Numerical Modeling of Fibre Suspensions
In Grid-Generated Turbulent Flow

By

Atanasis Plikas

A thesis submitted in conformity with the requirements
for the degree of Master of Applied Science
Graduate Department of Chemical Engineering and Applied Chemistry
University of Toronto

© Copyright by Atanasis Plikas 2000
The author has granted a non-exclusive licence allowing the National Library of Canada to reproduce, loan, distribute or sell copies of this thesis in microform, paper or electronic formats.

The author retains ownership of the copyright in this thesis. Neither the thesis nor substantial extracts from it may be printed or otherwise reproduced without the author’s permission.

L’auteur a accordé une licence non exclusive permettant à la Bibliothèque nationale du Canada de reproduire, prêter, distribuer ou vendre des copies de cette thèse sous la forme de microfiche/film, de reproduction sur papier ou sur format électronique.

L’auteur conserve la propriété du droit d’auteur qui protège cette thèse. Ni la thèse ni des extraits substantiels de celle-ci ne doivent être imprimés ou autrement reproduits sans son autorisation.

0-612-50361-5
Numerical Modeling of Fibre Suspensions In Grid-Generated Turbulent Flow

Master of Applied Science 2000

Atanasis Plikas

Graduate Department of Chemical Engineering and Applied Chemistry

University of Toronto

Abstract

Cellulose fibre floc formation and destruction by hydrodynamic forces in a grid-generated turbulent flow, such as that occurring downstream of turbulence generators in headboxes, is investigated using computational fluid dynamics (CFD) modeling. A Large Eddy Simulation was performed to elucidate the physics behind the break up of fibre flocs. Upon comparison with experimental data on fibre suspension flows, it was found that the minimum fibre flocculation coincided with the maximum time dependence and strain in the mean motion. The turbulent kinetic energy at these locations was negligible. A numerical model of the fibre flow was developed using an Eulerian multiphase flow model in where a transport equation for flocculation intensity was solved together with the momentum equations and turbulence models. Agreement with experimental data is good far downstream of the grids, but inadequate in the anisotropic flow immediately downstream of the grids.
Acknowledgements

I would like to thank my supervisor, Professor D.C.S. Kuhn, for taking me on and giving me a very challenging and rewarding project. Your advice, insight, and patience were much appreciated. I'd also like to acknowledge Professor P.E. Sullivan for his very prompt suggestions and ideas. Your expertise was invaluable.

Of course, the project would not have been possible without the financial assistance of the Paper Machine Science and Technology Consortium. To all the corporate members, thank you very much. I would also like to mention Balaji Devulapalli, Walter Schwarz, and Lanre Oshinowo, all from Fluent™ Incorporated, who helped me with my software training.

A great deal of gratitude goes out to our network administrator, Dan Tomchyshyn, for his very prompt solutions to all our computer related problems. Dan is an invaluable member of this department.

Finally, I'd like to thank Amir Raghem Moayed for providing me with excellent experimental results and for his knowledgeable insight on fibre flows.
# Table of Contents

Abstract .......................................................................................................................... ii

Acknowledgements .......................................................................................................... iii

Table of Contents .............................................................................................................. iv

List of Figures .................................................................................................................... vi

Nomenclature ..................................................................................................................... ix

1 Introduction ...................................................................................................................... 1

1.1 Motivation and objectives ......................................................................................... 1
1.2 Outline of Thesis ......................................................................................................... 3

2 Literature Review .......................................................................................................... 5

2.1 The headbox ................................................................................................................. 5
2.1.1 Fluid mechanics in the headbox ........................................................................... 5
2.1.2 Application of CFD in headbox design ............................................................... 8
2.1.3 Numerical Models of headbox flows .................................................................. 9

2.2 Transient pulp flocculation in a decaying turbulence flow field ............................ 11

2.3 Turbulence Modeling ................................................................................................. 13
2.3.1 Direct Numerical Simulation (DNS) .................................................................. 14
2.3.2 Large Eddy Simulation (LES) ........................................................................... 16
2.3.3 Reynolds Averaged Navier-Stokes (RANS) equations ....................................... 18
2.3.4 Zero equation models ....................................................................................... 20
2.3.5 One and two equation models ......................................................................... 20
2.3.6 Reynolds Stress Models (RSM) ....................................................................... 25
2.3.7 Near-wall modeling .......................................................................................... 27

2.4 Two-Phase Modeling ................................................................................................. 29
2.4.1 Direct Numerical Simulation ............................................................................ 29
2.4.2 Lagrangian Approach ....................................................................................... 30
2.4.3 Eulerian Approach ............................................................................................ 30
### 3 Development of Fibre Suspension model

- 3.1 Derivation of transport equation for flocculation intensity ........................................ 35
- 3.2 Modeling source terms in equation for fl ................................................................. 41
- 3.3 Determination of model constants .................................................................................. 50
- 3.4 Summary ....................................................................................................................... 51
- 3.5 Turbulence Modulation ................................................................................................ 51
  - 3.5.1 Mechanisms of modulation in fibre suspension flows .............................................. 51
  - 3.5.2 Application of existing methods to fibre suspension flows ..................................... 53

### 4 Numerical Solution

- 4.1 The Finite Volume method .......................................................................................... 56
  - 4.1.1 Discretization of governing equations .................................................................... 57
  - 4.1.2 Iterative solution procedure and the SIMPLE algorithm ...................................... 62
- 4.2 Numerical model of flow-cell ...................................................................................... 66
  - 4.2.1 Geometry and boundary conditions ....................................................................... 66
  - 4.2.2 Mesh and solver specifications ................................................................................ 68
  - 4.2.3 Physical model specifications ................................................................................. 70
  - 4.2.4 Implementation of fibre suspension model .............................................................. 71

### 5 Results and Discussion

- 5.1 Validation of turbulent flowfield .................................................................................... 73
  - 5.1.1 Large Eddy Simulation results ................................................................................ 73
  - 5.1.2 Sensitivity of RANS solution to numerical parameters .......................................... 87
  - 5.1.3 Mean flow and turbulence quantities ........................................................................ 90
- 5.2 Validation of fibre suspension model .............................................................................. 95
  - 5.2.1 Sensitivity of solution to numerical parameters ....................................................... 95
  - 5.2.2 Flocculation intensity results .................................................................................. 98
  - 5.2.3 Qualitative results .................................................................................................. 110

### 6 Practical Implications

- 113

### 7 Conclusions

- 116

- 7.1 Large Eddy Simulation .................................................................................................. 116
- 7.2 Fibre flocculation model .............................................................................................. 117
- 7.3 Recommendations for future work ............................................................................... 119

### References

- 120

### Appendix

- 125
List of Figures

1.1 A hydraulic headbox (From Valmet™). .................................................. 2
2.1 A simplified schematic of a hydraulic headbox. Not to scale. ................. 6
2.2 Schematic of grid-generated turbulence flow cell (Raghem and Kuhn 2000). ................................................................................................. 12
2.3 Hierarchy in the Numerical Simulation of Turbulence. .......................... 15
4.1 Shaded area is the Control Volume, also called a cell. Adjacent control Volumes also shown. ................................................................. 58
4.2 The SIMPLE algorithm (From Versteeg and Malalasekera 1995). ......... 65
4.3 Simplified geometry of flow cell and boundary conditions. .................. 67
4.4 188,160 cell computational mesh. ............................................................ 68
5.1 Velocity magnitude vectors on z/d=0 plane at 0.523 seconds. ............... 74
5.2 Velocity magnitude vectors on z/d=0 plane at 1.8238 seconds. .......... 75
5.3 Velocity magnitude vectors on z/d=0 plane at 2.6738 seconds. .......... 75
5.4 Velocity magnitude vectors on z/d=0 plane at 3.8238 seconds. .......... 76
5.5 Velocity magnitude vectors on z/d=0 plane at 5.0988 seconds. .......... 76
5.6 Velocity magnitude vectors on z/d=0 plane at 5.9988 seconds. .......... 77
5.7 x-velocity vs. time at selected x/d positions along centreline of channel, y/d=z/d=0. ................................................................. 78
5.8 Power Spectrum at (a) x/d=3.9970 and (b) x/d=6.001. ......................... 79
5.9 Power Spectrum at (a) \( x/d = 7.6108 \) and (b) \( x/d = 9.2101 \). ........................................ 79
5.10 Power Spectrum at (a) \( x/d = 10.09 \) and (b) \( x/d = 12.02 \). ........................................ 79
5.11 Power Spectrum at (a) \( x/d = 16.1924 \) and (b) \( x/d = 20.0029 \). .................................. 80
5.12 Power Spectrum at (a) \( x/d = 39.9960 \) and (b) \( x/d = 60.2488 \). .................................. 80
5.13 Turbulence Intensity vs. \( x/d \). Comparison between RANS and LES Models. ......................... 82
5.14 LES time-averaged velocity magnitude vectors on \( z/d = 0 \) plane. .......................... 83
5.15 Normalized mean streamwise velocity vs. \( x/d \). Comparison between models and experiment. ......................................................... 84
5.16 Instantaneous contours of \( z \)-velocity on \( z/d = 0 \) plane at 6.9988 seconds. ... 86
5.17 Turbulence Intensity vs. \( x/d \). RNG \( k - \varepsilon \) model. \( U_b = 0.45 \) m/s. .................. 88
5.18 Convergence history for RANS simulations. \( U_b = 0.45 \) m/s. ............................. 89
5.19 Comparison between predicted and experimental values of normalized Axial velocity vs. \( x/d \). \( U_b = 0.45 \) m/s. ................................................................. 91
5.20 Comparison between predicted and experimental values of turbulence Intensity vs. \( x/d \). \( U_b = 0.45 \) m/s. ................................................................. 91
5.21 Contours of velocity magnitude along the centre plane, \( z/d = 0 \), \( U_b = 0.45 \) m/s. ................................. 93
5.22 Contours of velocity magnitude along the centre plane, \( z/d = 0 \), \( U_b = 0.26 \) m/s. ................................................................. 94
5.23 Flocculation intensity vs. \( x/d \) for various inlet values of \( f \). \( U_b = 0.45 \) m/s, \( C_m = 0.54\% \). ................................................................. 96
5.24 Flocculation intensity vs. \( x/d \). Comparison of results computed on two different mesh sizes. \( U_b = 0.45 \) m/s, \( C_m = 0.54\% \). ................................................................. 96
5.25 Flocculation intensity vs. \( x/d \) at \( y/d = 0 \). \( U_b = 0.45 \) m/s, \( C_m = 0.37\% \). .................. 98
5.26 Flocculation intensity vs. \( x/d \) at \( y/d = 0 \). \( U_b = 0.45 \) m/s, \( C_m = 0.42\% \). .................. 99
5.27 Flocculation intensity vs. \( x/d \) at \( y/d = 0 \). \( U_b = 0.45 \) m/s, \( C_m = 0.50\% \). .................. 99

vii
Flocculation intensity vs. x/d at y/d=0. U_b=0.45 m/s, C_m=0.54%.

Flocculation intensity vs. x/d at y/d=0. U_b=0.26 m/s, C_m=0.42%.

Flocculation intensity vs. x/d at y/d=0. U_b=0.26 m/s, C_m=0.50%.

Flocculation intensity vs. x/d at y/d=0. U_b=0.26 m/s, C_m=0.54%.

Flocculation intensity vs. x/d at y/d=0.5. U_b=0.45 m/s, C_m=0.42%.

Flocculation intensity vs. x/d at y/d=0.5. U_b=0.45 m/s, C_m=0.50%.

Flocculation intensity vs. x/d at y/d=0.5. U_b=0.45 m/s, C_m=0.54%.

Flocculation intensity vs. x/d at y/d=0.21. U_b=0.45 m/s, C_m=0.50%.

Flocculation intensity vs. y/d at x/d=0.21. U_b=0.26 m/s, C_m=0.50%.

Flocculation intensity vs. y/d at x/d=0.12. U_b=0.45 m/s, C_m=0.37%.

Production and destruction of fl vs. x/d. U_b=0.45 m/s, C_m=0.50%.

Production and destruction of fl vs. x/d. U_b=0.45 m/s, C_m=0.37%.

Production and destruction of fl vs. x/d. U_b=0.26 m/s, C_m=0.50%.

(a) Optical image of the suspension at exit of grids (from Raghem Moayed 1999), (b) Contours of turbulent strain rate, $\varepsilon / k$, at exit of grids.

Contours of Flocculation intensity along the xy plane at z/d=0. U_b=0.45 m/s, C_m=0.50%.

Cross-sectional (yz plane) contours of flocculation intensity at various x/d positions downstream of grids. U_b=0.45 m/s, C_m=0.50%.
Nomenclature

- \(c\) instantaneous consistency
- \(c'\) fluctuating consistency
- \(C\) mean consistency
- \(C_m\) suspension consistency
- \(C_{1n}\) constant in flocculation intensity equation
- \(C_{2n}\) constant in flocculation intensity equation
- \(d\) grid width, \(= 0.008\) m
- \(D\) diffusion coefficient in flocculation intensity equation
- \(f_l\) flocculation intensity, \(= \frac{c'^2}{C_m^2}\)
- \(k\) turbulent kinetic energy, \(= \frac{1}{2}\overline{u_i' u_i'}\)
- \(L_s\) mixing length in LES
- \(n\) constant in flocculation intensity equation
- \(p\) pressure
- \(q\) turbulent velocity scale
- \(Re\) Reynolds number based on bulk velocity, grid width, and water properties
- \(S_n\) source term in flocculation intensity equation
- \(S_{ij}\) mean strain rate
- \(t_p\) particle response time
- \(Tu\) turbulence intensity, \(\sqrt{2k/3}/U_b\)
- \(u_i\) instantaneous velocities in \(x, y,\) and \(z\) directions
- \(u_i'\) fluctuating velocities in \(x, y,\) and \(z\) directions
- \(U_i\) mean velocities in \(x, y,\) and \(z\) directions
\( \overline{u'_i u'_j} \) \( \text{Reynolds Stresses} \)

\( U_b \) \( \text{bulk velocity} \)

**Greek Symbols**

\( \delta_{ij} \) \( \text{Kronecker delta} \)

\( \varepsilon \) \( \text{dissipation rate of turbulent kinetic energy, } \varepsilon = \nu \left( \partial u'_i / \partial x_j \right)^2 \)

\( \phi \) \( \text{dependent variable in general discretized equation} \)

\( \Gamma \) \( \text{diffusion coefficient in general discretized equation} \)

\( \eta \) \( \text{ratio of mean to turbulent strain rate} \)

\( \lambda \) \( \text{Taylor microscale} \)

\( \lambda_f \) \( \text{Taylor microscale for flocculation intensity} \)

\( \mu \) \( \text{molecular viscosity} \)

\( \mu_t \) \( \text{turbulent viscosity} \)

\( \nu \) \( \text{kinetic viscosity} \)

\( \rho \) \( \text{density} \)

\( \sigma_n \) \( \text{constant in equation for flocculation intensity} \)

\( \tau_{ij} \) \( \text{stress tensor} \)
Chapter 1

Introduction

1.1 Motivation and objectives

The first unit on an industrial paper machine is called the headbox. Its function is to convert the flow of a dilute cellulose fibre suspension from pipe flow to jet flow. Typically, the suspension contains no more than 1.0% fibre mass, which means that paper is formed using very dilute fibre suspensions. Figure 1.1 shows a typical hydraulic headbox, with the red areas indicating suspension flow. The fluid mechanics inside the headbox is complex, and is discussed in greater detail in Chapter 2. Modern headboxes are capable of delivering a very fast, thin jet onto a moving wire that drains water to form sheets of paper. Unfortunately, as a result of their large length to diameter ratios, fibres in suspension tend to aggregate and form dense fibre networks or flocs, which deteriorate the quality of the final paper produced.

