are approximately 1000 and 500 wall-units, which is sufficient to capture the near-wall
6.4. Results

Table 6.1: Parameters used in the simulations. $Re_f$ is the frictional Reynolds number, $Re$ is the bulk Reynolds number, $\alpha$ is the concentration parameter [Eq. (6.5d)], $L_x$ is the ratio of the streamwise and wall-normal channel dimensions, $L_z$ is the ratio of the spanwise and wall-normal channel dimensions, $N_y$ is the number of grid-points in wall-normal direction, $\kappa$ is the artificial diffusivity [Eq. (6.5f)], $\Delta t$ is the computational time step, $DR$ is drag reduction [Eq. (6.9)], $\delta_E^+$ is the elastic layer [Eq. (6.1)], $\epsilon$ is the relative difference between simulated $DR$ and model [Eq. (6.11)] and the symbols corresponds to those used in Figs. 6.1(b), 6.2(b) and 6.3.

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<td>0.05</td>
<td>0</td>
<td>0.054</td>
<td>-</td>
<td>+</td>
</tr>
<tr>
<td>6</td>
<td>1000</td>
<td>25</td>
<td>50</td>
<td>2</td>
<td>192</td>
<td>2</td>
<td>0.05</td>
<td>0.44</td>
<td>11.7</td>
<td>0.02</td>
<td>▼</td>
</tr>
<tr>
<td>7</td>
<td>1000</td>
<td>28</td>
<td>100</td>
<td>3</td>
<td>192</td>
<td>4</td>
<td>0.1</td>
<td>0.55</td>
<td>21.4</td>
<td>0.03</td>
<td>□</td>
</tr>
<tr>
<td>8</td>
<td>1000</td>
<td>34</td>
<td>300</td>
<td>6</td>
<td>96</td>
<td>4</td>
<td>0.1</td>
<td>0.71</td>
<td>60.3</td>
<td>0.05</td>
<td>○</td>
</tr>
<tr>
<td>9</td>
<td>3000</td>
<td>115</td>
<td>300</td>
<td>2</td>
<td>288</td>
<td>6</td>
<td>0.06</td>
<td>0.69</td>
<td>65.1</td>
<td>0.02</td>
<td>●</td>
</tr>
</tbody>
</table>

Vortical structures (Jiménez and Pinelli 1999). These structures increase in size with increasing drag reduction (Li et al. 2006). To capture these increasingly large structures the channel dimensions were adapted accordingly. The artificial diffusivity $\kappa$ is chosen as small as possible while maintaining a smooth numerical solution to Eq. (6.5e). The grid is non-uniform in $y$-direction such that $y$ of the $i$th grid-point is given by

$$y_i = \frac{D}{2} \left[ 1 + \frac{\arctan \left( \frac{3i}{N_y} - \frac{3}{2} \right)}{\arctan \left( \frac{1}{2} \right)} \right].$$

6.4 Results

The simulation results are presented in Fig. 6.3, showing the velocity profiles for all runs. The Newtonian profiles (runs 1 and 5) are well described by Eq. (6.1) with $\delta_E^+ = 0$, i.e. linear in the viscous layer and logarithmic with slope 2.5 in the inertial layer. Also the non-Newtonian profiles (runs 2-4 and 6-9) are in good agreement with Eq. (6.1). Drag reduction is accompanied by a parallel shift of the inertial layer and the elastic layer is approximately logarithmic with slope 11.7. The offset appears to be somewhat smaller than the empirical value of −17. Another important observation regarding these profiles is illustrated in Fig 6.1(b), showing the simulated bulk properties in PK-coordinates. The friction factors are obtained by averaging the non-dimensional velocity profiles over the channel cross section:

$$\frac{1}{\sqrt{f}} = \frac{2}{Re_f} \int_0^{Re_f/2} \bar{u}^+ dy^+.$$  (6.6)
Figure 6.3: Velocity profiles in channel flow simulations. Symbols correspond to parameters listed in Table 6.1.
6.4. Results

Fig 6.1(b) also shows the empirical parameterization for channel flow, which is obtained by inserting Eq. (6.1) into Eq. (6.6). It appears that when $\alpha$ is fixed, $\delta_E^+$ is independent of $Re\sqrt{\chi}$, which agrees with the experimental evidence presented in Fig. 6.1(a). The lack of a $Re\sqrt{\chi}$ dependence implies that the friction data can be fully parameterized by relating $\delta_E^+$ to $\alpha$, which is done in Fig. 6.2(b). The $\delta_E^+$-values are obtained from solving the equation between the simulated $1/\sqrt{\chi}$ and the parameterized $1/\sqrt{\chi}$, where the latter is obtained by inserting Eq. (6.1) into Eq. (6.6). A linear relationship can be seen to accurately describe the data:

$$\delta_E^+ \approx 0.2\alpha \approx 0.02nl^3.$$  (6.7)

The linear dependence agrees with the experimental data presented in Fig. 6.2(a), which further confirms that our numerical model is able to predict the correct physics. This suggest that the rheology of turbulent fibre solutions at large Reynolds number can be described by constitutive equations, which are based on the assumption of diluteness.

Rigid polymers exist in many varieties. The chemical structures have a great impact on their hydraulic properties and Eq. (6.7) is not expected to be applicable to all of them. To understand which polymers can be considered hydraulically rod-like requires detailed chemical and rheological analysis, which is outside the scope of the present work. We restrict ourselves to comparing our principle result [Eq. (6.7)] to available experimental data. Using $nl^3 = c_m \rho l^3 N_A/M_w$, Eq. (6.7) can be written as

$$\frac{\delta_E^+}{c_m} \approx \frac{0.02\rho l^3 N_A}{M_w}.  \quad (6.8)$$

The comparison goes as follows. Experimental values for $\delta_E^+/c_m$ are extracted from Fig. 6.2(a). After inserting $\delta_E^+/c_m$ into Eq. (6.8), we obtain the hydraulic length $l$, which is basically the fibre length for which our numerical model produces the corresponding experimentally measured $\delta_E^+/c_m$. To determine the agreement between our model and the experiment, we compare $l$ to the contour length $l^*$, the physical length of the polymer used in the experiment. Unfortunately the available experimental data are very sparse. Only three papers seem to present the required information, given in Table 6.2. For the experiments of Sasaki (1991b), the agreement is nearly perfect, which suggests that these polymers behave hydraulically as rods with $l \approx l^*$. Discrepancies for the other experiments might be related to the larger molecular weight, and contour length of the polymers used. As an effect, these polymers might have appreciable levels of flexibility in contrast to what is assumed in the simulations.