Flocs are formed and destroyed continuously in a headbox. They move as distinct entities in the flow and if allowed to pass onto the moving wire for water drainage, can
result in paper with poor printing quality and opacity. Destruction of flocs and dispersion of fibres is highly desirable to prohibit the formation of paper with these characteristics.

Figure 1.1: A hydraulic headbox (From Valmet™).

It has been recognized for some time that turbulence of high intensity and small scale is necessary to break apart flocs that form in the headbox, and this is what drives the design of what are called turbulence generators, also shown in Figure 1.1. Although the turbulence generated is sufficient to break apart flocs, it decays very rapidly downstream of the generators, allowing flocs to reform prior to their arrival at the slice opening. Hence, at the exit of the headbox, the suspension does not have the optimum fibre dispersion.
Improvements to headbox designs through on-line measurements are tedious and the high velocities involved make it difficult to obtain reliable data inside the headbox. This is further complicated by the fact that most techniques are intrusive and often do not provide an accurate representation of the flow. An alternative is to use computational fluid dynamics (CFD) methods to solve for the flow field inside the headbox. This can provide a better understanding of the relationships between the fluid turbulence and the fibres, which can then ultimately lead to improved headbox design.

The objectives of this study are to determine some of the mechanisms by which fibre flocs are created and destroyed in a grid-generated turbulent flow using numerical solution methodologies. The work is divided in two parts: (1) To perform a Large Eddy Simulation (LES) for the purposes of capturing the relevant physics involved in the downstream section of the grids with implications for floc destruction, and (2) To develop a numerical model of fibre suspension flow applicable in the decay portion of the grid-generated turbulent flow.

1.2 Outline of Thesis

Chapter 2 provides a comprehensive background on headbox flows with special attention paid to the numerical modeling of fibre flows and use of computational fluid dynamics for headbox design optimization. Also included is the description of the modern approaches to turbulence modeling and two-phase flow modeling.

A rigorous development of the fibre suspension model is given in Chapter 3. It is based on time-averaged bulk quantities in grid-generated turbulent flow. It is followed by a general discussion on turbulence modulation.
Chapter 4 outlines the numerical solution methods used to solve the governing equations, as well as the numerical details behind the modeling of the grid-generated turbulent flowcell.

The results for both the Large Eddy Simulation and the fibre suspension model are given in Chapter 5. Quantitative and qualitative comparisons are made with previously obtained experimental data on fibre suspension flows in grid-generated turbulent flow. There is a comprehensive discussion of the effects of hydrodynamic forces, both mean and turbulent, on the dispersion of fibres.

The practical implication of the results are given in Chapter 6 accompanied by the pertinent conclusions and recommendations in Chapter 7.
Chapter 2

Literature Review

2.1 The headbox

2.1.1 Fluid mechanics in the headbox

The flow inside a headbox is complex. It is three dimensional, unsteady, and involves many regions of separated flow, adverse pressure gradients, and wake formation. The addition of fibres changes the rheology of the fluid making it Non-Newtonian. Figure 2.1 shows a simplified hydraulic headbox. Although several different variants are used in industrial applications, the basic components remain the same. The pulp suspension is delivered into the headbox through a tapered manifold. The stock makes an abrupt 90° turn into the diffuser tubes, which are also turbulence generators. The large pressure drop that accompanies this helps to disperse the flocs that formed in the pipe flow and create flow uniformity in the tubes (Pantaleo 1994).
Figure 2.1: A simplified schematic of a hydraulic headbox. Not to scale.

Depending on the type of headbox, the diffuser tubes can be either circular or rectangular in cross-section, and can expand gradually downstream or abruptly via sudden expansions. In either case, the expansion produces an adverse pressure gradient that promotes flow separation and dispersion of flocs. As the suspension exits the tubes, the flow separates to form turbulent wakes between adjacent tube exits. Although these wakes may help in dispersing fibres, they create a very non-uniform velocity and consistency profile in the spanwise (cross-machine) direction. This means that the converging section needs to be of a minimum length to allow the suspension to become uniform at the jet exit. The size of the wakes can be reduced if the tubes are of rectangular cross-section (Soderberg 1999), since the land area between the tube exits is smaller. The jets that exit from the tubes merge together downstream causing considerable mixing in the spanwise direction. This turbulence is fairly isotropic and homogeneous in the spanwise direction, but decays very rapidly downstream. The small turbulent scales in this portion of the flow are believed to be beneficial in destroying flocs and creating uniformity in the spanwise, or cross-machine direction. Some headboxes
have a stilling chamber, which damps out pressure pulsations, others simply allow the flow from the tube bank to enter the converging section.

Because of the rectangular cross-section, secondary flows develop within the headbox. These are flows in the plane normal to the flow direction, and are said to contribute to non-uniform fibre orientation and shear on the forming wire (Aidun and Kovacs 1995). Secondary flows move in a circular fashion and produce streamwise vorticity, rendering the flow fully three-dimensional.

The final stage of the headbox involves the converging channel, which serves the function of delivering the dispersed fibre suspension from the turbulence generators onto the forming wire as a thin jet. The fibre orientation and distribution, especially in the cross machine direction, determines the mass distribution on the forming wire, and then on the final sheet of paper. Therefore, careful design of the converging section is needed if good quality is required. As noted by Nordstrom (1994), the acceleration of a fluid through a converging channel can result in a loss of turbulent kinetic energy to the mean motion, which would be detrimental to floc destruction. In a converging flow, it can be shown that the only two production terms that appear in the equation for turbulent kinetic energy are (McComb 1990):

\[
\text{production} = -u'_i u'_j \frac{dU_i}{dx_j} - u'_i^2 \frac{dU_i}{dx_i}
\]  \hspace{1cm} (2.1)

The first term will always be positive. But, since \( u'_i^2 \) is always positive and \( \frac{dU_i}{dx_i} > 0 \), the second term becomes negative, implying a conversion of turbulent energy back to the mean motion. Clearly, the strength of each term determines the overall effect, and that each is dependent on factors such as the convergence angle, Reynolds number, and length of channel. Clearly, this kind of flow requires further study.
It is generally agreed upon that turbulence of small scale and high intensity is beneficial in breaking apart flocs and dispersing fibres. However, this kind of turbulence is difficult to achieve due to some conceptual issues. First, it is difficult to attain small scales with high intensity, or high energy. In a typical energy spectrum, at high wavenumbers (small scales), the dissipation of turbulent kinetic energy increases more rapidly with increasing wavenumber than at intermediate wavenumbers, such as the inertial sub-range, for instance. Secondly, the size of the smallest eddies in a flow are determined by the viscosity of the medium. One effect of adding fibres to the flow is seen as an increase in the apparent viscosity of the suspension. Fibres suppress the generation of small scales, and it is likely that the smallest scales in a fibre suspension are of the same size as the fibres. Therefore, the size of the smallest eddy in a pulp suspension is larger than the smallest eddy in a fibre free suspension (Kerekes 1983). In practice, then, the generation of fine-scale high energy turbulence is constricted by these two conceptual problems.

2.1.2 Application of CFD in headbox design

Obtaining quantitative information on pulp suspension flows is difficult experimentally, whether it is in a laboratory or in an operational headbox. Measurement techniques are often intrusive. For example, sensors cannot be used because fibres staple to the sensors. The opacity of the suspension prohibits the use of visual techniques (Luo et. al. 1999). Much of the current headbox design is accomplished through empirical and heuristic means. An alternative is to use CFD in the design process. With CFD, there are no restrictions on geometry and flow conditions, and detailed information can be
obtained at any location in the headbox. The flow in a full-scale headbox under operational conditions can be simulated. Moreover, much more information is obtainable from a numerical analysis than from experiment. Rather than building physical models and pilot machines, appropriate geometrical changes can be made on the computer and their impact on performance analyzed.

CFD provides the capability to study the hydrodynamics in the headbox to determine where the flow conditions are adversely affecting performance. As an example, and, as seen in the previous section, the flow in the converging section involves complex physics which, depending on the design, may or may not be producing the most dispersed jet.

Another important section is the decaying flowfield downstream of the turbulence generators. Although the turbulence generated is sufficient to break apart flocs and disperse fibres, the rapid decay that follows allows the flocs to reform before they exit the headbox at the slice. The main conclusion that was drawn from the experiments by Kerekes (1995) on flocculation in grid generated turbulent flow was that coherent flocs formed prior to their arrival at the exit of the converging channel. This implies that the jet impinging on the forming wire does not have the optimum fibre dispersion.

Since the grid-generated turbulent flow precedes the converging section, it is desirable to simulate the flow in this section first. This was the focus of this study.

2.1.3 Numerical Models of headbox flows

Although much experimental work has been done on pulp flows, very little has been done in the area of modeling. This is due primarily to a lack of constitutive
mathematical models that describe the physics of fibre suspension flow. Even models that use stiff rod-like cylinders are not applicable to cellulose fibre flows. The issue of modeling fibres is further discussed in section 2.4. Most numerical work has concentrated on solving for the continuous phase only, neglecting the two-phase nature of the flow.

Jones and Ginnnow (1988) used CFD to model the flow in an experimental headbox as well as in a grid generated turbulence flowcell. They used the standard $k - \varepsilon$ model for turbulence modeling but did not model the fibres. The results are in adequate agreement with experiment, with turbulence quantities providing the largest discrepancies. No grid dependency analysis was done, making it difficult to discriminate between modeling errors and numerical errors.

Aidun and Kovacs (1995) used a non-linear $k - \varepsilon$ turbulence model to model the flow in the converging section of a full-scale headbox under operational conditions. With this turbulence model, which is capable of predicting a non-isotropic eddy viscosity, they were able to predict the secondary motion produced by the rectangular geometry and anisotropy of the Reynolds Stresses. The results are in good qualitative agreement with Direct Numerical Simulation (DNS) data. No model was presented for the fibres.

More recently, Hua et. al. (1999) solved for the flow distribution in an inlet tapered manifold and the diffuser tubes. They used a curvilinear grid and the standard $k - \varepsilon$ turbulence model. Simulations were run on two grids to verify grid independence. Although the model appears to capture much of the relevant three-dimensional flow patterns, most of the information presented was qualitative, and no comparison was made
against any experimental measurements. Again, there was no discussion on fibre modeling.

Thus far, the only model presented which accounts for the presence of the fibres is the model by Steen (1991). He models the fibre particles as a continuum and solves a conservation equation for flocculation intensity. For the aggegration of flocs, Steen uses a model analogous to kinetic rate expressions in chemical reactions. He suggests that small turbulent eddies weaken the large floc structures to form smaller flocs. These smaller flocs are transported by the large turbulent eddies, and upon collision with other flocs, form larger flocs. He notes that these two processes occur at the same locations, but at different times. The numerical results presented for pipe flow are in good qualitative agreement with the general trends observed experimentally. However, there is no direct quantitative comparison against any experimental data, which is necessary due to errors associated with the mathematical modeling of both the fibres and the turbulence.

2.2 Transient pulp flocculation in a decaying turbulence flow field

Raghem Moayed (1999) studied the flow of a dilute pulp suspension in a grid-generated turbulent flow. Figure 2.2 shows a schematic of the flowcell with the dimensions. Experiments were run at bulk velocities of 0.26 m/s and 0.45 m/s, and at consistencies of 0.37, 0.42, 0.5, and 0.54%. There are ten grids aligned parallel to the flow. Each grid is 8 mm in width, and the grids are separated by 8 mm. The Reynolds numbers are 2080 and 3600, based on the bulk velocities, grid width, and properties of pure water. The turbulence generated by the grids is fairly isotropic and homogeneous in
the spanwise and normal planes. The local mass density variation downstream of the two central grids was measured using a Dynamic Panoramic View (DPV) technique (Raghem Moayed and Kuhn 2000). The measurement area is showed in Figure 2.2 as the rectangular boxes indicated by the Z abbreviation. A Charged Coupled Device (CCD) video camera was used to continuously capture 500 images at each measurement location. The temporal variation of the images of the selected areas of measurement were computed and converted to mass variability, which was called flocculation intensity, and

![Diagram of grid-generated turbulence flow cell]

**Figure 2.2:** Schematic of grid-generated turbulence flow cell (Raghem Moayed and Kuhn 2000).

is given by,

\[
fl = \frac{(c - C)^2}{C_n^2}
\]

(2.2)
Where, \( c \) is the instantaneous consistency, \( C \) is mean local consistency, and \( C_m \) is the mean consistency of the suspension. Therefore, flocculation intensity values were obtained along the centreline of the channel as well as at spanwise positions up to the centre of the two adjacent central grids. This data will be used for the validation of the numerical model developed in Chapter 3.

2.3 Turbulence Modeling

Turbulence modeling represents one of the most important problems in all of computational fluid dynamics. The characteristics of turbulent flow make it highly non-deterministic. For a flow to be classified as turbulent, it must be three dimensional, unsteady, rotational, and highly irregular. The irregularity is attributed to the non-linearity of the Navier-Stokes equations. The evolution of a turbulent flow is highly dependent on the initial conditions that caused it, as well as on the boundaries that enclose it. This makes the task of developing universal models exceedingly difficult. There has been much work done in this area over the last half-century, and an enormous amount of empirical relations and phenomenological models have been developed. Figure 2.3 displays the current state of the art in the simulation of turbulence. Excellent reviews and descriptions of turbulence modeling are given by Chen and Jaw (1998), Ferziger (1987), Moin and Mahesh (1998), Nallasamy (1987), Rodi (1993), and Speziale (1991). The remainder of the chapter is devoted to the description of each of the more common modeling approaches in more detail.
2.3.1 Direct Numerical Simulation (DNS)

A complete description of a turbulent flow can be obtained by solving the time-dependent Navier-Stokes equations and continuity equation. For the incompressible flow of a Newtonian fluid, these are given by, and written in conservative form,

\[
\frac{\partial u_j}{\partial x_j} = 0
\]

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial u_i}{\partial x_j} \right) - \frac{\partial p}{\partial x_i} + \rho g_i
\]

Where \( u_i \) and \( p \) represent the instantaneous velocity and pressure respectively. These equations, which model the flow as a continuum, are still valid for a turbulent flow because even the smallest length scales in turbulence, the Kolmogorov scales, contain enough molecules to allow statistically significant point averages of velocity, density, etc., which can vary continuously in space (Tennekes & Lumley 1972). Of course, to resolve all the motion, from the largest eddies dictated by the flow enclosure to the smallest scales dictated by the viscosity, a computational mesh of exceedingly large size would have to be constructed.