Eqs. (6.10) and (6.7) comprise a complete description of fibre-induced drag reduction. The exact pre-factor in Eq. (6.7) is expected to depend on specific chemical properties or effects of non-diluteness and must be considered as an order-of-magnitude estimate. The elastic layer thickness is a rather abstract concept. More practical is the relative decrease of the friction factor:

$$DR = 1 - \frac{f^P}{f^N}.  \quad (6.9)$$

where the polymer solution $f^P$ and in the Newtonian fluid $f^N$ are evaluated at the same frictional Reynolds number $Re_\tau$. Physically, $DR$ measures the relative increase of the squared bulk velocity, while maintaining a constant pressure drop over the channel. To arrive at expressions for the friction factors, we insert Eq. (6.1) into Eq. (6.6). In the limit $Re_\tau \to \infty$ this yields:

$$\frac{1}{\sqrt{\chi}} = 2.5\log Re_\tau + 9.2\log \left(1 + 0.086\delta_E^+\right) + 1.2.  \quad (6.10)$$
Table 6.2: Characterization of rigid polymers used in experimental studies. Distilled water was always used as solvent. Polymer abbreviations are: PAA-Na (Na-polyacrylate) and PAHM (partially hydrolyzed polyacrylamide). $M_w$ is molecular weight given in Mg mol$^{-1}$. The values for $\delta^+ / c_m$ are obtained from Fig. 6.2(a) and given in millions. The hydraulic length $l$ is obtained from Eq. (6.8). The contour length $l^* = aM_w/M_a$, where $M_a$ is the molecular weight of the repeat unit and $a$ is the length of the repeat unit, $a = 2 \times (1.5 \text{Å}) \cos 35^\circ = 2.5 \text{Å}$(Flory 1969). For PAMH: $M_a = 72 \text{ g mol}^{-1}$ and for PAA-Na: $M_a = (83 \pm 11) \text{ g mol}^{-1}$. Both $l$ and $l^*$ are given in $\mu$m.

<table>
<thead>
<tr>
<th>Source</th>
<th>Polymer</th>
<th>$M_w$</th>
<th>$\delta^+ / c_m$</th>
<th>$l^*$</th>
<th>$l$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sasaki (1991b)</td>
<td>PAA-Na</td>
<td>1.7</td>
<td>1.4</td>
<td>5.1 ± 0.7</td>
<td>5.8</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>2.4</td>
<td>4.4</td>
</tr>
<tr>
<td>Virk (1975a)</td>
<td>PAMH</td>
<td>15</td>
<td>2.1</td>
<td>52</td>
<td>14</td>
</tr>
<tr>
<td>Virk et al. (1997)</td>
<td></td>
<td>20</td>
<td>5.1</td>
<td>70</td>
<td>20</td>
</tr>
</tbody>
</table>

Expressions for $f^N$ and $f^P$ are obtained by substituting $\delta^+_E = 0$ and $\delta^+_E = 0.02nl^3$ respectively. We finally obtain

$$DR \approx 1 - \left(1 + \frac{9.2 \log (1 + 0.0017nl^3)}{2.5 \log Re_r + 1.2}\right)^{-2}.$$ (6.11)

The result for pipe flow is similar with 1.2 replaced by 0.3. The relative difference $\epsilon$ between Eq. (6.11) and the simulated $DR$-values is listed in Table 6.1. The rather low values reflect the good quality of this relation.

6.5 Discussion and Conclusion

We have conducted DNS of turbulent drag reduction in fibre solutions. In the numerical model, interactions between fibres are neglected, conflicting with realistic conditions. To study the implications of this non-physical assumption, the simulations are compared to experimental data from the literature. It is shown that the simulations accurately reproduce three crucial physical observations: (i) the velocity profiles are well described by the empirical parameterization proposed by Virk (1971); (ii) the drag reduction efficiency, measured by the elastic layer $\delta^+_E$ is independent of the frictional Reynolds number and (iii) increases linearly with fibre mass fraction.

From the agreement it is inferred that the rheology in drag-reduced fibre solutions can be described accurately by the dilute equations and the relevant parameter to describe drag reduction is $nl^3$. In this regard, the simulation results can be summarized by a linear relationship between $\delta^+_E$ and $nl^3$.

The problem of predicting the friction factor for a given fibre solution now becomes that of determining the fibre hydraulic length $l$. To relate this quantity to easily accessible input data requires detailed knowledge on the molecular structure. Extensive experimental work combining turbulent friction analysis and chemical characterization is therefore needed to determine the full implications of the present work.
Chapter 7

Comparing Simulation to Experiment at Maximum Drag Reduction

Direct Numerical Simulation is used to compute fibre-induced drag reduction in turbulent channel flow. The simulations correspond to relatively small drag reduction (SDR) and maximum drag reduction (MDR). The results are compared to the experimental data of Escudier et al. (2007), involving the profiles of the mean velocity, the Reynolds stress and the turbulent kinetic energy (TKE). At SDR there is reasonable, qualitative agreement, while at MDR there are large differences in TKE. These discrepancies suggest that interactions between fibres, which are neglected in the numerical model, are important at MDR.

7.1 Introduction

In this chapter we compare Direct Numerical Simulations (DNS) of drag-reduced flows to experimental data from the literature. We focus on polymers which have a negligible level of flexibility referred to as fibres. By excluding flexibility the complexity of the modeling is considerably reduced which is beneficial for the reliability of the simulations.

Owing to computer restrictions, effects of entanglement and hydrodynamic interactions are not taken into account in the numerical model. Therefore the model applies only to dilute solutions, in which interactions between fibers play no part. However, it can be shown that in principle drag reducing solutions are non-dilute. The aim of the present work is to determine the implication of neglecting interactions by comparing simulations to experimental data.

In the previous chapter we have presented such a comparison. The computed velocity profiles were shown to be in close agreement with the experimentally based parameterization [Eq. (6.1)]. Furthermore, in accord with experimental data, the elastic layer thickness $\delta_E^+$ was independent of the frictional Reynolds number $Re_f$ and linearly related to the fibre number density $n$.

The agreement with experimental data implies that the constitutive equations describing suspensions of non-interacting rods [Eqs. (6.5)] correctly reproduce experimental friction data for solutions of rigid polymers. This suggests that hydrodynamic interactions, which are neglected
Table 7.1: Parameters used in the simulations. $Re$ is the bulk Reynolds number, $\alpha \approx 0.1 m^3$ is the concentration parameter, where $n$ is the fibre number density and $l$ is the fibre length. $L_x$ is the ratio of the streamwise and wall-normal channel dimensions, $L_z$ is the ratio of the spanwise and wall-normal channel dimensions, $N_x$, $N_y$ and $N_z$ are the number of grid-points in streamwise, wall-normal and spanwise directions, and drag reduction is defined as $DR = 1 - \frac{f_F}{f_N}$ where the friction factor in the fibre solution $f_F$ and in the Newtonian fluid $f_N$ are evaluated at the same frictional Reynolds number $Re_f$.

<table>
<thead>
<tr>
<th>RUN</th>
<th>$Re \times 10^{-3}$</th>
<th>$\alpha$</th>
<th>$L_x = 2L_z$</th>
<th>$N_x = N_z$</th>
<th>$N_y$</th>
<th>$DR$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>18</td>
<td>0</td>
<td>1</td>
<td>96</td>
<td>384</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>28</td>
<td>100</td>
<td>3</td>
<td>96</td>
<td>192</td>
<td>0.55</td>
</tr>
<tr>
<td>3</td>
<td>45</td>
<td>1600</td>
<td>18</td>
<td>192</td>
<td>96</td>
<td>0.83</td>
</tr>
</tbody>
</table>

in the numerical model, are not important in the mechanisms leading to drag reduction. The comparison however was restricted to the small drag reduction (SDR) regime. In the present work we wish to extend the comparison to the maximum drag reduction (MDR) regime. For this purpose we compare simulation results to the experimental data acquired by Escudier et al. (2007), involving the profiles of first- and second-order fluid velocity statistics. Escudier et al. (2007) performed channel flow experiment using a Newtonian fluid and aqueous solutions of carboxymethyl cellulose (CMC) and xanthan gum (XG). Owing to the high rigidity of their backbone structures these polymers can be considered as rod-like particles. To our knowledge this is the only paper presenting measured velocity statistics in drag-reduced channel flow using rigid polymers.

We have carried out three simulations of Eqs. (6.5). Details of the numerical methods can be found in Chapter 6. The fibre concentration parameter [Eq. (6.5d)] was chosen $\alpha = 0$, 100 and 1600, corresponding to Newtonian flow, SDR and MDR, respectively. All calculations are based on the same frictional Reynolds number $Re_f = 1000$. Additional parameters are listed in Table 7.1. For the Newtonian flow calculation the streamwise and spanwise channel dimensions are 1000 and 500 wall-units, which are sufficient to capture the near-wall vortical structures, responsible for the friction factor (Jiménez and Pinelli 1999). These structures increase in size with increasing drag reduction (Li et al. 2006). Therefore we have used larger channel dimensions for the drag-reduced flow calculations.

### 7.2 Results

#### 7.2.1 Mean Flow

The computed velocity profiles are presented in Fig. 7.1(a). The profiles are in good qualitative agreement with the experimental data presented in Fig. 7.1(b). The velocity profile for $\alpha = 100$ agrees qualitatively with that of the CMC solution. The logarithmic profile is displaced from the Newtonian profile, while the slope is kept at the Newtonian value of 2.5. These trends are typical for SDR and have been observed many times in experiments using flexible polymers, such as Warholic et al. (1999). The flow for $\alpha = 1600$ is at MDR. The mean flow compares well with the measurement of the XG solution. The slope of the logarithmic profile is increased over
7.2. Results

The whole domain to a value which is in reasonable agreement with the empirical value of 11.7.

7.2.2 Shear Stress

To further assess the physical significance of the numerical simulations we consider the various contributors to the shear stress balance. This balance is obtained after integrating the $x$-component of the Reynolds averaged Navier-Stokes equations over the $y$-direction. In non-dimensional form the result reads:

$$1 - \frac{2y^+}{Re_r} = \frac{du^+}{dy^+} - \overline{uv^+} + \overline{xy^+}.$$ (7.1)

The driving pressure gradient force on left hand side balances the dissipating forces on the right hand side. Energy dissipation is divided into viscous stress $du^+/dy^+$, Reynolds stress $-\overline{uv^+}$ and polymer stress $\overline{xy^+}$. Drag reduction is equivalent to an increase of the non-dimensional velocity gradient $d\overline{u^+}/dy^+$. According to Eq. (7.1) this is realized when the additional polymer stress is overwhelmed by the reduction of the Reynolds stress. In Fig. 7.2(a) we show the computed Reynolds stresses and polymer stresses. These results are compared to the experimental data, which is given in Fig. 7.2(b). At SDR there is a small discrepancy between simulation and experiment, where the simulation shows a smaller Reynolds stress in the outer region ($y/D \gtrsim 0.2$) and a larger Reynolds stress in the inner region ($y/D \lesssim 0.2$). These differences however may be attributed to the different Reynolds numbers and levels of drag reduction in the simulation and the experiment. At MDR there is good agreement between simulation and experiment. Both predict a nearly identical level of Reynolds stress.
Chapter 7. Comparing Simulation to Experiment at Maximum Drag Reduction

7.2.3 Turbulent Kinetic Energy

A very interesting characteristic of drag reduction is the modifications of the turbulent kinetic energy (TKE), measured by the standard deviation of the fluid velocity vector $u_{\text{rms}}$. Simulation and experiment are compared in Fig. 7.3, showing the profiles corresponding to the streamwise ($x$) and the wall-normal ($y$) velocity components. For both Newtonian flow and drag-reduced flow most of the energy is contained in the streamwise velocity component. The anisotropy is largest near the wall, while in the channel center the TKE is evenly distributed over the different directions. The kinetic energy peaks at $y^+ \approx 10$ and decreases thereafter towards the center. For Newtonian flow, simulation and experiment agree perfectly, while for drag-reduced flow, significant differences are observed in $u_{\text{rms}}$. In contrast to the experimental data, the simulations show a substantial increase in $u_{\text{rms}}$, reaching a maximum of approximately 5.5 at MDR, two times as large as being measured experimentally. The discrepancy is surprising, considering that the mean flow and the Reynolds stress profiles are in good agreement. These inconsistencies reflect the imperfections of the numerical model and are probably due to neglecting interactions between the fibres.

7.3 Conclusions

We have compared DNS of drag-reduced turbulent channel flow to the experimental data of Escudier et al. (2007), concerning the profiles of the mean flow, the Reynolds stress and the turbulent kinetic energy. At SDR the trends are in reasonable agreement, indicating that the
7.3. Conclusions

Figure 7.3: (a) Standard deviation of streamwise fluid velocity (open symbols) and wall-normal fluid velocity (filled symbols) in channel flow simulations for Newtonian flow and drag-reduced flow using rigid polymers. The polymers are modeled as non-interacting massless rods. The polymer number density is \( n \) and the polymer length \( l \) is smaller than the Kolmogorov length-scale. The polymer concentration parameter \( \alpha \approx 0.1nl^3 \) equals \( \alpha = 0 \) (circles), \( \alpha = 100 \) (squares) and \( \alpha = 1600 \) (triangles). For clarity the symbols are shown for only one tenth of the grid-points. (b) Standard deviation of streamwise fluid velocity (open symbols) and wall-normal fluid velocity (filled symbols) in aqueous channel flow experiments for Newtonian flow (circles) and drag-reduced flow using solutions of carboxymethyl cellulose (squares) and xanthan gum (triangles) (Escudier et al. 2007). The channel height \( D = 25 \times 10^{-3} \) m.