It can be shown (Tennekes and Lumley 1972) that the number of grid points required is proportional to the turbulent Reynolds number to the 9/4\(^{th}\) exponent. The disparity in scales increases with increasing Reynolds number, which then exponentially increases the mesh requirements. Furthermore, in addition to spatial resolution, small time steps are needed to resolve time evolution due to the inherent unsteadiness of the flow. For example, in the grid-generated turbulent flow of Raghem Moayed (1999), the relevant
turbulent Reynolds number is 3600 based on the width between grids. Using the 9/4\textsuperscript{th} rule, this would require 100 million computational nodes for a complete description of this flow. In an operational headbox where Reynolds numbers are much higher, DNS becomes unmanageable. Clearly, DNS is only applicable to flows with moderate Reynolds numbers and simple geometries. At present, it is used mainly to study the physics of turbulence and to aid in the development of the more common phenomenological turbulence models. It was not used in this study.
2.3.2 Large Eddy Simulation (LES)

In almost all industrial applications, DNS is not feasible, and alternative approaches such as modeling need to be employed. Large Eddy Simulation represents a compromise between direct solution and modeling. In this approach, the unsteady Navier-Stokes equations are filtered to produce a set of equations that govern the large scale motion. The small scales are modeled. The justification for using LES is that the large scales tend to be more anisotropic and dependent on the initial and boundary conditions, whereas the small scales tend to be more isotropic and hence, universal. The large scales also transport most of the energy, so they represent the more relevant scales in a turbulent flow. LES, then, involves solving directly for the large scales and modeling the small scales.

A filtered variable is given as (Ferziger and Peric 1999),

\[ \bar{\phi}(\bar{x}) = \int_D \bar{\phi}(\bar{x}) G(\bar{x}, \bar{x}') d\bar{x}' \]  

(2.5)

Where, D is the fluid domain, and G is the filter function. In the finite volume method, D becomes the control volume, CV, and G equals 1/CV. Therefore, the smallest scale that is resolved directly is equal to the size of the control volume. All other scales smaller that the size of the control volume must be modeled. Filtering the incompressible Navier-Stokes equations gives,

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \bar{u}_i) = 0 \]  

(2.6)

\[ \frac{\partial (\rho \bar{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \bar{u}_i}{\partial x_j} \right) - \frac{\partial \bar{p}}{\partial x_i} - \frac{\partial \tau_{ij}}{\partial x_j} \]  

(2.7)
Where, \( \tau_{ij} = \rho \bar{u}_i \bar{u}_j - \rho \bar{u}_i \bar{u}_j \) is the subgrid-scale stress, which must be modeled. The usual model used is an eddy viscosity model,

\[
\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2 \mu_t \bar{S}_{ij}
\]  

(2.8)

Where, \( \mu_t \) is the subgrid-scale turbulent viscosity and,

\[
\bar{S}_{ij} = \frac{1}{2} \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)
\]  

(2.9)

is the rate of strain tensor. Models for turbulent viscosity include the Smagorinsky-Lilly model and the ReNormalized Group (RNG) based model. In the former, the viscosity is set as, \( \mu_t = \rho L_s^2 \bar{S} \), where \( L_s^2 \) is a mixing length. This model is analogous to the Prandtl mixing length model used for the Reynolds stresses. The model used in this study was the RNG based model, which is given by,

\[
\mu_{eff} = \mu \left[ 1 + H \left( \frac{\mu^2 \mu_{eff}}{\mu_s^3} - C \right) \right]^{1/3}
\]  

(2.10)

where,

\[
\mu_s = (C_{mg} V_{1/3})^2 \sqrt{2 \bar{S}_{ij} \bar{S}_{ij}}
\]  

(2.11)

and,

\[
H(x) = \begin{cases} 
    x, & x > 0 \\
    0, & x \leq 0 
\end{cases}
\]  

(2.12)

The RNG theory gives \( C_{mg} = 0.157 \) and \( C = 100 \). This model was used because of its ability to model low Reynolds number effects encountered in near wall regions. LES was applied to the grid-generated turbulent flow using the exact geometry shown in Figure 2.2 to determine the large scale turbulent motion. The results are presented in Chapter 5.
2.3.3 Reynolds Averaged Navier-Stokes (RANS) equations

Although LES is less computationally intensive than DNS, it still requires a fairly large mesh and small timestep, making it very time-consuming. Moreover, it produces much more information than is required for engineering purposes. An alternative, and in fact a much more widely used approach in industry, is to use the Reynolds Averaged Navier-Stokes (RANS) equations. In this approach, all scales of motion are modeled. The unsteadiness of the flow is removed, or filtered, leaving an equation for the Reynolds Averaged flow variables. A steady state solution can be obtained despite the unsteadiness of the flow. Also, a much larger mesh can be used since the average flow variables vary much more gradually in space than the instantaneous variables. The instantaneous velocity and pressure field is decomposed into a mean (Reynolds average) and fluctuating component:

\[ u_i = U_i + u_i' \quad \text{and} \quad p = P + p' \quad (2.13) \]

The Reynolds average can be of several forms. In a statistically steady flow, it becomes the time average (Speziale 1991),

\[ U_i(\bar{x}) = \frac{1}{T} \int_{t}^{t+T} u_i(\bar{x}, t) dt \quad (2.14) \]

Where \( T \) is a time scale much larger than the time scale of turbulence. For a spatially homogeneous flow, a volume average is used,

\[ U_i(t) = \frac{1}{V} \int_{V} u_i(\bar{x}, t) dV \quad (2.15) \]

For turbulent flows which are neither of the above, the ensemble average can be used. This is the most general average,
Where the average is taken over $N$ repeated experiments (Speziale 1991). Regardless of which of the three is used, the resulting form of the RANS equation is the same. Of course, although the equation is the same, conceptually, each average is different.

Substituting equation (2.13) into equation's (2.3) and (2.4) give the RANS equations,

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

(2.17)

$$
\frac{\partial}{\partial t} (\rho U_i) + \frac{\partial}{\partial x_j} (\rho U_i U_j) = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial U_i}{\partial x_j} \right) - \frac{\partial P}{\partial x_i} + \rho g_i + \frac{\partial}{\partial x_j} (-\rho \overline{u_i' u_j'})
$$

(2.18)

Where, $-\rho \overline{u_i' u_j'}$ is the Reynolds Stress tensor, not to be confused with the subgrid-scale stress given in section 2.3.2. This term arises as a result of the non-linearity of the Navier-Stokes equations, and since it is unknown, the equations cannot be solved. This is the so-called turbulence closure problem. A model must be used for the Reynolds Stress tensor in order to close the equations. Note that the solution of equation's (2.17) & (2.18) yield only the mean quantities, and give no details about the turbulence. The details have been lost as a result of the averaging process. To recover this information, a model must be used, and it must be calibrated with experiment. The effects of the turbulence are important only in as much as how they affect the mean quantities. The Reynolds stresses are tantamount to having additional stresses imposed on the motion, i.e., simply adding extra viscosity. In fact, it is this extra viscosity which enables a stable, steady state numerical solution to equation's (2.17) and (2.18).
2.3.4 Zero Equation Models

The first models to be used for the Reynolds Stresses were zero equation models. Zero implies that no additional partial differential equations are used. Analogous to the Stokes relations for the viscous stresses, the Boussinesq eddy viscosity model is used, which assumes that the Reynolds stress is proportional to the mean strain. For incompressible flow the general form is,

\[-\rho u'_i u'_j = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \]  

(2.19)

Where, \( \mu_t \) is the turbulent viscosity. In zero equation models, the turbulent viscosity is an algebraic function of the mean strain rate, with the constant of proportionality being equal to the length scale of turbulence. The most popular models are the Prandtl mixing length model and the Baldwin-Lomax models. Although the computational effort required with these models is minimal, the applicability is very limited, and as such, they are seldom used.

2.3.5 One and two equation models

A major shortcoming of zero equation models is that the turbulent length scale must be prescribed. However, it is flow dependent and not known a priori. An alternative, which has become very popular, is to solve transport equations describing some mean quantities of turbulence. For example, if the turbulent velocity scale is given by \( q \), and the length scale given by \( \ell \), then it can be shown by dimensional analysis (Kolmogorov 1942) that the turbulent viscosity is given by,

\[ \mu_t = C q \ell \]  

(2.20)
Where, $C$ is a dimensionless constant. Therefore, $\mu_i$ can be evaluated if both these scales are known. Both $q$ and $\ell$ can be related to more physically identifiable quantities such as the turbulent kinetic energy, $k$, and the dissipation rate of turbulent kinetic energy, $\varepsilon$. These are defined as,

$$k = \frac{1}{2} \frac{u'_i u'_i}{\varepsilon}$$

$$\varepsilon = \nu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_j}{\partial x_i}$$

The relationships are,

$$q = k^{\nu^2}$$

and,

$$\ell = C_D k^{3/2} \varepsilon$$

Where, $C_D$ is a dimensionless coefficient. The second relation comes from the assumption that at high Reynolds numbers there is a balance between the production of turbulent kinetic energy and the dissipation (Rodi 1993). Substituting these expressions into equation (2.20) gives,

$$\mu_i = \rho C_{\mu} \frac{k^2}{\varepsilon}$$

Where, $C_{\mu}$ is a dimensionless constant. In a one-equation turbulence model, a transport equation is solved for the turbulent kinetic energy, and the length scale of turbulence is prescribed. Equation (2.24) is then used to determine $\varepsilon$. This procedure, however, suffers from the same problems which plague the zero equations models, that is, the value of the length scale must be given. The alternative is to solve another transport equation, either
for \( \ell \) or \( \varepsilon \). The more popular choice has been for the later. Solving two equations, one for \( k \) and the other for \( \varepsilon \), enables \( \mu \) to be calculated from equation (2.25). Once this is known, then all the Reynolds Stresses can be computed using equation (2.19).

Exact equations that describe the transport of turbulent kinetic energy and the dissipation rate of turbulent kinetic energy can be derived. The procedure for the \( k \) equation is as follows:

- Multiply equation (2.18) by \( U_i \) to obtain an equation for the mean turbulent kinetic energy, \( K \).
- Multiply equation (2.4) by \( u_1 = U_i + u' \) and take the ensemble average of this equation.
- Subtract the \( K \) equation from this equation.

This leaves the equation for the turbulent kinetic energy,

\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial}{\partial x_j} \left( \rho U_j k \right) = \frac{\partial}{\partial x_j} \left( -\frac{\rho u'_i u'_j u'_j}{2} - \overline{p' u'_j} + \mu \frac{\partial k}{\partial x_j} \right) - \rho u'_{i} u'_{j} \frac{\partial U_{i}}{\partial x_{j}} - \mu \frac{\partial u'_{i}}{\partial x_{j}} \frac{\partial u'_{i}}{\partial x_{j}} \tag{2.26}
\]

The physical interpretation of each term is as follows:

- 1\(^{st}\) term and 2\(^{nd}\) terms on the R.H.S are the diffusion of \( k \) due to turbulent and pressure fluctuations.
- 3\(^{rd}\) term on the R.H.S is the diffusion of \( k \) due to molecular viscosity.
- 4\(^{th}\) term on the R.H.S accounts for the production of \( k \).
- 5\(^{th}\) term on the R.H.S. accounts for the dissipation of \( k, \varepsilon \).
1st term on the L.H.S. is the accumulation term and the 2nd term is the convective transport of $k$ due to the mean motion.

The 1st, 2nd, 4th, and 5th terms on the R.H.S. are all unknown, and to close the equation, must be modeled. Equation (2.19) is used for the correlation in the 4th term. The 1st and 2nd terms are usually modeled together using a gradient type approach (Launder and Spalding 1974),

$$
\frac{\partial}{\partial x_j} \left( \frac{-\rho u'_i u'_j u'_j}{2} - p'u'_j \right) = \frac{\partial}{\partial x_j} \left( \frac{\mu^+}{\sigma + \sigma_k} \frac{\partial k}{\partial x_j} \right)
$$

(2.27)

Where $\sigma_k$ is the turbulent Prandtl number. Rather than model the 5th term, which is the dissipation rate of $k$, a similar transport equation is derived for it. An exact equation can also be derived for $\epsilon$. The equation contains so many unknown correlation’s that almost every term requires modeling. Only the modeled equation is given here,

$$
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial (\rho U_j \varepsilon)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \frac{\mu^+}{\sigma} \frac{\partial \varepsilon}{\partial x_j} \right) - \rho \frac{u'_i u'_j}{2} \frac{\partial \nu}{\partial x_j} \frac{\partial U_j}{\partial x_j} C_{\epsilon 1} \frac{\varepsilon}{k} - \rho C_{\epsilon 2} \frac{\varepsilon^2}{k}
$$

(2.28)

Equations (2.26) and (2.28) make up the two-equation standard $k-\varepsilon$ model. The constants in the model have the following values:

$C_{\mu} = 0.09; \quad \sigma_k = 1.0; \quad \sigma_\varepsilon = 1.3; \quad C_{\epsilon 1} = 1.44; \quad C_{\epsilon 2} = 1.92$

Several variants of the $k-\varepsilon$ model have been proposed in recent years. A more popular version is the RNG $k-\varepsilon$ model, developed by Orszag and Yakhot (1986). It has the same form as the standard model, but the model constants are derived analytically from a mathematical method referred to as renormalization group theory. In addition, a second term also appears in the $\varepsilon$ equation. The RNG $k-\varepsilon$ model is given by,
\[
\frac{\partial (\rho k)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j k) = \frac{\partial}{\partial x_j} \left( \alpha_k (\mu + \mu_a) \frac{\partial k}{\partial x_j} \right) + \mu_s S^2 - \rho \varepsilon \tag{2.29}
\]

\[
\frac{\partial (\rho \varepsilon)}{\partial t} + \frac{\partial}{\partial x_j} (\rho U_j \varepsilon) = \frac{\partial}{\partial x_j} \left( \alpha_\varepsilon (\mu + \mu_a) \frac{\partial \varepsilon}{\partial x_j} \right) + C_{\varepsilon 1} \frac{\varepsilon}{k} \mu_s S^2 - \rho C_{\varepsilon 2} \frac{\varepsilon^2}{k} - R \tag{2.30}
\]

Where,

\[
S = \sqrt{2S_{ij} S_{ij}} \tag{2.31}
\]

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j} \right) \tag{2.32}
\]

\[
R = \frac{C_\mu \rho \eta^3 (1 - \eta / \eta_0) \varepsilon^2}{1 + \beta \eta^3 k} \tag{2.33}
\]

\[
\eta = \frac{Sk}{\varepsilon} \tag{2.34}
\]

and, \( \alpha_k = \alpha_\varepsilon = 1.393, C_{1\varepsilon} = 1.42, C_{2\varepsilon} = 1.68, \eta_0 = 4.38, \beta = 0.012 \).

The effect of the extra strain term, \( R \), in the \( \varepsilon \) equation can be seen as follows. The last two terms on R.H.S. of equation (2.30) can be lumped together to give the following term,

\[-C_{2\varepsilon}^{*} \rho \frac{\varepsilon^2}{k} \]

where,

\[
C_{2\varepsilon}^{*} = C_{2\varepsilon} + \frac{C_\mu \rho \eta^3 (1 - \eta / \eta_0)}{1 + \beta \eta^3} \tag{2.35}
\]

Now, \( \eta \), is the ratio of the mean to turbulent strain rate. In regions where \( \eta < \eta_0 \), the second term in equation (2.35) is positive and increases the value of \( C_{2\varepsilon}^{*} \) close to the value of 1.92 used in the standard \( k-\varepsilon \) model (Choudhury et al. 1993). Therefore, in
moderately strained flows, the two models yield similar results. The differences lie when the value of $\eta$ becomes larger than $\eta_0$. In this case, the second term in equation (2.35) becomes negative, and the value of $C'_2$ becomes smaller than $C_2 = 1.68$. This reduced value means that the destruction of $\varepsilon$ in equation (2.30) is also reduced. This leads to higher values of $\varepsilon$, and subsequently, lower values of $k$ and $\mu_1$. Therefore, the RNG model gives better results in regions of the flow where the mean strain rates are high because it is more responsive to the effects of rapid strain than the standard $k-\varepsilon$ model (Choudhury et. al. 1993). For this reason, the RNG $k-\varepsilon$ model was chosen over the standard model for application in the grid-generated turbulent flow simulations. The model will not over-predict the values of $k$ in the massive flow separation that occurs when the jet exits the channels between the grids.

### 2.3.6 Reynolds Stress Models (RSM)

Two equation turbulence models have become very popular in industrial applications because they are easy in implement into a code, require little extra computational effort, and are very robust in solving a variety of industrial problems. However, they are based on the eddy viscosity model, which conceptually, is not a good representation of turbulent flow. The eddy viscosity concept is based on an analogy with the Stokes hypothesis for the viscous stresses. It implies that turbulent eddies, like molecules, collide and exchange momentum (Rodi 1993). Therefore, turbulence is assumed to be a diffusive type process. This, however, can not be correct. Unlike molecules, eddies are not rigid bodies that retain their size and identity (Rodi 1993). Most of the turbulent energy is transported by the largest eddies in the flow, who's size is
comparable to the size of the boundaries which enclose the flow. Therefore, the momentum exchange between these large eddies cannot be assumed to behave in a diffusive type process. Since the eddy viscosity model assumes that it is, this implies that the turbulent viscosity, $\mu_r$, is isotropic, and hence, a scalar quantity. This means that it takes on the same value for the different Reynolds stresses, $-\rho \overline{u_i u_j}$ (Nallasamy 1987). Experiments show, that in three dimensional flows, it becomes highly anisotropic, and can no longer be regarded as a scalar, in fact, it is a tensor quantity (Ferziger 1999).

The inability of two-equation models to predict anisotropic flows such as the secondary motion in rectangular channels has lead to the development of the so-called Reynolds Stress Models (RSM). In this approach, the eddy viscosity concept is abandoned altogether, and conservation equations are derived from the Navier-Stokes equations for all the Reynolds stresses, $-\rho \overline{u_i u_j}$. Since this model was not used in this study, the equations will not be given here, only a brief description will be given instead. Complete derivations and modeling techniques for RSM models are given in Chen and Jaw (1998) and Rodi (1993).

Analogous to the exact $k$ and $\varepsilon$ equations, additional unknown correlation's appear in the exact equations that require modeling to close the system of equations. Unlike in the $k$ and $\varepsilon$ equations, however, additional terms appear that account for some of the relevant physics. For example, a pressure-strain term arises in the derivation, which has the role of redistributing energy among the different velocity components, i.e., it tends to isotropize the flow. In addition, the effects of buoyancy and rotation are included in the equations (Rodi 1993). The premise of RSM models is that, by solving for the different Reynolds stresses, the anisotropy and inhomogeneity of the turbulence can be
accurately predicted. Of course, all the extra terms which account for this physics require modeling, making the task of developing a universal RSM model a difficult one. A major drawback is that seven additional partial differential equation's need to be solved, six for the six independent Reynolds Stresses, and one for the dissipation rate of turbulent kinetic energy, making the computational effort much more demanding. Furthermore, RSM models have not been tested as extensively as two-equations models, so their applicability in different industrial applications remains uncertain. It is for this reason, and the fact that grid-generated turbulence tends to be fairly isotropic and homogeneous, that RSM was not used in this study.

2.3.7 Near-wall modeling

Because of the no-slip boundary condition at wall surfaces, the velocity gradients near walls are especially large. Solving the transport equations all the way to the wall requires a very fine grid to resolve the boundary layer accurately. In most numerical codes, this is avoided by using what is referred to as a wall function to bridge the gap between the wall and the flow immediately outside the boundary layer. Thus, a computationally expensive mesh is avoided. The most common wall function is the standard logarithmic law of the wall. It is derived based on the fact that at high Re numbers, there is an equilibrium between the production and dissipation of turbulent kinetic energy. The mean velocity profile is given by (Nallasamy 1987),

$$\frac{U}{u_r} = U^+ = \frac{1}{\kappa} \ln \left( \frac{E u_r \sigma y}{\mu} \right) = \frac{1}{\kappa} \ln(Ey^+)$$  (2.36)
Where, \( u_r = \sqrt{\tau_w / \rho} \) = friction velocity, \( \kappa = 0.41 \), \( E = 9.81 \), \( y^+ = u_r \rho y / \mu \), and \( y \) is the distance from the wall. Equation (2.36) is generally valid for: \( 30 < y^+ < 500 \). The first grid point needs to be within this region. Near the wall where \( y^+ < 11 \), the following equation is used,

\[
U^+ = y^+ \tag{2.37}
\]

Although the standard wall function is easy to implement and reduces the computational effort involved, it has limited ability in handling flows that have separated at the wall or that deviate from the assumption of turbulence equilibrium (Chen and Patel 1987). The non-equilibrium wall function was devised to remedy this situation. This model still assumes a logarithmic velocity profile, but incorporates additional terms to account for non-equilibrium boundary layers and pressure gradients that lead to separation. The velocity profile is given as,

\[
\frac{\bar{U}C_{\mu}^{1/4}k^{1/2}}{\tau_w / \rho} = \frac{1}{\kappa} \ln \left( E \frac{\rho C_{\mu}^{1/4}k^{1/2}y}{\mu} \right) \tag{2.38}
\]

Where,

\[
\bar{U} = U - \frac{1}{2} \frac{dp}{dx} \left[ \frac{y_v}{\rho \kappa^* k^{1/2}} \ln \left( \frac{y}{y_v} \right) + \frac{y - y_v}{\rho \kappa^* k^{1/2}} + \frac{y_v^2}{\mu} \right] \tag{2.39}
\]

\[
y_v = \frac{\mu y_v^*}{\rho C_{\mu}^{1/4}k_p^{1/2}} \tag{2.40}
\]

\[
y_v^* = 11.225 \tag{2.41}
\]

Note that the log-law mean velocity is sensitized to pressure gradients.
2.4 Two-Phase Modeling

This section describes the methods used to model two-phase flow mixtures with emphasis on applications to fibre suspension flows. The different approaches will be discussed in context of applicability to fibre flows. A good general review of multiphase flow modeling is given by Crowe et. al. (1996).

2.4.1 Direct Numerical Simulation

The ideal numerical model for a fibre suspension flow would allow for the calculation of the velocity and position of each fibre at any instant in time. This would require solving a particle equation of motion,

\[
m_p \frac{d\vec{v}_p}{dt} = \sum \vec{f}_p \tag{2.42}
\]

\[
\frac{d\vec{x}_p}{dt} = \vec{v}_p \tag{2.43}
\]

All the forces that act on a fibre need to be determined. This includes, in addition to hydrodynamic drag, the forces exerted by fibres on each other. These forces can be mechanical, through the action of friction, or electrostatic, caused by the addition of chemical additives. The inability of fibres to support bending stresses makes them flexible, further complicating the force balance. It is clear that such an equation would be extremely difficult to construct, even if major simplifications are made, such as assuming a fibre to be a stiff, rod-like cylinder. A second major complication is that some forces, such as drag, are a function of the local instantaneous velocity of the carrier, or continuous, fluid. The only way to obtain this information, is through a Direct Numerical Simulation. Therefore, the fact that the equations of motion for fibres are unknown, and
that a DNS of the continuous phase requires immense computational requirements, makes the use of this method far from becoming a reality any time soon. Alternative approaches must be used.

2.4.2 Lagrangian Approach

In this approach, the continuous phase is determined by solving the RANS equations, and an equation of motion is used for the particles. These are usually referred to as Stochastic models, which can track the trajectories of many particles in space and time. The instantaneous fluid velocity is determined by adding a fluctuating velocity to the mean velocity calculated randomly from a Gaussian distribution related to the turbulent kinetic energy. Of course, the problem of solving an equation of motion for a fibre is still present. Lagrangian models have found application mainly in dilute gas-liquid flows, where the density of the particles is much greater than that of the carrier fluid. As a result, hydrodynamic drag becomes the dominant force affecting the particle motion. Also, all particles are spherical with low concentrations in suspension, making particle-particle interactions unimportant. Adeniji-Fashola and Chen (1990) and Durst and Milojevic (1984) give Lagrangian models applied successfully to gas-liquid flows.

2.4.3 Eulerian Approach

Clearly, deriving an equation of motion for fibre particles in turbulent flow is difficult. Also, it is not particularly necessary, since the exact position and velocity of every fibre in the flow need not be known. An alternative, is to treat the particulate phase as a continuum, this is the basis behind Eulerian models. Analogous to that of the carrier
fluid, properties of the particulate phase are assumed to vary continuously in space. Ideally, for a two-phase mixture to be considered a continuum, the smallest dynamical scale of motion, the smallest turbulent eddies, must contain within it enough particles to allow statistically significant local averages of particle density, concentration, etc. (Lumley 1976). In reality, however, no two-phase mixture can satisfy this criterion, unless the size of the particles approaches those of molecules. The cellulose fibres used in the experiments of Raghem Moayed (1999) were approximately 1 mm in length, which coincides with the length scale of the smallest eddies in the grid-generated turbulent flow. Therefore, the smallest dynamical scale is of the same order of magnitude as the particle scale.

The Eulerian continuum model encompasses both a single-fluid and two-fluid model. In the single-fluid model, the particles are treated as passive, with a relative velocity between the carrier fluid and particles being close to zero. A single conservation equation can be written describing the transport of a relevant quantity related to the particulate phase, such as mass fraction or concentration, for instance. In the two-fluid model, additional mass and continuum momentum equations need to be solved for the particulate phase, since the particle velocities differ from those of the carrier fluid. An indication of whether a two-phase flow can be accommodated by the single-fluid model is to examine the magnitude of the Stokes number.

This is ratio of the particle response time to the characteristic time of the carrier fluid motion,

\[ St = \frac{t_p}{t_c} \]  

(2.44)
If the Stokes number is much less than unity, the velocity differences between the particles and fluid are negligible, and the single-fluid model is applicable. If the Stokes number is much larger than unity, the velocity differences are larger (Crowe et. al. 1996), and the two-fluid model needs to be used. The particle response time is the time it takes for a particle at rest to accelerate to within 63% of the carrier fluid velocity (Hestroni 1989). It is given by,

\[
t_r = \frac{d^2 \rho_p}{18 \mu_f} \tag{2.45}
\]

Where, \(d\) is the particle diameter, \(\rho_p\) is the particle density, and \(\mu_f\) is the carrier fluid viscosity. The definition of the characteristic time of the fluid motion is less clear. If it is based on bulk quantities, then for the grid-generated turbulent flow of Raghem Moayed (1999) it is equal to \(d/\bar{U}_b\), which then becomes 0.008 m/0.45 m/s = 0.0178 s. The fibres used in the experiments of Raghem Moayed (1999) had an average diameter of 1 mm, and average length of 50 \(\mu\)m. If the density of the fibres is assumed to be 1,500 kg/m³ and the viscosity of the carrier fluid equal to 0.001 Pa·s, then the particle response time for the fibres becomes 0.000283 s, and the Stokes becomes 0.016. This low value is attributed to the small fibre diameter and fibre density. The fibre density is very close to that of water, which means the fibres are neutrally buoyant and their inertia is unimportant. Although the magnitude of the Stokes number implies that there is a negligible velocity difference between the fibres and carrier fluid, it is known that there exist strong fibre-fibre interactions due to the large L/D ratios associated with fibres, and this interaction is what causes floculation. The possible alternative is to use a two-fluid model, which involves solving additional mass and momentum equations for the fibres. If
the volume fraction of the fibres in the flow is given by $\theta$, then the particulate phase loading is given by,

$$\rho_p = \rho_s \theta$$  \hspace{1cm} (2.46)

Where, $\rho_s$ is the fibre material density, i.e., 1,500 kg/m$^3$. If the velocity of the particulate fibre phase is given by $u_p = U_p + u_p'$, then the following mass and momentum equations can be written for the fibre phase for steady, incompressible flow,

$$\frac{\partial}{\partial x_j}(\rho_p U_{p_i}) + \frac{\partial}{\partial x_j}(\rho_p' u'_p) = 0$$  \hspace{1cm} (2.47)

$$\frac{\partial}{\partial x_j}(\rho_p U_{p_i} u_{p_i}) = -\frac{\partial}{\partial x_j}(\rho_p u'_p u'_{p_i}) - \frac{\partial}{\partial x_j}(\rho_p' u'_p U_{p_i})$$

$$-\frac{\partial}{\partial x_j}(\rho_p' u'_p u'_{p_i}) - F_{pi}$$  \hspace{1cm} (2.48)

Equations (2.47) and (2.48) are applicable only if the suspension is dilute, that is, the volume fraction of the particulate phase is much smaller than unity, so that the volume fraction of the carrier phase is equal to unity. This assumption is valid for a fibre suspension in a headbox since at consistencies of 0.5% the volume fraction of fibres in the suspension is low. Unfortunately, $\rho_p' u'_p, u'_p u'_{p_i}, \rho_p' u'_p u'_{p_i},$ and $F_{pi}$ are all unknown, and must be modeled. Without detailed experimental measurements of these correlations, modeling these terms would be very difficult. $F_{pi}$ represents the inter-phase interaction force that accounts for the exchange of momentum between the fibre particulate phase and the carrier phase. In a fibre suspension, it is difficult to define this term since hydrodynamic drag is not the dominant force affecting the momentum exchange. The
forces exerted by the fluid on the fibres to build and destroy flocs are likely to be much larger. At present, these forces are not well understood.

It was concluded, based on all the above arguments, that a single-fluid Eulerian multiphase flow model may be used to account for the fibres in the suspension. As mentioned previously, it is not important to determine the instantaneous locations of each and every fibre in the flow, but rather to determine local variations of fibre mass by solving a conservation equation describing the transport of some quantity indicative of the amount of fibre mass present. This quantity will be called the flocculation intensity, its exact definition will be given in the next chapter. The magnitude of flocculation intensity and its spatial variation indicates the level of mass variability present in the suspension, and hence, the degree to which the suspension is flocculated. The hydrodynamic forces exerted by the turbulent motion will govern the magnitude of flocculation intensity and its transport. The next chapter describes the derivation of the transport model for the flocculation intensity.
Chapter 3

Development of Fibre Suspension Model

3.1 Derivation of transport equation for flocculation intensity

The rules of time averaging for a scalar variable $\phi$ in a turbulent flow are as follows:

\[
\bar{\phi} = \phi^0 ; \quad \overline{\phi + \phi} = \overline{\phi} + \overline{\phi} ; \quad \overline{\phi'} = 0 ; \quad \overline{\phi'^2} \neq 0 ;
\]

\[
\frac{\partial \phi}{\partial s} = \frac{\partial \bar{\phi}}{\partial s} ; \quad \overline{\phi \phi} = \bar{\phi} \bar{\phi}
\]

The conservation equation describing the steady transport of instantaneous fiber mass is,

\[
\rho u_j \frac{\partial c}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c}{\partial x_j} \right)
\]

(3.1)

where,

$\rho$ = density of the suspension, kg suspension/m$^3$ (assumed to that of water)

$c$ = mass fraction of fiber (consistency), in kg fibre/kg suspension

$D$ = molecular diffusivity, in m$^2$/s
Using Reynolds decomposition, introduce $c = C + c'$ and $u = U + u'$ into equation (3.1) and time average according to the rules above to give,

$$\rho U_j \frac{\partial C}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) - \frac{\partial}{\partial x_j} \left( \rho \overline{u'_j c'} \right)$$

Equation (3.2) is the exact equation describing the transport of the mean fibre mass. Analogous to the Reynolds Averaged Navier Stokes (RANS) equations, the solution of equation (3.2) requires the determination of $\rho \overline{u'_j c'}$, the turbulent mass flux. This term accounts for the transport of $C$ by turbulent fluctuations. However, in turbulent pulp suspensions, gradients of the mean mass fraction, $C$, are usually quite small, and so the solution of equation (3.2) would yield little information concerning the mass variability responsible for flocculation. Of more interest, is the flocculation intensity, as defined by Raghem Moayed and Kuhn (1999),

$$fl = \frac{\text{variance}}{C_m^2} = \frac{(c - C^2)}{C_m^2} = \frac{c'^2}{C_m^2}$$

The flocculation intensity indicates the level of mass variability. If there are flocs, then there is a lot of variability since mass is concentrated in the flocs rather than in between them. The remaining section describes the derivation of a conservation equation which describes the steady state transport of flocculation intensity.