At MDR we observe large discrepancies in the turbulent kinetic energy. Probably interactions between polymers, which are neglected in the numerical model, are important at MDR. It is noted that the comparison is restricted to only one set of experimental data and we should be careful in drawing conclusions. Further experimental research is required to fully determine the potentials of the present numerical model.
Chapter 7. Comparing Simulation to Experiment at Maximum Drag Reduction
Chapter 8

Polymer Flexibility and Turbulent Drag Reduction

Polymer-induced drag reduction is the phenomenon where the friction factor of a turbulent flow is reduced by the addition of small amounts of high-molecular-weight, linear polymers, which conformation in solution at rest can vary between randomly coiled and rod-like. It is well-known that drag reduction is positively correlated to viscous stresses, which are generated by extended polymers. Rod-like polymers always assume this favorable conformation, while randomly-coiling chains need to be unraveled by fluid strain rate in order to become effective.

The coiling and stretching of flexible polymers in turbulent flow produces an additional elastic component in the polymer stress. The effect of the elastic stresses on drag reduction is unclear. To study this issue we compare Direct Numerical Simulations (DNS) of turbulent drag reduction in channel flow using constitutive equations describing solutions of rigid and flexible polymers. When compared at constant $\phi r^2$ both simulations predict the same amount of drag reduction. Here $\phi$ is the polymer volume fraction and $r$ is the polymer aspect ratio, which for flexible polymers is based on average polymer extension at the channel wall. This demonstrates that polymer elasticity plays a marginal role in the mechanism for drag reduction.

8.1 Introduction

Turbulence puts severe limitations on fluid transport processes and it is therefore of practical relevance that the addition of small concentrations ($\sim 10^{-5}$ in weight) of high-molecular-weight ($\sim 10^6 \text{ g mol}^{-1}$), linear polymers to turbulent flow inhibits turbulent momentum transfer and consequently induces a reduction of the drag (Toms 1948). In addition to economical advantages polymer-induced drag reduction is interesting from a fundamental point of view and many scientific efforts have been devoted to gain a deeper understanding of wall-bounded turbulence and polymer dynamics (Lumley 1969, Virk 1971, De Gennes 1986, Ryskin 1987, Benzi, De Angelis, L’vov and Procaccia 2005).

Owing to their large molecular weight polymers which are effective in drag reduction are usually highly flexible. In solution at rest, these flexible chains assume a randomly coiled

\footnote{A slightly different version of this chapter has been submitted for publication as an article in Physical Review E (Gillissen et al. 2008b)}
configuration and in a statistical sense can be thought of as spherical particles. Exceptions are polyelectrolytes in de-ionized water (Sasaki 1991b) or polymers with a helical backbone structure (Sasaki 1991a). Owing to a negligible level of flexibility these polymers assume an extended conformation in solution at rest. Virk et al. (1997) induced drag reduction using polymers with varying flexibility. He observed an increase in drag reduction with decreasing flexibility and concluded that the extended conformation is responsible for drag reduction. A similar conclusion was drawn by Den Toonder et al. (1997) who performed a numerical simulation of drag reduction by rigid polymers. Drag reduction was observed to diminish after the polymer model was modified to account for polymer flexibility.

In order for a flexible polymer to become an effective drag reducer it needs to be unraveled to an extended conformation by the action of the fluid rate of strain. This phenomenon is reflected by the so-called onset phenomenon. Drag reduction sets in above an onset Reynolds number corresponding to a critical rate of strain required to unravel the flexible polymers (Virk 1971). Since rigid polymers are always in the favorable extended conformation, no onset phenomenon is observed. Instead they induce a more or less constant drag reduction efficiency as a function of the Reynolds number.

Drag reduction is the effect of forces between the polymers and the solvent molecules, referred to as polymer stresses. In general, polymers induce so-called viscoelastic stresses. In addition to having a capacity for dissipating mechanical energy, polymers have a capacity for storing energy, like springs. The elastic component of the polymer stress is related to polymer flexibility. When subjected to a varying fluid rate of strain, flexible polymers tend to stretch and coil, storing and releasing fluid mechanical energy. Rigid polymers, on the other hand, have a negligible level of flexibility and therefore induce purely viscous stresses. The viscous stress induced by polymers has an anisotropic character. This means that the magnitude of the viscosity induced by the polymers, referred to as the polymer viscosity, depends on the alignment of the polymer w.r.t. the fluid rate of strain. In simple shear flow, polymers tend to align in the flow direction. Since the polymers experience no fluid deformation along this direction, the polymer stress is negligible in the viscous sublayer of a turbulent boundary layer. Further away from the wall, the polymers experience straining motion, resulting in large polymer viscosity. Lumley (1973) reasoned that the combination of an increased viscosity in the turbulent region and a negligible effect in the viscous layer results in a thickening of the viscous layer, with the net effect of a reduced drag coefficient. Benzi, De Angelis, L’vov and Procaccia (2005) quantified these ideas and formulated a model for drag reduction, based on the Reynolds averaged equations of fluid momentum, turbulent kinetic energy and polymer stress, where the latter was represented by a polymer viscosity.

As previously mentioned, a viscous representation for the polymer stress is not complete. In general, flexible polymers induce not only viscous stresses but also elastic stresses. A mechanism for drag reduction based on elastic stresses has been put forward by De Gennes (1986), who assumed that the polymers absorb energy above a certain cut off frequency, corresponding to the polymer relaxation time. Unfortunately these ideas have not been validated experimentally nor numerically and therefore remain speculative.

In this work we aim to clarify the role of elastic polymer stresses on drag reduction. We use direct numerical simulations (DNS) to study drag reduction induced by polymers having different levels of flexibility. For this purposes we use constitutive equations representing solutions of rigid and elastic dumbbells (Bird et al. 1977). Owing to the hypothetical nature of
these representations, the simulations cannot be used for quantitative predictions. However the
equations are considered conceptually correct and the predicted flow properties are in qualita-
tive agreement with experiments. The simplicity of the equations allows performing simulations
using relatively little computer resources. Therefore a large number of simulations could be
conducted, such that the effect of polymer flexibility could be explored over a wide parameter
range.