Multiply equation (3.2) by $\rho C$ to give,

$$\rho^2 C U_j \frac{\partial C}{\partial x_j} = \rho C \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) - \rho C \frac{\partial}{\partial x_j} \left( \rho \overline{u'_j c'} \right)$$

or equivalently written as,
\[ \rho^2 U_j \frac{\partial}{\partial x_j} \left( \frac{C^2}{2} \right) = \rho C \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) - \rho C \frac{\partial}{\partial x_j} \left( \rho u_j c' \right) \]  

(3.3)

Next, multiply equation (3.1) by \( \rho c \) and introduce \( c = C + c' \) and \( u_j = U_j + u_j' \) to give,

\[ + \rho^2 (C + c') (U_j + u_j') \frac{\partial (C + c')}{\partial x_j} = \rho (C + c') \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial (C + c')}{\partial x_j} \right) \]

Next, time average this equation to give,

\[ \rho^2 C U_j \frac{\partial C}{\partial x_j} + \rho^2 C \bar{u}_j \frac{\partial C}{\partial x_j} + \rho^2 \bar{c} \bar{u}_j \frac{\partial C}{\partial x_j} + \rho^2 \bar{c'} \bar{u}_j' \frac{\partial C}{\partial x_j} \]

\[ + \rho^2 C U_j \frac{\partial c'}{\partial x_j} + \rho^2 C \bar{u}_j \frac{\partial c'}{\partial x_j} + \rho^2 U_j \bar{c'} \frac{\partial c'}{\partial x_j} + \rho^2 \bar{c'} \bar{u}_j' \frac{\partial c'}{\partial x_j} \]

\[ = \rho C \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) + \rho C' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'}{\partial x_j} \right) + \rho C \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial \bar{c'}}{\partial x_j} \right) + \rho C' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial \bar{c'}}{\partial x_j} \right) \]

(3.4)

The 2\textsuperscript{nd}, 3\textsuperscript{rd}, and 5\textsuperscript{th} terms on the L.H.S. and the 3\textsuperscript{rd} and 4\textsuperscript{th} terms on the R.H.S. are zero from the rules of time averaging. Therefore, equation (3.4) reduces to,

\[ \rho^2 C U_j \frac{\partial C}{\partial x_j} + \rho^2 \bar{c} \bar{u}_j \frac{\partial C}{\partial x_j} + \rho^2 \bar{c'} \bar{u}_j' \frac{\partial C}{\partial x_j} + \rho^2 U_j \bar{c'} \frac{\partial c'}{\partial x_j} \]

\[ + \rho^2 \bar{c'} \bar{u}_j' \frac{\partial c'}{\partial x_j} = \rho C \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) + \rho C' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'}{\partial x_j} \right) \]

or equivalently written as,

\[ \rho^2 U_j \frac{\partial (C^2 / 2)}{\partial x_j} + \rho^2 \bar{c} \bar{u}_j' \frac{\partial C}{\partial x_j} + \rho^2 C \bar{u}_j' \frac{\partial c'}{\partial x_j} + \rho^2 U_j \bar{c'} \frac{\partial (C^2 / 2)}{\partial x_j} + \rho^2 \bar{c'} \bar{u}_j' \frac{\partial (c'^2 / 2)}{\partial x_j} \]

\[ = \rho C \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial C}{\partial x_j} \right) + \rho C' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'}{\partial x_j} \right) \]

(3.5)

Subtract equation (3.3) from equation (3.5) to give,
\[
\rho^2 c' u'_j \frac{\partial c}{\partial x_j} + \rho^2 C u'_j \frac{\partial c'}{\partial x_j} + \rho^2 U_j \frac{\partial (c'^2 / 2)}{\partial x_j} \\
+ \rho^2 u'_j \frac{\partial (c'^2 / 2)}{\partial x_j} = \rho c' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'}{\partial x_j} \right) + \rho C \frac{\partial}{\partial x_j} \left( \rho u'_j c' \right)
\]

(3.6)

The 2\textsuperscript{nd} and 4\textsuperscript{th} terms on the L.H.S. can be written as,

2\textsuperscript{nd} term: \[ \rho^2 C u'_j \frac{\partial c'}{\partial x_j} = \rho^2 C \frac{\partial (u'_j c')}{\partial x_j} \]

4\textsuperscript{th} term: \[ \rho^2 u'_j \frac{\partial (c'^2 / 2)}{\partial x_j} = \rho^2 \frac{\partial (u'_j c'^2 / 2)}{\partial x_j} \]

Since \( \frac{\partial u'_j}{\partial x_j} \equiv 0 \) from continuity.

Making the substitutions into equation (3.6) and rearranging and simplifying,

\[
\rho^2 U_j \frac{\partial (c'^2 / 2)}{\partial x_j} = \rho c' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'}{\partial x_j} \right) - \rho^2 c' u'_j \frac{\partial c}{\partial x_j} - \rho^2 \frac{\partial (u'_j c'^2 / 2)}{\partial x_j}
\]

(3.7)

Also, if D is constant (i.e., assumed independent of the flow), it can be shown that,

\[
\rho c' \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'}{\partial x_j} \right) = \rho \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial (c'^2 / 2)}{\partial x_j} \right) - \rho^2 D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j}
\]

Making the substitution into equation (3.7) and multiplying the entire equation by 2 gives,

\[
\rho^2 U_j \frac{\partial c'^2}{\partial x_j} = \rho \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial c'^2}{\partial x_j} \right) - 2 \rho^2 D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} \\
-2 \rho^2 c' u'_j \frac{\partial c}{\partial x_j} - \rho^2 \frac{\partial (u'_j c'^2)}{\partial x_j}
\]

(3.8)
Other than that $D$ & $\rho$ are constant, equation (3.8) represents the exact conservation equation for the transport of $\bar{c}^{\prime 2}$. It represents a conservation of the mean square of the fluctuations in consistency. It is analogous to the exact conservation equation for the turbulent kinetic energy. The turbulent kinetic energy is defined as the sum of the mean square of the fluctuations in the three components of velocity. The term on the L.H.S. represents the convective flux of $\bar{c}^{\prime 2}$. The 1st term on the R.H.S. represents the molecular diffusion of $\bar{c}^{\prime 2}$, the 2nd term, the dissipation, $\varepsilon_r$, of fluctuations due to molecular processes (Lauder, 1976) (analogous to $\varepsilon$ in the turbulent kinetic energy equation), the 3rd term, the production, $P_r$, due to gradients in $C$ (Lauder, 1976), and the 4th term, the convective transport of $\bar{c}^{\prime 2}$ due to turbulent fluctuations. Equation (3.8) cannot be solved since the last three terms on the R.H.S. contain unknown quantities ($\frac{\partial \bar{c}^{\prime}}{\partial x_j} \frac{\partial \bar{c}^{\prime}}{\partial x_i}, \bar{c}^{\prime} u^{\prime}_i u^{\prime}_j, u^{\prime}_i \bar{c}^{\prime 2}$).

Therefore, the closure problem which plagues the RANS also afflicts equation (3.8). Exact equations can be derived in a similar fashion as above for the three unknown quantities, but this will introduce even more higher order (triple and fourth order) correlation's which are also unknown, hence the closure problem in turbulence. Alternatively, these terms can be measured and empirical correlation's can be produced. This would require a complete record of both the turbulent and mass fraction statistics both temporal and spatial. However, most often the only option is to simply model these terms, which is what is done in the turbulent kinetic energy equation.

To be used in the finite volume method, equation (3.8) must be converted into the standard conservative form. It is customary to group all the source terms together. Let,
\[ S_n = -2c'u_j \frac{\partial C}{\partial x_j} - 2D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} - \frac{\partial (u'c'^2)}{\partial x_j} + S_{add} \]

\( S_{add} \) represents any additional source terms which may need to be added. Since \( \rho \) is constant, equation (3.8) can be re-written as,

\[ \rho U_j \frac{\partial (c'^2)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial (c'^2)}{\partial x_j} \right) + \rho S_n \]  

(3.9)

The term on the L.H.S. can be written as,

\[ \rho U_j \frac{\partial (c'^2)}{\partial x_j} = \frac{\partial (\rho U_j c'^2)}{\partial x_j} \]

Since \( \frac{\partial U_j}{\partial x_j} = 0 \) from continuity.

Making the substitution gives,

\[ \frac{\partial (\rho U_j c'^2)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial (c'^2)}{\partial x_j} \right) + \rho S_n \]  

(3.10)

Equation (3.10) is in the standard form with

\[ \phi = c'^2 \quad ; \quad \Gamma = \rho D \quad ; \quad S = \rho S_n \]

Furthermore, dividing equation (3.10) by \( C_m^2 \) and letting \( fl = c'^2 / C_m^2 \),

\[ \frac{\partial (\rho U_j fl)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial fl}{\partial x_j} \right) + \frac{\rho S_n}{C_m^2} \]  

(3.11)

Where,

\[ fl = c'^2 / C_m^2 \]

\[ S_n = -2c'u_j \frac{\partial C}{\partial x_j} - 2D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} - \frac{\partial (u'c'^2)}{\partial x_j} + S_{add} \]
Equation (3.11) is the final form of the conservation equation for flocculation intensity. Note the equation has the units of kg/m³s. All the source terms in $S_n$ have units of s⁻¹.

### 3.2 Modeling source terms in equation for $f_l$

The three terms from equation (3.11) which require modeling are,

\[
(3.12) \quad -2\frac{\rho}{C_m^2} c'u'_j \frac{\partial C}{\partial x_j}; \quad (3.13) \quad 2\frac{\rho}{C_m^2} D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j}; \quad (3.14) \quad -\frac{\rho}{C_m^2} \frac{\partial (u'_j c'^2)}{\partial x_j}
\]

Term (3.12)

For a passive scalar, this term is usually the production term, which assumes that the production of fluctuations are governed by mean gradients in $C$. However, for a pulp suspension, this is not necessarily the case. Moreover, $C$ is assumed to remain uniform over the entire flowfield\(^1\), which means that gradients in $C$ are zero. Therefore, this term can be neglected,

\[
-2\frac{\rho}{C_m^2} c'u'_j \frac{\partial C}{\partial x_j} \equiv 0
\]

However, in the flow of a pulp suspension in a decaying turbulence flowfield, a production term must be included since the experimental observations made by many researchers have shown the flocculation process (increasing flocculation intensity) exists, and that flocculation is governed in part by the hydrodynamics of the mean flow and the turbulent flow. Other factors of course included fibre type, length/diameter ratio, surface characteristics, etc. Furthermore, large stable flocs with no change in size tend to form

\[^1\] This assumption is valid over most of the flow except near the walls where the shear is strong enough to cause a variation in the mean consistency. For this study, however, these near-wall effects are ignored.
indicating a balance between production and destruction.

The flocculation process has been studied extensively by many, Anderson (1966), Beghello (1998), D’Incau (1983), Hourani (1988), Kerekes (1983) & Kerekes et. al (1985), Mason (1950), Norman et. al. (1977) and Takeuchi et. al (1983). Although a wide range of theories have been proposed concerning the mechanisms responsible for flocculation, consensus amongst researchers is limited. One conclusion, however, that is generally agreed upon, is that shear flow, or gradients in the mean fluid velocity, cause fibres to rotate, collide, and entangle to form flocs, the basic mechanisms behind mechanical flocculation. Also, it is generally accepted that the destruction of flocs is determined by turbulence of small scale and high intensity. Therefore, it is postulated here that the floc formation (production of fl) is governed by the bulk or mean properties of the flow, such as mean strain, Reynolds number, consistency, etc., and that the destruction of flocs (dissipation of fl) is determined by the small scale turbulence of high intensity.

The role of mean strain in the production of flocs is described next. Kerekes (1983) notes that mean strain will cause a transient floc to form, and this transient floc will turn into a permanent floc if the strain further downstream in the flow is less than it was at the point where the floc formed. This condition appears to be occurring in the decaying turbulence experiments conducted by Raghem Moayed (1999). From both visual observations and through quantitative estimates of flocculation intensity, it appeared that flocs formed very quickly in the decay section of the flow and that these flocs persisted downstream with little growth in size. The dominant strain occurring is
\( \partial U/\partial y \), which reaches a maximum at \( x/d = 7 \), and then decays very rapidly further downstream.

Therefore, based on the above observations, it appears that the production of flocculation intensity (formation of flocs) is proportional to the magnitude of local strain in particular, \( \partial U/\partial y \) (\( \partial V/\partial x \) is small relative to it). This is consistent with the postulation that the strain is responsible for the production of the floc, and as the strain diminishes downstream, along with a simultaneous reduction in turbulent energy, the floc can sustain its size because the magnitude of both the strain and turbulent energy are not high enough to enlarge and rupture it respectively. Therefore, a type of equilibrium or steady state is attained. Furthermore, as the turbulent energy decreases downstream, the collisions among fibres will result in the production of flocs since the forces exerted by the turbulence necessary to rupture them are diminished. Therefore, a *decreasing turbulent kinetic energy acts a source for floc production*. Let this effect be represented by some function of \( k, f(k) \), the exact form is to be determined later. Combining these two effects, the following production term is added to the conservation equation,

\[
S_{add} = A_t \left| \frac{\partial U}{\partial y} \right| \frac{U_b}{d} \left( \frac{U_b}{d} \right)^n f(k) \tag{3.15}
\]

Where,

\( A_t = \) dimensionless constant of proportionality

\( 0 < n < 1 \) (must be determined empirically)

\( f(k) = \) a function of the turbulent kinetic energy

It is worth noting at this point, that the recent work of Raghem Moayed (1999) will be used to determine the constants and \( f(k) \) which appear in equation (3.15).
It is anticipated that the value of \( n \) will likely be less than 1 since the spatial variations of \( \bar{c}^2 \) are much more gradually than those of the strain. This means that the strain must be normalized with respect to the bulk strain, \( U_b/d \), to be made dimensionless. To retain the proper units, the entire equation needs to be multiplied by \( U_b/d \).

To determine the unknown function in equation (3.15), it is useful to examine the relationship between \( \bar{c}^2 \) and \( k \) presented by the results of Raghem Moayed and Kuhn (1999). The profiles of \( \bar{c}^2 \) for the different conditions of mean consistency and bulk velocity appear to be all of the same shape, the magnitude simply shifted up or down. Therefore, all the data was collapsed into a single relationship given as follows,

\[
\bar{c}^2 = \frac{A_2}{(k/k_o)^{0.19609}}
\]  

(3.16)

Where, the dimensionless constant \( A_2 \) is a function of \( C_m \) and Re\(^2 \) only, to account, separately, for the effects of mean consistency and Reynolds number on flocculation intensity, and \( k_o \) is the turbulent kinetic energy at the flow inlet. The kinetic energy is that computed from a fibre free flow field at the same bulk velocities. Of the seven cases, the smallest exponent was 0.1249, the largest was 0.2765, the average was 0.19609. The following correlation was developed by Raghem Moayed (1999) for flocculation intensity in the decay portion of the flow \((x/d>9)\),

\[
\bar{c}^2 \propto \left(\frac{x}{d}\right)^{0.42}
\]  

(3.17)

The theoretical prediction of turbulence intensity as a function of dimensionless length in an isotropic decaying turbulence is given by (Roach 1986),

\(^2\)The Reynolds number is defined as \( Re=U_b d/\nu \), where \( \nu \) is based on the properties of water.
\[ Tu = \left( \frac{x}{d} \right)^{0.7} \]  

(3.18)

Substituting \( Tu \approx k^{1/2} \) into equation (3.18), rearranging for \( x/d \) and substituting that into equation (3.17) gives,

\[ \overline{c'^2} \approx \frac{1}{k^{0.28}} \]  

(3.19)

The exponent is close to the value 0.19609 obtained in equation (3.16). In both cases, the kinetic energy is determined from the fibre free fluid. The correlation in equation (3.17) however, is obtained from the pulp suspension. The relative correspondence of the two results indicates that an inverse relationship between \( \overline{c'^2} \) and \( k \) exists, as well as a good isotropic turbulence decay. Furthermore, the numerical results of Steen (1991) conducted for pipe flow also show that the flocculation intensity exhibits an inverse relationship to the turbulent kinetic energy. It appears then that the function in equation (3.15) may be best represented by an inverse relationship, and that this is a general result characteristic of pulp suspensions, the exponent, likely varying from flow to flow. Setting this function equal to equation (3.16) and substituting into equation (3.15) gives the final result for the production term,

\[ \frac{\rho}{C_m^2} S_{add} = C_{1f} \left| \frac{\partial U}{\partial y} \right| U_b \left( \frac{U_b}{\rho^2} \right)^{0.19609} \overline{c'^2} d \]  

(3.20)

The two coefficients, \( A_1 \) and \( A_2 \) have been lumped together into \( C_{1f} \) (a function of Re and \( C_m \)). The effects of the bulk quantities Re and \( C_m \) on the production are taken into account through \( C_{1f} \).
Term (3.13)

This term accounts for the dissipation of $\bar{c'}^2$. Physically, it represents the breaking up of flocs into smaller flocs or individual fibres. Expanding this term into its Cartesian components,

$$-\frac{2\rho}{C_m^2} D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} = -\frac{2\rho}{C_m^2} D \left( \frac{(\partial c')^2}{\partial x} + \frac{(\partial c')^2}{\partial y} + \frac{(\partial c')^2}{\partial z} \right)$$  \hspace{1cm} (3.21)

Under isotropy and homogeneity,

$$\left( \frac{\partial c'}{\partial x} \right)^2 = \left( \frac{\partial c'}{\partial y} \right)^2 = \left( \frac{\partial c'}{\partial z} \right)^2$$

Therefore, equation (3.21) becomes,

$$-\frac{2\rho}{C_m^2} D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} = -\frac{6\rho}{C_m^2} D \frac{(\partial c')^2}{\partial x}$$  \hspace{1cm} (3.22)

Furthermore, for isotropic and homogeneous turbulence (Tennekes & Lumley 1972, Hinze 1975),

$$\left( \frac{\partial c'}{\partial x} \right)^2 = \frac{c'^2}{\lambda_f^2}$$  \hspace{1cm} (3.23)

where,

$$\lambda_f = \text{Taylor microscale for flocculation intensity}$$

The Taylor microscale is also referred to as the dissipative scale of turbulence since it exists only when dissipation is occurring. The relationship between the microscale for a scalar and that of the fluid turbulence is given as (Tennekes & Lumley 1972, Hinze 1975),
\[ \lambda_r^2 = C_{2n} \frac{D}{\nu} \lambda^2 \]  

(3.24)

where,

- \( C_{2n} \) is a dimensionless constant (determined empirically),
- \( D \) = molecular diffusivity of suspension,
- \( \nu \) = kinematic viscosity of continuous phase.

It appears plausible that this relationship also holds for a pulp suspension, since at this dissipative range, which is also the Kolmogorov equilibrium range, the flocs sizes would be very small and would follow or trace the fluid very closely. In this case, as noted by Lee and Brodley (1987), the velocity differential between the fibres and fluid is reduced, implying the fibres act as a passive scalar. Equation (3.24) is also consistent with the notion that small scale turbulence (i.e., sizes order of \( \lambda \)) is necessary for dispersion of flocs, since the smaller \( \lambda \) is, the smaller \( \lambda_r \) becomes, and the larger the dissipation of fluid through equation (3.24).

It is well known that in a decaying turbulent flowfield the turbulent kinetic energy dissipation is given by (Roach 1986, Mohamed & LaRue 1990),

\[ \varepsilon = 15\nu \frac{\overline{u'^2}}{\lambda^2} \]  

(3.25)

Rearranging for \( \lambda^2 \) and substituting into equation (3.24) gives,

\[ \lambda_r^2 = 15DC_{2n} \frac{\overline{u'^2}}{\varepsilon} \]  

(3.26)

Also, under isotropy,

\[ \overline{u'^2} = \frac{2}{3} k \]  

(3.27)

Substituting into equation (3.26) gives,
\[ \lambda_i^3 = 10D C_{2n} \frac{k}{\varepsilon} \]  \hspace{1cm} (3.28)

Substituting this expression into equation (3.23) and that into equation (3.22) gives the final result,

\[ -\frac{2\rho}{C_m^2} D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} \equiv -\frac{0.6\rho \varepsilon c''}{C_{2n} C_m^2 k} \]

Or, using the definition of flocculation intensity,

\[ -\frac{2\rho}{C_m^2} D \frac{\partial c'}{\partial x_j} \frac{\partial c'}{\partial x_j} \equiv -\frac{0.6\rho \varepsilon f_1}{C_{2n} k} \]  \hspace{1cm} (3.29)

This is the same model used by Steen (1991) to model the dissipation term in his conservation equation for flocculation intensity. The flocculation intensity remains in the equation so that it can be treated implicitly rather than be an explicit source term. This adds an additional term to the coefficient, \( a_p \), of \( \phi_p \) which improves convergence (See section 4.2.4 in Chapter 4).

If the velocity of an eddy is given by \( u' = k^{1/2} \), and the length scale by, \( \ell = C_{\mu}^{3/4} k^{3/2} / \varepsilon \), then,

\[ \frac{u'}{\ell} = \frac{k^{1/2} \varepsilon}{C_{\mu}^{3/4} k^{3/2}} = \frac{1}{C_{\mu}^{3/4} k} \]  \hspace{1cm} (3.30)

represents the turbulent strain rate. Therefore, the destruction of flocs is governed by the strain imposed by the turbulent motion. The larger the turbulent kinetic energy and the smaller the scale, the greater the turbulent strain rate and the greater the destruction through equation (3.30).
Term (3.14)

This term accounts for the convective transfer of $c'c^2$ by turbulent fluctuations. It re-distributes energy along the spectrum, and acts neither to produce nor dissipate $c'c^2$. An accurate determination of this term would require the measurement of the $u'c'c^2$ triple correlation. This was not done experimentally, and in fact is difficult to do so, because it requires a simultaneous measurement of the velocity and consistency. As a result, the conventional model used for this term will also be included here, it is given by (Rodi, 1993)

$$-\rho u'c^2 = (\mu_t / \sigma_n) \frac{\partial c^2}{\partial x_j}$$  \hspace{1cm} (3.31)

Where,

$$\sigma_n = \text{Turbulent Prandtl number for flocculation intensity}$$

This approach is analogous to how triple correlations are modeled in the exact equation for turbulent kinetic energy (See Launder & Spalding, 1974). Substituting into term (3.14) gives the final result,

$$- \rho \frac{C_m^2}{C_m^2} \frac{\partial (u'c^2)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( (\mu_t / \sigma_n) \frac{\partial \eta}{\partial x_j} \right)$$  \hspace{1cm} (3.32)

It is expected that this term is small relative to the production and dissipation terms, and hence, a very accurate model is not required. Note that this term can be lumped together with the diffusion term in the conservation equation for flocculation intensity.
3.3 Determination of model constants

The following constants appear in the transport equation for flocculation intensity:

\[ D, n, \sigma_n, C_{1n}, \& C_{2n} \]

**Value for D**

The value for molecular diffusion coefficient \( D \) was chosen according to measured values for a scalar contaminant in water (Tennekes & Lumley, 1972),

\[
\frac{\nu}{D} = 0.7
\]

which gives,

\[ D = 1.428 \times 10^{-7} \text{ m}^2/\text{s} \] (3.33)

**Values for \( C_{1n} \) and \( C_{2n} \)**

These coefficients appear in the production term (3.20) and dissipation term (3.29) from the last section. In a steady, fully developed flow, homogeneous shear flow, the production must equal the dissipation. These conditions are achieved far downstream of the grid. Therefore, setting the production equal to the dissipation at this location will determine the relationship between \( C_{1n} \) \& \( C_{2n} \). Furthermore, these constants are functions of \( \text{Re} \) and \( C_m \), and hence differ among the results obtained with varying \( U_b \) and \( C_m \). Based on the comparisons with the experimental data of Raghem Moayed (1999), the following correlation's were developed,

\[ C_{1n} = 0.011012 C_m^{0.1272} \text{ Re}^{-0.52735} \] (3.34)

\[ C_{2n} = 19.76613 C_m^{0.04579} \text{ Re}^{-0.34767} \] (3.35)
Value for $n$

The optimum value for $n$ was found to be 0.02.

Value for $\sigma_n$

The optimum value for $\sigma_n$ was found to be 7.5

3.4 Summary

The final form of the transport equation for flocculation intensity is given by,

$$\frac{\partial (\rho U_j f_l)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \left( \rho D + \frac{\mu_t}{\sigma_n} \right) \frac{\partial f_l}{\partial x_j} \right) +$$

$$C_{1n} \left| \frac{\partial U}{\partial y} \right| U_b \left( \frac{\rho U_b}{k \kappa} \right)^{0.19609} C_m^2 \frac{\rho \sigma n}{C_2 n} - \frac{0.6 \rho \sigma n}{C_2 n}$$

(3.36)

Where, $D = 1.428 \times 10^{-7}$ m$^2$/s, $\sigma_n = 7.5$, $n = 0.02$, $C_{1n} = 0.011012C_m^{-0.1728} Re^{-0.52735}$,

$C_{2n} = 19.76613C_m^{-0.04379} Re^{-0.34767}$, and $fl = \frac{c^2}{C_m}$.

3.5 Turbulence Modulation

3.5.1 Mechanisms of modulation in fibre suspension flows

The fibre suspension equation is solved independently of the turbulent flow field. In other words, there is one-way coupling in which the turbulence affects the fibre motion, but not vice versa. It is likely that in a fibre suspension, the presence of the fibres alters, or modulates, the turbulence to some degree. The interactions between the particles and fluid are not well understood and have been the focus of the much more recent work in two-phase flow modeling. Some knowledge has been gained for dilute
gas-liquid flows. Unfortunately, the extension to fibre flows has not been so straightforward.

In a two-phase system involving spherical particles, it is generally thought that the following mechanisms are responsible for turbulence modulation (Bennington 1993, Hestroni 1989, and Yuan and Michaelides 1992):

- Dissipation of turbulent kinetic energy by the acceleration of a particle by an eddy.
- Enhancement of turbulent kinetic energy by the shedding of vortices or the presence of wakes behind particles.
- Mean flow alteration by fluid moving as added mass in particle wake.

If the particles are fibres, the following effects may also contribute:

- Turbulent kinetic energy dissipation by fibre-fibre collisions that lead to floc formation.
- Turbulent kinetic energy dissipation to break apart fibre network (flocs).

In a fibre suspension, some or all of the above may be occurring. In decaying turbulence, the interactions of the fibres with the carrier fluid are complex. The flocs are destroyed by the turbulent stresses or by other mechanisms to be discussed in Chapter 5, and subsequently reform as the turbulent stresses diminish in magnitude downstream.

D'Incau (1983) compared the turbulence intensity between a fibre suspension and pure water along the centreline downstream of the grids. From his results, it appeared that the greatest reduction in turbulence intensity from the pure water result occurred at \( x/d = 7.5 \). There was no appreciable difference in turbulence intensities far downstream of the grids where the flocs are the largest. These results would indicate that the energy
reduction to break apart flocs is greater than the energy reduction to form flocs. Even if this is the case, it is not clear which scales of turbulence are being attenuated.

The energy spectra of Kerekes and Garner (1982) conducted on the same flow cell geometry indicate that there is a suppression of energy at high wavenumbers or small scales, and not so much at smaller wavenumbers. This would suggest that the smaller scales of turbulence are responsible for floc destruction.

The results of Steen (1989) obtained from vertical pipe flow measurements would seem to contradict the Kerekes and Garner result. He observed that in the near wall region, there was an increase in turbulence intensity over that of pure water. An explanation, as he notes, is that in this high shear region, most flocs are destroyed, and individual fibres are able to rotate causing the generation of small scale eddies.

Clearly, the interactions between the fibres and the turbulent eddies are complex. Further enlightenment can only be obtained through more systematic experimental studies where the turbulent statistics of a fibre suspension are compared to that of a fibre free suspension. It will be shown that the currently available modeling approaches are not applicable to fibre suspension flows.