8.2 Numerical model

8.2.1 Fluid

We consider polymer-induced drag reduction in turbulent channel flow, where a fluid of density
\( \rho \) is driven by a constant pressure gradient \(-d\Pi/dx\) between two no-slip walls separated in the
\( y \)-direction by a distance \( D \). Periodic boundary conditions are imposed in the streamwise (\( x \))
and spanwise (\( z \)) directions. The flow is governed by the incompressible Navier-Stokes equations,
supplemented by the divergence of the polymer stress tensor \( \tau \).

\[
\frac{D\mathbf{u}}{Dt} = \nabla \cdot (-\Pi \delta + 2\mu S + \tau),
\]

(8.1a)

\[
\nabla \cdot \mathbf{u} = 0.
\]

(8.1b)

Here \( \mathbf{u} \) is the fluid velocity vector, \( t \) is time, \( \nabla \) is the nabla operator, \( \delta \) is the unit tensor,
\( D/Dt = \partial / \partial t + \mathbf{u} \cdot \nabla \) is the material derivative, \( S = \frac{1}{2}(\nabla \mathbf{u}^T + \nabla \mathbf{u}) \) is the rate of strain tensor,
\( \Pi \) is the pressure and \( \mu = \nu \rho \) is the solvent dynamic viscosity and \( \nu \) is the solvent kinematic
viscosity. Without polymers \( \tau = 0 \) the flow is fully characterized by the Reynolds number
\( Re_{\tau} = U_{\tau} D/\nu \) based on the friction velocity \( U_{\tau} = \left[-\frac{1}{2}(d\Pi/dx)(D/\rho)\right]^{1/2} \).

We use a pseudo-spectral flow solver. Spatial derivatives are computed with a Fourier-
basis for the wall-parallel directions and a second-order, central, finite-differences scheme for
the wall-normal direction. Time integration is achieved with the second-order, explicit Adams-
Bashforth scheme, except for the non-linear term on the r.h.s. of Eq. (8.3b) (given below) which
is treated with the second-order, implicit Crank-Nicholson scheme (Ptasinski et al. 2003).

We conducted one simulation of a Newtonian flow and several simulations of drag-reduced
flow. For the Newtonian flow the channel dimensions and number of grid-points are \( 3D \times D \times 1.5D \)
and \( 96 \times 128 \times 96 \) in the \( x \), \( y \) and \( z \)-direction. To capture the larger near-wall vortical structures
in the drag-reduced flows, we use larger dimensions \( 4.5D \times D \times 2.25D \) and coarser resolutions
\( 96 \times 96 \times 96 \). To study the role of polymer flexibility on drag reduction we conducted simulations
using two different constitutive equations describing solutions of rigid and flexible polymers.

8.2.2 Rigid Polymers

Rigid polymers are modeled as mass-less, neutrally buoyant, non-Brownian, non-interacting rigid
dumbbells, which are smaller than the Kolmogorov length-scale (Bird et al. 1977). The rigid
dumbbell displayed in Fig. 8.1(a) consists of two spheres of diameter \( d \) which are connected
by a rigid rod of length \( l \). The spheres interact with the flow by Stokes forces. The dumbbell
volume fraction is \( \phi \) and the aspect ratio is \( r = l/d \). The stress generated by the dumbbells \( \tau \)
Chapter 8. Polymer Flexibility and Turbulent Drag Reduction

\begin{equation}
D^{\langle pp \rangle}_t - \nabla u^T \cdot \langle pp \rangle - \langle pp \rangle \cdot \nabla u + 2 \nabla u : \langle pppp \rangle = \kappa \nabla^2 \langle pp \rangle, \tag{8.2b}
\end{equation}

is a viscous stress, with viscosity depending on the orientation of the dumbbells relative to the axes of fluid deformation.

\begin{equation}
\tau = \frac{9}{2} \mu \phi r^2 S : \langle pppp \rangle. \tag{8.2a}
\end{equation}

Here \( p \) is the polymer orientation unit vector and \( \langle \cdots \rangle \) is an average over polymers contained in a (small) volume centered at the point where the stress is to be determined. The concentration parameter \( \phi r^2 \) measures the importance of the polymer stress relative to the Newtonian stress and determines the amount of drag reduction.

Computing the stress requires the fourth-order moment of the polymer orientation distribution function \( \langle pppp \rangle \). We approximate this quantity by solving the equation of change for the second-order moment \( \langle pp \rangle \):

\begin{equation}
D^{\langle pp \rangle}_t - \nabla u^T \cdot \langle pp \rangle - \langle pp \rangle \cdot \nabla u + 2 \nabla u : \langle pppp \rangle = \kappa \nabla^2 \langle pp \rangle, \tag{8.2b}
\end{equation}

and applying the closure developed in Wetzel (1999) to express \( \langle pppp \rangle \) in terms of \( \langle pp \rangle \). This closure model relates the principal values of \( \langle pppp \rangle \) to the principal values of \( \langle pp \rangle \) by means of a fit to exact solutions. The fit coefficients are constrained to reproduce correct \( \langle pppp \rangle \) for the three limiting cases of isotropic, bi-axial and uni-axial distribution functions.

The diffusive term \( \kappa \nabla^2 \langle pp \rangle \) models unresolved spatial variations where \( \kappa \) is the artificial diffusivity (Gillissen et al. 2007b).
8.2.3 Flexible Polymers

In addition to rigid polymers we have simulated drag reduction by flexible polymers. Flexible polymers are modeled as FENE-P (finitely extensible non-linear elastic with the Peterlin approximation) dumbbells (Bird et al. 1977). As drawn in Fig. 8.1(b) the elastic dumbbell consists of two spheres of diameter $d$ which are separated by a vector $l$ and connected by a FENE spring, which accounts for the tendency of Brownian fluctuations to drive the polymer to its equilibrium coiled configuration. The maximum and equilibrium lengths of the spring are $l_{\text{max}}$ and $l_{\text{eq}}$. As for rigid dumbbells, the flexible dumbbells are assumed mass-less, non-interacting and smaller than the Kolmogorov length-scale. The polymer stress:

$$\tau = \frac{9\mu \phi r_{\text{eq}}^2}{4\lambda} \left( \frac{c}{1 - \frac{c}{l_{\text{eq}}} - \delta} \right), \quad (8.3a)$$

is determined by the conformation tensor $c = \langle U \rangle / l_{\text{eq}}^2$, which evolves according to:

$$\frac{Dc}{Dt} - \nabla u^T \cdot c - c \cdot \nabla u = \frac{1}{\lambda} \left( \delta - \frac{c}{1 - \frac{c}{l_{\text{eq}}} - \delta} \right) + \kappa \nabla^2 c. \quad (8.3b)$$

The polymer stress is determined by three dimensionless parameters: the concentration parameter at equilibrium $\phi r_{\text{eq}}^2 = \phi l_{\text{eq}}^2/d^2$, the extensibility parameter $b = l_{\text{max}}^2/l_{\text{eq}}^2$ and the Weissenberg number $We_\tau = \gamma \lambda$, where $\gamma = U^2/t^+/\nu$ is the mean shear rate at the wall and $\lambda = \frac{3\pi}{2} \mu d l_{\text{eq}}^2/4 k_B T$ is the polymer relaxation time, with $k_B$ the Boltzmann constant and $T$ the temperature. For small $We_\tau$, the polymers are randomly coiled. The conformation tensor is isotropic: $c = \delta$ and the polymer stress attains the form of a Newtonian viscous stress: $\tau = \frac{3}{2} \mu \phi r_{\text{eq}}^2 S$. The resulting flow is equivalent to a Newtonian flow, with an increased viscosity. Obviously there will be no drag reduction, but rather a drag increase. Significant drag reduction requires the polymers to be extended, which happens when $We_\tau \gg 1$.

8.2.4 Parameters

We have conducted one simulation of Newtonian (polymer-free) flow, three simulations of drag-reduced flow using rigid polymers and twelve simulations of drag-reduced flow using flexible polymers. The Reynolds number was always $Re_\tau = 360$.

In the rigid polymer solutions, the concentration parameter was chosen $2 \phi r^2 = 10, 25$ and 50, resulting in approximately 0.2, 0.3 and 0.4 drag reduction $DR$, defined as the relative decrease of the friction factor $f$:

$$DR = 1 - \frac{f^P}{f^N}. \quad (8.4)$$

Here $f^P$ and $f^N$ correspond to the polymer solution flow and the Newtonian flow, respectively. The friction factor is related to the non-dimensional bulk velocity $U^+$ as $1/\sqrt{f} = U^+$, which is obtained by averaging the simulated velocity profiles over the non-dimensional channel height $D^+ = Re_\tau = Du_+ / \nu$.

$$U^+ = \frac{2}{Re_\tau} \int_0^{Re_\tau} y^+ dy^+. \quad (8.5)$$

It is noted that variables indicated with the superscript $+$ are given in wall-units, being scaled with the friction velocity $U_\tau$ and the solvent kinematic viscosity $\nu$. 
Table 8.1: Parameters used in the simulations. Types N, R and E correspond to simulations of Newtonian flow, drag-reduced flow using rigid dumbbells and drag-reduced flow using elastic dumbbells. For type E the value given for $\frac{2}{7} r_{eff}^2$ is based on the Reynolds average at $y^+ = 0$, as given by Eq. (8.7).

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8.3. Results

The mean velocity profiles $\overline{u^+}(y^+)$ for all simulations are shown in Fig. 8.2(a). For clarity we show the inertial layer in detail in Fig. 8.2(b). As explained in the legend of Fig. 8.2(a) the symbols correspond to the different simulations. The symbols are superimposed on the lines for only one tenth of all grid-points. The Newtonian profile (run 16) is linear for $y^+ \lesssim 10$ and logarithmic with slope 2.5 for $y^+ \gtrsim 10$, referred to as the viscous layer and the inertial layer respectively. In the polymer solution flows, the observed increase in non-dimensional velocity is equivalent to a reduced friction factor $f$. The increased velocity is realized by an upward, parallel shift of the inertial layer, due to the formation of a third layer in between the viscous layer and the inertial layer. With increasing $DR$ the velocity profile in this intermediate layer approaches a logarithm of slope 11.7, asymptotically.

This intermediate, logarithmic layer was discovered experimentally and was termed the elastic layer Virk (1971). According to this concept the velocity profile in drag-reduced flow can be described by a three layer model.

$$\overline{u^+} = \begin{cases} 
  y^+ & \text{if } 0 < y^+ < 11.6 \\
  11.7 \log y^+ - 17 & \text{if } 11.6 < y^+ < 11.6 + \delta_E^+ \\
  2.5 \log y^+ + 9.2 \log (11.6 + \delta_E^+) - 17 & \text{if } 11.6 + \delta_E^+ < y^+ < Re_e/2 
\end{cases}$$  

(8.6)
Chapter 8. Polymer Flexibility and Turbulent Drag Reduction

Figure 8.3: (a) Elastic layer thickness $\delta_E^+$ versus concentration parameter $\phi r^2$ for rigid dumbbells. (b) Elastic layer thickness $\delta_E^+$ versus equilibrium concentration parameter $\phi r_{eq}^2$ for elastic dumbbells having $We_\tau = 50$ (downward triangles), $We_\tau = 150$ (upward triangles), $We_\tau = 450$ (squares) and $We_\tau = 1500$ (circles).

Figure 8.4: Polymer extension normalized by maximum extension as a function of the distance to the wall. Symbols correspond to different simulations as explained in Fig. 8.2(a).
Figure 8.5: Elastic layer thickness $\delta_E^+$ versus effective concentration parameter $\phi r_{eff}^2$, for rigid dumbbells (diamonds) and elastic dumbbells having $We_\tau = 50$ (downward triangles), $We_\tau = 150$ (upward triangles), $We_\tau = 450$ (squares) and $We_\tau = 1500$ (circles).
Chapter 8. Polymer Flexibility and Turbulent Drag Reduction

From the wall outward, these layers are referred to as the viscous layer, the elastic layer and the inertial layer. In the following we use the elastic layer thickness $\delta_E^+$ to quantify the amount of drag reduction and explore its dependence on the various polymeric properties. We compute $\delta_E^+$ (numerically) from the equation between the simulated bulk velocity and the parameterized bulk velocity, where the latter is defined as the average of Eq. (8.6) over the channel cross-section.

In Fig. 8.3(a) $\delta_E^+$ is plotted versus $\phi r^2$ for the rigid polymer cases (runs 1, 6 and 11). The linear relation indicates that the drag reduction efficiency per polymer, measured by $\delta_E^+/\phi r^2$, is independent of the amount of drag reduction.

For flexible polymers the situation is more complicated. Besides polymer concentration $\phi r^2_{eq}$, there is an additional dependency on polymer flexibility $We_{\tau}$. Fig. 8.3(b) presents the data in the $(\phi r^2_{eq}, \delta_E^+)$-plane. The dashed curves connect points of constant $We_{\tau}$. The data for $We_{\tau} = 450$ and 1500 collapse on a single curve, which is in good approximation linear. This implies that for $We_{\tau} > 450$, elastic dumbbells behave as rigid dumbbells. This observation is understood by considering the level of polymer extension, which is shown in Fig. 8.4. It is seen that for $We_{\tau} = 450$ and 1500, the polymers are nearly fully stretched and therefore behave as rigid rods.