3.5.2 Application of existing methods to fibre suspension flows

Most work in turbulence modulation has been done in the area of dilute gas-liquid flows. Here, particle-particle interactions are assumed negligible due to the low concentrations involved and the spherical nature of the particles. This simplifies the problem considerably. The hydrodynamic drag becomes the predominant force acting on the particles, and hence, the mechanism by which the fluid loses its momentum.
In this approach, a hydrodynamic drag force is added to the time dependent momentum equations. The exact equations for the turbulent kinetic energy ($k$) and the dissipation rate of turbulent kinetic energy ($\varepsilon$) are derived from the momentum equations. They produce, after some simplifying assumptions, the following additional terms in the $k$ and $\varepsilon$ equations respectively (Chen and Wood 1985),

$$S_k = \frac{\overline{\rho_p}}{t_p} \left( u'_{p} u'_{p} - \overline{u'_{p} u'_{p}} \right)$$  \hspace{1cm} (3.37)

$$S_\varepsilon = \frac{2 \overline{\rho_p}}{\rho} \left[ \nu \frac{\partial u'_{i}}{\partial x_j} \left( \frac{\partial u'_{p} \partial x_j}{\partial x_j} - \frac{\partial u'_{p} \partial x_j}{\partial x_j} \right) \right]$$  \hspace{1cm} (3.38)

where, $\overline{\rho_p}$ = particulate phase density, $u'_{p}$ = velocity fluctuation of carrier fluid, $u'_{p_i}$ = velocity fluctuation of particulate phase, and $t_p$ is the particle response time, given by equation (2.45). Of course, the correlation's in equation's (3.37) and (3.38) are unknown and must be modeled. The most commonly used models for these terms are (Chen and Wood 1985),

$$S_k = -\frac{2k}{t_p} \left( \frac{\overline{\rho_p}}{\rho} \left[ 1 - \exp\left( -0.5t_p \frac{\varepsilon}{k} \right) \right] \right)$$  \hspace{1cm} (3.39)

$$S_\varepsilon = -\frac{2\overline{\rho_p}}{\rho} \frac{\varepsilon}{t_p}$$  \hspace{1cm} (3.40)

To examine the usefulness of equation's (3.39) and (3.40), it is relevant only to consider the magnitude of the term inside the exponential, $-0.5t_p \frac{\varepsilon}{k}$, which is the ratio of the particle response time to the eddy response time. The largest reduction in $k$ due to equation (3.39) will occur when this ratio has its largest magnitude. As was mentioned in Chapter 2, $t_p$ is the particle response time. It is the time it takes for a particle at rest to
accelerate to within 63% of the fluid velocity (Hestroni 1989). The particle response time for the fibres used in the experiments of Raghem Moayed (1999) was calculated to be 0.000283 seconds (See Chapter 2). From the Reynolds Averaged Navier Stokes simulation results (to be presented in Chapter 5), the largest value of $\varepsilon/k$ is 173.01. Therefore, the ratio of response times becomes equal to $-0.02448$, which then makes the term $1 - \exp(-0.02448)$ equal to 0.02418. This, when multiplied by the first term in equation (3.39) results in a very small number for $S_k$.

Therefore, the reduction in the turbulent kinetic energy due to hydrodynamic drag appears negligible in a fibre suspension. Models used for the gas-liquid systems are not applicable. As mentioned previously, more understanding of mechanisms behind the attenuation of the turbulence by the fibres can only be obtained through detailed experimental measurements of the turbulence statistics.
Chapter 4

Numerical Solution

This chapter outlines the numerical methodology used to solve the governing partial differential equations (PDE). Section 4.1 briefly describes the Finite Volume method and the general solution algorithm. The details behind the modeling of the flow cell are given in Section 4.2. This section also describes the implementation of the fibre suspension model into Fluent™.

4.1 The Finite Volume method

Fluent™ uses the Finite Volume method to solve the governing equations. This is just one of many numerical solution methods used to solve partial differential equations. A few others include: Finite Difference, Finite Element, Spectral method, and Boundary Element. Essentially, each differs in the method used to discretize the PDE’s. There are numerous texts on each method with application to fluid flow. The Finite Volume method, which is the most widely used for fluid flow, will be described in detail here.
4.1.1 Discretization of governing equations

All the PDE's which govern the transport of mass, momentum, turbulent kinetic energy, dissipation rate of turbulent kinetic energy, and flocculation intensity can be expressed in a generic form, written here for steady flow in Cartesian tensor notation,

$$\frac{\partial}{\partial x_j} (\rho u_j \phi) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + S$$ \hspace{1cm} (4.1)

or in vector notation,

$$\nabla \cdot (\rho \vec{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S$$ \hspace{1cm} (4.2)

where, \(\phi = u, v, w, k, \varepsilon, \& \text{fl}\). The diffusion coefficient \(\Gamma\) is the viscosity in the momentum equations, the effective viscosity in the turbulent transport equations, and the turbulent diffusion coefficient the fl equation. All terms that can not be included in the two partial derivative terms are included in the source term. In the momentum equations, this would be the pressure gradient and gravity forces. In the turbulent transport equations and the flocculation intensity equation, it would be the production and destruction terms.

In Fluent\textsuperscript{TM} 5.1, an unstructured Finite Volume solver is employed. This entails solving equation (4.1) on fully unstructured meshes which can be of any particular shape, i.e., arbitrary polyhedra in three dimensions. Solution on these types of meshes do not require a coordinate transformation (Zingg et. al. 1998). This is in contrast to structured meshes, which require a coordinate transformation to be used on complex geometries.

The first step in the Finite Volume method is to split the entire computational domain into small control volumes (CV), which collectively, make up the entire domain. Figure 4.1 shows a typical control volume in two dimensions. In three dimensions, the control volume is a closed volume, in two dimensions, it is a closed contour. The control
volume in Figure 4.1 is quadrilateral, although triangular control volumes can also be applied. For all the simulations conducted in this study, three dimensional meshes with hexahedral CV where used because of the relatively simple geometry of the flow cell (See section 4.2).

![Figure 4.1: Shaded area is the Control Volume, also called a cell. Adjacent control volumes also shown.](image)

The PDE's are discretized over each control volume to produce a set of nonlinear algebraic equations which, upon solution, will yield the values of the dependent variables at the centre of each control volume, i.e., at P, N, S, W, and E and in Figure 4.1.

In the Finite volume method, it is not the PDE's themselves which are discretized, but the integral form of the PDE's, obtained by integrating equation (4.2) over each control volume,

\[
\iiint_{CV} \nabla \cdot (\rho \vec{u} \phi) dV = \iiint_{CV} \nabla \cdot (\Gamma \nabla \phi) dV + \iint_{CV} \mathbf{S} \cdot dV \quad (4.3)
\]

The Gauss' divergence theorem is used for the convective and diffusive terms to transform the volume integrals to surface integrals,

\[
\iint_{S} (\rho \vec{u} \phi) \cdot \hat{n} dS = \iint_{S} (\Gamma \nabla \phi) \cdot \hat{n} dS + \iiint_{CV} \mathbf{S} \cdot dV \quad (4.4)
\]
The finite volume method approximates each of these terms as applied to every control volume in the computational domain. Note that because of the integral formulation in equation (4.4), the method is conservative, i.e., mass, momentum, etc. are conserved in a discrete sense. This is one of the chief advantages of the method.

Various methods are used to approximate each term. For the source terms, it is assumed that the cell averaged source term holds over the entire control volume. For example, if the source term is a function of the dependent variable, $\phi$, then the value of $\phi$ at the cell centre is assumed over the entire CV. This is a second order\(^1\) accurate approximation (Ferziger and Peric 1999). Therefore, this term is written as the product of the cell averaged source term and the CV volume (in this case, the area),

$$\iiint_S (\rho \bar{u} \phi) \cdot \hat{n} dS = \iiint_S (\Gamma \nabla \phi) \cdot \hat{n} dS + \bar{S} \cdot V$$  \hspace{1cm} (4.5)

For the convective and diffusive terms, the surface integral is evaluated on each surface which encloses the control volume (in Figure 4.1 there are 4 surfaces or faces), and summed up to give the total surface integral. Furthermore, since the values of the dependent variables are not known along each surface, they are represented by the cell face centre values, i.e., e, w, n, and s in Figure 4.1. Again, this is a second order accurate representation (Ferziger and Peric 1999). Making these substitutions in equation (4.5) gives,

$$\sum_{f}^{N_{faces}} (\rho \bar{u} \phi \cdot \hat{n})_f A_f = \sum_{f}^{N_{faces}} (\Gamma \nabla \phi \cdot \hat{n})_f A_f + \bar{S} \cdot V$$  \hspace{1cm} (4.6)

\(^1\) The order of a scheme indicates how the discretization error is reduced when the mesh size is reduced. For example, if $\Delta x$ is the mesh size and $n$ is the order, then the error reduces as $(\Delta x)^n$. Therefore, the higher the order, the greater the reduction in the error when the mesh size is reduced.
where, \( f \) is the index for each face, and \( A_f \) is the area of each face. In equation (4.6), the velocity, dependent variable \( \phi \), and the gradient of \( \phi \) must all be prescribed at the centre of each face, i.e., at e, w, n, and s. Since these values are not produced as a part of the solution, they must be interpolated from the cell centred values, i.e., at P, N, S, E, and W. The approximation used to relate the cell face values to cell centred values is called the discretization scheme. Several different schemes have been devised for this interpolation.

For the diffusive terms, the most commonly used scheme is the second order accurate central differencing scheme, which assumes that the face value is a linear interpolation of adjacent cell centred values. For example, referring to Figure 4.1, the diffusive flux at the face e is given by (Patankar 1980),

\[
\left( \Gamma \frac{\partial \phi}{\partial x} \right)_e \equiv \Gamma_e \frac{\phi_E - \phi_P}{x_E - x_P}
\]  

(4.7)

Fluent\textsuperscript{TM} retains this scheme for the diffusive terms in all the discretized equations.

Choosing the appropriate discretization scheme for the convective terms is more cumbersome. It can be shown (Patankar 1980 and Versteeg and Malalasekera 1995) that if the same central differencing scheme is used, non physical oscillatory solutions can result. An alternative scheme is to use upwind differencing. Here, the face value is assumed to be equal to the upstream value only. For example, if the flow in Figure 4.1 is from right to left, then \( \phi_e \equiv \phi_E \). This scheme is very stable and easy to implement. Unfortunately, it is only first order accurate and introduces a significant amount of numerical or artificial diffusion. Zingg (1998) gives a detailed mathematical description of numerical diffusion introduced using upwind differencing schemes. Neither the 1st order upwind or 2nd order central differencing schemes were used in this study.
Instead, a 2\textsuperscript{nd} order upwind scheme was used. Here the face value is computed using the following formulation (Barth and Jespersen 1989),

\[ \phi_f = \phi + \nabla \phi \cdot \Delta \bar{s} \]  

(4.8)

where,

\( \phi \) = is the cell centred value in the upstream cell,

\( \Delta \bar{s} \) = displacement vector from the upstream cell centroid to face centroid

\( \nabla \phi \) = gradient of \( \phi \) in upstream cell

\[ \frac{1}{V} \sum_{f} ^{N_{face}} \tilde{\phi}_f \bar{A} \]  

(4.9)

where, the face values \( \tilde{\phi}_f \) are calculated by averaging \( \phi \) from the two cells adjacent to the face (Barth and Jespersen 1989). The inclusion of the second term in equation (4.8) gives the scheme its second order accuracy. This scheme was used for all the equations in RANS simulations, including the equation for flocculation intensity.

For the Large Eddy Simulation, which involves a transient solution, time discretization was performed using the following 2\textsuperscript{nd} order accurate scheme,

\[ \frac{3\phi^{n+1} - 4\phi^n + \phi^{n-1}}{2\Delta t} = F(\phi) \]  

(4.10)

where, the superscript \( n \) refers to the current time step, and \( F(\phi) \) refers to all the spatially discretized terms including source terms. \( F(\phi) \) is also calculated at the current time step making the scheme implicit.

After all the discretization schemes are incorporated into equation (4.6), a nonlinear algebraic equation is constructed at the centre of each control volume, \( P \), for each dependent variable,
\[ a_p \phi_p = \sum a_{nb} \phi_{nb} + b \]  

(4.11)

where, the subscript \( nb \) refers to the neighbouring values of \( \phi \) in adjacent control volumes. Equation (4.11) is nonlinear since the coefficients, \( a_{nb} \) and \( a_p \), are also a function of the dependent variable. For example, if \( \phi \) is equal to \( u_i \) in the momentum equation, then all the a’s are also a function of \( u_i \). Solution of equation (4.11) requires an iterative process. The b term contains all discretized source terms. In the momentum equations, this will include the pressure gradient and Reynolds stresses, in the case of the RANS equations.

### 4.1.2 Iterative solution procedure and the SIMPLE algorithm

The three momentum equations and the continuity equation constitute four equations with four unknowns. The pressure, however, does not appear in the continuity equation, and in fact, only its gradient appears in the three momentum equations. To solve the equations, a sequential procedure is used where each equation is solved in succession, treating the other dependent variables as temporally known. In Fluent\textsuperscript{TM}, this is referred to as the segregated implicit solver. Of course, this procedure requires an iterative process.

The most popular and most tested method is the Semi Implicit Method For Pressure Linked Equations (SIMPLE) method of Patankar and Spalding (1972). A detailed derivation will not be given here. This can be found in the text by Patankar (1980), and in more recent texts on Finite Volume methods by Ferziger and Peric (1999) and Versteeg and Malalasekera (1995). A brief description of the method will follow.
In the SIMPLE algorithm, an initial pressure is assumed at all grid points which make up the computational domain. Using this as the temporary pressure field, the discretized momentum equations, which have the form of equation (4.11), are solved to produce a temporary velocity field. Since the pressure field was arbitrarily guessed at, the resulting velocity field will not satisfy the continuity equation. There will be a residual, or an additional fictitious mass, produced. The premise behind the method is to use this continuity equation and its residual to correct the pressure field such that when the solution converges, the velocity field will satisfy the continuity equation and produce a zero residual in the continuity equation.

From the momentum equations and the continuity equation, a pressure correction equation can be derived (Patankar 1980),

\[ a_p p' = \sum a_{ab} p'_{ab} + b_m \]  \hspace{1cm} (4.12)

where, \( p' \) is the pressure correction to be computed and \( b_m \) is the residual in the continuity equation resulting from the incorrect velocity field. After this equation has been computed, all pressures and velocities are updated using the pressure correction. For example, by referring to the CV in Figure 4.1, these corrections are made to pressure and velocities at point P (using the notation of Ferziger and Peric (1999)),

\[ p_P = p^*_P + p'_P \]  \hspace{1cm} (4.13)

\[ u_{i,P} = u^*_P + \left[ A_P \left( \frac{\delta p'}{\delta x_i} \right) \right]_P \]  \hspace{1cm} (4.14)

where, \( p^* \) and \( u^* \) are the guessed pressure and calculated velocities respectively, and \( \delta / \delta x_i \) represents a discretized spatial derivative. The exact form of the second term in equation (4.14) depends on the pressure-velocity coupling technique being used. It differs
depending on whether a staggered or non-staggered (co-located) computational mesh is used. Fluent™ uses a non-staggered mesh where all the variables are to be stored at the centre of each CV or cell.

Once the pressure and velocities have been updated through equations (4.13) and (4.14), all other discretized equations of the form in equation (4.11),

\[ a_p \phi_p = \sum a_{nb} \phi_{nb} + b \] (4.11)
can be solved.

As mentioned previously, the coefficients, \( a_{nb} \), and the source term, \( b \), are also functions of the dependent variables, \( \phi \), rendering the equations nonlinear. The iteration procedure to solve the equations is split into what is called an outer iteration and an inner iteration (Ferziger and Peric 1999).

The outer iteration involves updating the coefficients and source terms using the most recently available values. This makes equation (4.11) linear, temporally. The linear equations can actually be solved directly, i.e., without iteration. This is usually not done, however, since the coefficients are only temporarily known. Instead, these too are solved iteratively. This is what constitutes the inner iterations.

The iteration method used by Fluent™ is a point implicit Gauss-Seidel method, accelerated by an Algebraic Multigrid Method (AMG). More about Gauss-Seidel methods can be found in most texts on numerical methods, while the texts by Zingg (1998) and Ferziger and Peric (1999) give detailed descriptions of multigrid methods.