For smaller $We_{\tau}$ the data in the $(\phi r^2_{eq}, \delta_E^+)$-plane deviate from the rod-like, linear relation. As the concentration increases the flow becomes more drag-reduced, and less effective in stretching polymers, as can be seen in Fig. 8.4. Apparently, a decreases in polymer extension is related to a decrease in the drag reduction efficiency per polymer, measured by $\delta_E^+/(\phi r^2_{eq})$.

To quantify this relation, we define an effective concentration parameter based on polymer extension at the wall:

$$\phi r^2_{eff} = \phi r^2 |_{y^+ = 0} = \phi r^2_{eq} \frac{tr\tau}{y^+ = 0}.$$  

(8.7)

In Fig. 8.5 we plot our results in the $(\phi r^2_{eff}, \delta_E^+)$-plane for both elastic and rigid dumbbells. It is noted that for rigid dumbbells the aspect ratio is fixed: $\phi r^2_{eff} = \phi r^2$. A single linear relationship is seen to reasonably fit all the data. Apparently elastic dumbbells and rigid dumbbells induce identical drag reduction when compared at equal $\phi r^2_{eff}$. It is therefore concluded that the amount of drag reduction is related to the average polymer extension near the wall, while fluctuations have little or no effect. This indicates that elastic stresses have a marginal influence in the drag reduction mechanism.

8.4 Conclusions

We have used DNS to study drag reduction in turbulent channel flow induced by rigid and elastic polymers. In both systems drag reduction depends similarly on $\phi r^2$. Here $\phi$ is the polymer volume concentration and $r$ is the polymer aspect-ratio, which for flexible polymers is based on average polymer extension at the wall.

This similarity indicates that the mechanism for drag reduction is nearly identical for flexible and rigid polymers and it is therefore due to the viscous polymer stresses. The elastic polymer stresses, owing to polymer coiling and stretching, seem to play a minor part.

Obtaining a predictive relation between drag reduction and polymeric properties requires an expression for $\phi r^2$ at the wall. An estimate could be obtained by assuming simple shear conditions. Unfortunately, the FENE-P model does not reproduce correct stress characteristics.
in simple shear flow, and can therefore not be used for this purpose. Quantitative predictions as such must come from experiments.
Chapter 9

Conclusions

Over the past sixty years many scientific papers have been published, addressing the problem of polymer-induced drag reduction. Despite these numerous efforts there is still no satisfactory theory to describe the phenomenon. Drag reduction is the result of forces between the polymer and the solvent molecules. The fact that in turbulent flows these quantities cannot be measured directly initiated efforts to develop drag reduction simulations.

In drag reduction simulations the level of physical detail is limited by computational resources. At present only simple models can be used where polymer chains are modeled as two-point particles and interactions between different chains are excluded. Obviously the physical significance of these models is questionable and comparison to experimental data is needed to shed light on this issue.

In this work we have studied the potential of a relatively simple model to predict polymer-induced drag reduction in turbulent channel flow. To minimize the required modeling we focused on the special class of rigid polymers. As compared to flexible chains, the numerical modeling of rigid rods is far less complicated.

However, even in the absence of flexibility, there is still a number of difficulties. The polymer stress is related to a distribution function of polymer orientation angles. Because of computer restrictions, the distribution function cannot be solved directly. Therefore an approximate method must be used to compute the polymer stress. We have used the so-called moment approximation, involving the computation of low-order moments of the distribution function. The equations governing these moments contain unknown terms which are modeled using closure approximations. We have studied the performance of several closure schemes by comparing calculations of the moments to ‘exact’ calculations of the distribution function. From these studies we conclude that the closures do not introduce significant errors.

Instead of the closures, we believe that neglecting polymer interactions is the main source of errors in the present numerical model. To study the implications of this unphysical assumption we have compared the simulations to experimental data from the literature. The comparison involves the relation between the friction factor, the Reynolds number and the polymer concentration as well as the profiles of the mean flow, the Reynolds stress and the turbulent kinetic energy (TKE). We see that there is good agreement in all observable trends for relatively small levels of drag reduction (SDR). Therefore we conclude that interactions between polymers, which are excluded in the model, do not play a crucial part in the SDR regime.
In the maximum drag reduction (MDR) regime however the present numerical model does not correctly reproduce experimental data. The TKE in the simulation is four times as large as the TKE found in experiments. These discrepancies indicate that interactions between polymers are important at MDR. To obtain reliable MDR simulations therefore requires further development of the rheological model by including interactions.

It must be noted that experimental drag reduction data for fibres are very limited. It is therefore difficult to validate the present numerical model and to draw definite conclusions regarding its physical significance. Further experimental research is needed to validate and improve the present numerical model.

Besides the validation of the numerical model, we have studied the mechanism for drag reduction. We conclude that drag reduction can be considered to be an effect of an additional viscosity, which is defined in such a way that the resulting dissipation of fluid kinetic energy matches the dissipation predicted by the full constitutive equations. In contrast to Newtonian viscosity, this fibre viscosity depends on wall-distance, which is considered to be the key property leading to drag reduction. The fact that drag reduction can be induced by an additional Reynolds averaged viscosity, further suggests that the characteristic directions of the polymer stress tensor as well as its fluctuations in space and time are of minor importance.

Furthermore we have elucidated the effect of polymer flexibility on drag reduction. For this purpose we have compared simulations of constitutive equations describing solutions of flexible and rigid polymers. The results are almost equal when compared at constant \( \phi r^2 \). Here \( \phi \) is the polymer volume fraction and \( r \) is the polymer length to diameter ratio, which for flexible polymers is based on the Reynolds average at the wall. The agreement implies that polymer flexibility plays a passive part in the drag reduction mechanism.
Appendix A

The EBOF Closure

Figure A.1: (a) Possible orientational configurations on the plane spanned by the two largest eigenvalues of \( \langle pp \rangle \) fall within the bold triangle. (b) The triangle of possible configurations in 3D and representations of \( \Psi \) in three limiting cases, occurring at the corners of this triangle.

The EBOF closure, due to Cintra and Tucker (1995), relates the fourth moment to the second moment of the fibre orientation distribution function \( \Psi \). The closure is a quadratic fit to ‘exact’ solutions of the Fokker-Planck equation (2.9), for several simple flows. The closure is formulated in the principal frame of the second moment, which is also the principal frame of the fourth moment. In this frame \( \langle pp \rangle \) has three nonzero values, two of which are independent owing to normalization (Eq. 2.10). Similarly \( \langle pppp \rangle \) has nine nonzero values, six of which are unique due to symmetry and three are independent owing to normalization. The principle values of \( \langle pp \rangle \) are denoted \( a_{11} \), \( a_{22} \) and \( a_{33} \). The coordinates are such that \( a_{11} \geq a_{22} \geq a_{33} \). Furthermore normalization requires \( a_{11} + a_{22} + a_{33} = 1 \) and positiveness of the probability density.
Appendix A. The EBOF Closure

function implies that each principal value $a_{ii} \geq 0$.

The combinations of eigenvalues which fulfill these restrictions are confined within a triangular area, which is plotted on the $(a_{11}, a_{22})$-plane in Fig. A.1(a). The triangle corresponds to the physical region, in which $1 \geq a_{11} \geq a_{22} \geq a_{33} = 1 - a_{11} - a_{22} \geq 0$. A three-dimensional representation is given in Fig. A.1(b). That figure also shows the shape of $\Psi$ at the corners $A$, $B$ and $C$ of this triangle. At $A$ there is one non-zero eigenvalue. All fibres are aligned in the same direction. At $B$ one eigenvalue is zero and the other are equal. Fibre orientation is evenly distributed over a unit-circle. At $C$, all eigenvalues are equal and fibre orientation is evenly distributed over the unit sphere.

The principal values of $(pppp)$ are denoted $a_{ijkl}$. For simplicity the indices $ijkl$ of the six unique non-zero fourth-order components are abbreviated by $m'$ as follows:

\[
m' : \quad 1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6
ijkl : \quad 1111 \quad 2222 \quad 3333 \quad 1122 \quad 1133 \quad 2233
\]

The closure expresses these six components as quadratic functions of $a_{11}$ and $a_{22}$.

\[
a_{m'}^{\text{closure}} = C_{m'}^1 a_{11}^2 + C_{m'}^2 a_{11} a_{22} + C_{m'}^3 a_{22}^2 + C_{m'}^4 a_{11} a_{22} + C_{m'}^5 a_{11}^2 + C_{m'}^6 a_{22}^2.
\] (A.1)

The polynomial coefficients are obtained from a least square fit minimizing:

\[
\chi^2 = \sum_{i=1}^{N_{\text{DATA}}} \sum_{m'=1}^{6} (a_{m'}^{i} - a_{m'}^{i;\text{closure}})^2.
\] (A.2)

Here $N_{\text{DATA}}$ is the number of data points to which the closure is fitted, $a_{m'}^{i}$ is the $i^{th}$ data point obtained from the Fokker-Planck equation and $a_{m'}^{i;\text{closure}}$ is the corresponding value predicted by the closure (Eq. A.1). In addition to Eq. (A.2) the normalization constraint is satisfied:

\[
a_{1'} + a_{4'} + a_{5'} = a_{11}, \quad a_{2'} + a_{4'} + a_{6'} = a_{22}, \quad a_{3'} + a_{5'} + a_{6'} = a_{33}.
\] (A.3)

There are 36 fit coefficients $C_{m'}$, 18 of which are independent owing to normalization. These are the coefficients for $m' = 1, 2, 3$. Differentiating Eq. (A.2) to the independent coefficients and equating the results to zero yields a system of linear equations from which the independent coefficients are obtained. This procedure is applied to homogeneous solutions of the Fokker-Planck equation for several flow cases:

\[
\begin{align*}
\nabla u_T^T &= \gamma \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \nabla u_T^T &= \frac{\gamma}{4\sqrt{3}} \begin{pmatrix} -1 & 10 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, & \nabla u_T^T &= \frac{\gamma}{\sqrt{13}} \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \\
\nabla u_T^T &= \frac{\gamma}{2\sqrt{3}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}, & \nabla u_T^T &= \frac{\gamma}{2\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, & \nabla u_T^T &= \frac{\gamma}{2\sqrt{20}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\nabla u_T^T &= \frac{\gamma}{\sqrt{5}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \nabla u_T^T &= \frac{\gamma}{4} \begin{pmatrix} 1 & 0 & 2 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}, & \nabla u_T^T &= \frac{\gamma}{\sqrt{37}} \begin{pmatrix} 1 & 0 & 5 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
\end{align*}
\] (A.4)

For each case the evolution of the distribution is calculated using $N = 64$ (2145 basis functions), over a time interval of $\gamma t = 20$, starting from an isotropic fibre orientation.
Table A.1: EBOF closure parameters.

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EBOF50

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EBOF800

As explained in Sec. 4.3, the system of ODE’s (Eq. 4.11) can be written as:

$$\frac{\partial \mathbf{A}}{\partial t} = \mathbf{M} \cdot \mathbf{A},$$  \hspace{1cm} (A.5)

with $\mathbf{A}$ the vector of expansion coefficients and $\mathbf{M}$ the matrix representation of the advection and diffusion operator. For steady flow conditions the solution reads:

$$\mathbf{A}(t) = \mathbf{T} \cdot \exp^{\mathbf{Nt}} \cdot \mathbf{T}^{-1} \cdot \mathbf{A}(t=0),$$  \hspace{1cm} (A.6)

with $\mathbf{T}$ the matrix containing the eigenvectors of $\mathbf{M}$ and $\mathbf{A}$ the diagonal matrix containing the eigenvalues of $\mathbf{M}$. The closure is fitted to 100 samples per case, taken equidistant in time. This yields a total of $N_{DATA,A} = 900$. We have derived three closures at three different rotary Peclet numbers numbers: $Pe_r = 50$, $Pe_r = 200$ and $Pe_r = 800$, referred to as EBOF50, EBOF200 and EBOF800. The resulting fit-coefficients $C_{nm}$ are given in Table A.1.

Per closure the FORTRAN computer code took 75 minutes on one AMD Opteron 2.0 GHz processor.
Bibliography


Curriculum Vitae

Jurriaan Gillissen was born on 18 October 1977 in Sint Oedenrode, the Netherlands. He attended Zwijsen College Veghel where he obtained his pre-academic education in 1996. Jurriaan obtained his M. Sc. degree in Applied Physics at the Eindhoven University of Technology in 2003. The topic of his M. Sc. thesis concerned the mathematical modeling of the airflow through permeable airbag fabrics.

In 2004 he started his Ph.D. research at the Delft University of Technology. Supervised by Prof. F. T. M. Niewstadt and Prof. B. J. Boersma, he conducted research on turbulent drag reduction at the Laboratory for Aero- and Hydrodynamics of the faculty of Mechanical Engineering.

In 2008 he was appointed assistant professor at the Multi-Scale Physics department of the faculty of Applied Physics of the Delft University of Technology. Here he will continue working on turbulence related problems using numerical tools.