The entire SIMPLE algorithm is summarized in Figure 4.2. The notation differs slightly from that of Versteeg and Malalasekera (1995).
Start

Initial guess $p_r$

Step 1: Solve discretized momentum eqns
$$a_p u_{i,p} = \sum a_{nb} u_{i,nb} + b$$

Step 2: Solve pressure correction eqn
$$a_p p'_p = \sum a_{nb} p'_{nb} + b$$

Step 3: Update pressure and velocities
$$p_p = p'_p + p'_r$$
$$u_{i,p} = u_{i,p}^* + A_p \left( \frac{\delta p'}{\delta x_i} \right)_p$$

Step 4: Solve all other discretized eqn's
$$a_p \phi_p = \sum a_{nb} \phi_{nb} + b$$

Converged?

no

yes

Stop

Figure 4.2: The SIMPLE algorithm (From Versteeg and Malalasekera 1995).
4.2 Numerical model of flow-cell

To model the flow-cell illustrated in Figure 2.2, the turbulent flowfield was calculated using both a Large Eddy Simulation (LES) and Reynolds Averaged Navier Stokes (RANS) simulations. The fibre suspension model was applied to the RANS simulations only.

4.2.1 Geometry and boundary conditions

**Large Eddy Simulation**

The turbulent flow in the geometry shown in Figure 2.2 was calculated using a transient Large Eddy Simulation. The dimensions of the flow-cell were set to be exactly equal to the dimensions of the experimental flow-cell. At the flow inlet, the instantaneous velocity field was set by adding a fluctuating velocity component related to the intensity of turbulence to the user specified velocity of 0.45 m/s. At the flow outlet, zero gradients in the streamwise direction were used,

\[
\frac{\partial \phi}{\partial x} = 0
\]  

(4.15)

This boundary condition assumes that the flow in the streamwise direction is fully developed. Hence, the flow is locally parabolic.

The no-slip condition is used at the top and bottom walls of the channel as well as at all grid surfaces.
Reynolds Averaged Navier Stokes Simulations

The Large Eddy Simulation yields an instantaneous velocity field that exhibits transient behaviour. In fact, the flow downstream of the grids is periodic due to vortex shedding. If this instantaneous field is time-averaged, then a steady state solution is obtained, similar to that which would be produced by the solution of the RANS equations. This will be shown in Chapter 5. To simplify the geometry and reduce the computational effort, the RANS numerical model involved modeling only a portion of the channel, imposing symmetry boundary conditions at two planes along the centre of the two adjacent grids that make up the core of the channel. This simplified geometry is shown in Figure 4.3.

![Figure 4.3: Simplified geometry of flow cell and boundary conditions.](image)

At the inlet, the velocity, turbulence intensity, and characteristic length scale are all specified. At the outlet, the zero streamwise gradient boundary condition is used. The no-slip condition was used at all wall surfaces.
4.2.2 Mesh and solver specifications

Large Eddy Simulation

Although the geometry of the flow-cell is simply, fitting a high quality mesh is
difficult due to the large aspect ratio of the entire channel. Creating high mesh density
near the exit of the grids results in large cell aspect ratios further downstream. To capture
all the relevant large scale physics and to avoid using cells with large aspect ratios, a
large mesh needs to be constructed. As mentioned, the geometry is simply, in fact, all
surfaces are orthogonal to each other. As a result, the calculation domain was fitted using
a structured hexahedral mesh. Mesh density was made slightly greater near the exit of the
grids, however, not too excessively so as to create large aspect ratios in the cells far
downstream of the grids. The mesh has 221 grid points in the x-direction, 77 in the y-
direction, and 9 in the z-direction for 188,160 cells. An isometric view of the mesh is
given in Figure 4.4. Grid generation was done in Fluent™'s preprocessor, Gambit™.

Figure 4.4: 188,160 cell computational mesh
Due to the large computational times involved, the solution was not obtained on a finer mesh, therefore, it is not known if the results are grid independent. This analysis is recommended for future studies.

The equations were solved using the segregated implicit solver in Fluent\textsuperscript{TM} 5.1. As mentioned in section 4.1, this is a pressure-based solution strategy. The PISO algorithm was used for pressure-velocity coupling. This differs from the SIMPLE algorithm by solving an additional pressure correction equation (Versteeg and Malalasekera 1995) and is well suited for unsteady problems. The 3\textsuperscript{rd} order accurate QUICK scheme was used for the convection terms, while a 2\textsuperscript{nd} order accurate implicit scheme for used for time discretization. The time step chosen was 0.001 seconds. Unfortunately, time constraints did not allow for a time step independence test. However, convergence was achieved for all variables at each time step, indicating that a correct time step was chosen.

The simulation was run on a Windows NT workstation equipped with a dual Pentium 2 450 MHz processor with 512 Mb RAM. Convergence at each time step required approximately 11 min and 15 iterations. The simulation was run for over 6400 time steps and 96000 iterations.

**Reynolds Averaged Navier Stokes simulations**

A structured hexahedral mesh was also fitted to the simplified geometry shown in Figure 4.3. Three mesh sizes were used in the computations: 14,630 cells, 46,000 cells, & 72,400 cells. Grid independence studies are given in Chapter 5. Again, grid generation was done in Gambit\textsuperscript{TM}. 

As in the case for the Large Eddy Simulation, the solution was obtained using the segregated implicit solver in Fluent™ 5.1. The SIMPLE algorithm was used for pressure-velocity coupling. The 2nd order Upwind scheme was used for the convection terms. Convergence to a steady state solution was obtained by allowing the residuals to fall below $10^{-6}$. Convergence to $10^{-6}$ required approximately 4 hours and 800 iterations on a dual Pentium 2 450 MHz with 512 Mb RAM Windows NT workstation.

Since the transport equation for the flocculation intensity is not coupled with the RANS and RNG $k-\varepsilon$ equations, it was solved separately after the latter two had been solved. This greatly reduced the time involved for model validation.

4.2.3 Physical model specifications

**Large Eddy Simulation**

The fluid properties were assumed to that of water, with $\mu = 0.001$ Pa·s and $\rho = 1000$ kg/m³. The RNG subgrid scale model was used in the simulation to model the effects of small scales, and the standard wall function was used to resolve the boundary layers.

**Reynolds Averaged Navier Stokes Simulations**

The same fluid properties used in the Large Eddy Simulation were used for these simulations. The RNG $k-\varepsilon$ turbulence model was used to close the RANS equations. The non-equilibrium wall function was used to resolve the boundary layers.
4.2.4 Implementation of fibre suspension model

As mentioned previously, the fibre model was used in conjunction with the RANS simulations. To incorporate the fibre suspension model in Fluent™, user defined functions (UDF) needed to be used. A user-defined scalar transport equation of the following form was added,

$$\frac{\partial}{\partial x_j} (\rho U_j \phi) = \frac{\partial}{\partial x_j} \left( \Gamma \frac{\partial \phi}{\partial x_j} \right) + S_\phi \quad (4.16)$$

By referring to equation (3.36), the variables are defined as,

$$\phi = f_l$$
$$\Gamma = \rho D + \frac{\mu}{\sigma_n}$$

$$S_\phi = C_{1n} \left| \frac{\partial U}{\partial y} \right| \frac{U_b}{d} \left( k / k_a \right)^{0.1967} C_m d + \frac{0.6 \rho \varepsilon f_l}{C_{2n} k} \quad (4.17)$$

The diffusion coefficient, $\Gamma$, and the source term, $S_\phi$, were implemented using user defined functions written in C. The DEFINE_DIFFUSIVITY and DEFINE_SOURCE routines were used. These are the standard routines used by Fluent to implement user defined diffusivities and source terms. Since the second source term is a function of $f_l$, it was separated into an explicit and implicit part to improve convergence,

$$S = S_c + S_p \phi_p$$

Where,

$$S_c = -\frac{0.6 \rho \varepsilon f_l}{C_{2n} k}; \quad S_p = -\frac{0.6 \rho \varepsilon}{C_{2n} k} \quad (4.18)$$

The user defined functions for all the cases considered in this study are given in the Appendix.
The boundary conditions for the fibre suspension model were more difficult to define. At the inlet, the value of flocculation intensity must be given. Fortunately, as will be shown in Chapter 5, the flocculation intensity profile downstream of the grids is insensitive to the magnitude of fl at the flow inlet. This is particularly true in the decay portion of the flow, \( x/d > 10 \). Nonetheless, the inlet value of fl was set to be approximately equal to the predicted value far downstream of the grids. Note that this was a trial and error process. This was done to predict a more accurate value of fl immediately downstream of the grids (\( x/d < 10 \)).

At all wall surfaces, the gradient of fl was set equal to zero, implying no flux through the surface. At the symmetry and outflow boundary conditions, the flux was also set equal to zero.
Chapter 5

Results and Discussion

5.1 Validation of turbulent flowfield

Before solving the fibre suspension equation, it was necessary to validate the turbulent flowfield. Section 5.1.1 gives the results for the Large Eddy Simulation (LES) while sections 5.1.2 and 5.1.3 present the results for the Reynolds Averaged Navier Stokes (RANS) simulations.

5.1.1 Large Eddy Simulation Results

Instantaneous Quantities

A Large Eddy Simulation was done for the entire flow-cell shown in Figure 2.2 of Chapter 2. The bulk velocity for the flow was 0.45 m/s. The solution procedure involved solving the mass and momentum continuum equations over all control volumes at each time step. Due to the uncertainty in the initial conditions and inflow boundary condition, it was necessary to run the simulation long enough to allow the flow to approach a periodically repeating steady state. The residence time for the entire channel based on the
bulk quantities is 2.33 seconds. The simulation was run for 7.1488 seconds, or just over 3 residence times. The analysis will show that this was sufficient time for the flow to reach a periodically repeating steady state.

The solution was updated at every time step (1 ms), and the data was saved every 25 time steps. Convergence was achieved to $10^{-3}$ residual level at each time step. As mentioned, there is an initial period where the flow is still developing. It is not useful to include this "initial transient" for time averaging purposes. Figures 5.1 through 5.6 show the evolution of the velocity vector field along the centre plane ($z/d=0$) obtained at six different times. Note in particular, the development of the two large recirculation zones behind the grids, adjacent to the side walls.

Figure 5.1: Velocity vectors on $z/d=0$ plane at 0.523 seconds.
Figure 5.2: Velocity vectors on z/d=0 plane at 1.8238 seconds.

Figure 5.3: Velocity vectors on z/d=0 plane at 2.6738 seconds.
Figure 5.4: Velocity vectors on z/d=0 plane at 3.8238 seconds.

Figure 5.5: Velocity vectors on z/d=0 plane at 5.0988 seconds.
From the figures it can be seen that the flow approaches a periodic state in which the jets appear to oscillate over time in the xy plane. The jets that exit the grids expand slightly and merge together at some distance downstream. The x-velocity component was plotted versus time at various x/d positions along the centreline of the channel, i.e., at y/d=z/d=0. It was found that the largest amplitude in the x-velocity occurred at x/d=7.61. Figure 5.7 displays the x-velocity vs. time at selected x/d positions along the centreline of the channel. As mentioned, the most variation in time occurs at x/d=7.61, which roughly coincides with the minimum in fibre flocculation, which, according to the experiments of Raghem Moayed, occurs at x/d = 8.5. The flocculation intensity results will be given in later in section 5.2. Recall that the velocities shown in Figure 5.7 are the instantaneous
Figure 5.7: $x$-velocity vs. time at selected $x/d$ positions along centreline of channel, $y/d=z/d=0$.

velocities of the resolved large scale motion. The unresolved small scale motion is not represented directly in Figure 5.7, its effects on the large scale motion are included through the subgrid scale model. Physically, the time dependence shown in Figure 5.7 is due to the jet swaying back and forth in the $xy$ plane over a very short distance in the flow direction, between $x/d=5$ and $x/d=15$. The experiments of Raghem Moayed, done at the same bulk velocity of 0.45 m/s, show that a floc that gets trapped in this oscillating jet is destroyed and completely dispersed.

The velocity field in Figure 5.7 appears very regular, especially at $x/d=7.61$. It is difficult to ascertain whether the flow at this point is very turbulent or not, since the time dependence may be a result of variations in the mean motion as opposed to the presence
Figure 5.8: Power Spectrum at (a) x/d=3.9970 and (b) x/d=6.001

Figure 5.9: Power Spectrum at (a) x/d=7.6108 and (b) x/d=9.2101

Figure 5.10: Power Spectrum at (a) x/d=10.09 and (b) x/d=12.02
Figure 5.11:  Power Spectrum for (a) x/d=16.1924 and (b) x/d=20.0029

Figure 5.12:  Power Spectrum for (a) x/d=39.9960 and (b) x/d=60.2488

of large scale turbulent eddies. To investigate this further, the time dependent velocities
were converted to power spectra. The spectra at various x/d positions are shown in
Figures 5.8 to 5.12. It is clear from the figures that the periodicity occurs at a very distinct
low frequency, and that the rest of the spectrum shows additional peaks of very low
energy. This would appear to imply that most of the kinetic energy is contained in the
mean motion, rather than in the turbulent motion. Examining the spectra far downstream
of the grids (Figure 5.12) shows further support of this. Here, the high amplitude peak has
subsided, and the energy in the remainder of the spectrum, which may represent the turbulence, is very low.

The intensity of turbulence can be obtained by removing the high amplitude peaks that corresponds to the mean motion, and performing an inverse Fourier transform to the spectra to obtain the fluctuating velocity components. It should be recalled here that LES is incapable of predicting the fluctuating velocity components associated with the small scales, which corresponds to an absence of energy at the higher frequencies. However, the fluctuations occurring at the lower frequencies, if they exist, should be predicted by the LES.

The turbulent intensity is defined as \( \sqrt{\langle u'^2 \rangle} / U_b \). Figure 5.13 shows the variation of the turbulence intensity with \( x/d \). Also plotted is the turbulence intensity predicted by the RANS simulation, which was done on the simplified geometry shown in Figure 4.3. The turbulent kinetic energy predicted by the LES is substantially lower than that predicted by the RANS model. As mentioned in Chapter 4, the RANS model solves the steady state RANS equations with turbulence models, and is therefore unable to predict transient behaviour. It appears that the effect of the time varying mean motion, as predicted by the LES, is seen as an increase in the turbulent kinetic energy predicted by the RANS simulation.

In addition, both the instantaneous and the time-averaged strain rate predicted by the LES exhibits a maximum at \( x/d = 7 \). Its magnitude drops further downstream.

In terms of the implications for fibre dispersion, the present results suggest that the strains imposed by the mean motion are responsible for the destruction of flocs. The action of small scale turbulence to destroy flocs seems negligible. This contradicts the
conventional wisdom that deflocculation is caused by the small scales of high intensity. Rather, it may be that as the jet sways back and forth, the combination of tensile and shear strain in the mean velocity is what causes the floc breakup. Of course, this conclusion is based on a LES result obtained at one Reynolds number and on one mesh size. The Reynolds number of 3600 used here is based on a bulk velocity of 0.45 m/s, which is typical in hydraulic headboxes. It may be that as the Reynolds number increases, the turbulent kinetic energy makes up a greater proportion of the total kinetic energy. Clearly, more work needs to be done to evaluate the influence of Reynolds number on the total kinetic energy.

![Turbulence Intensity vs. x/d. Comparison between RANS and LES models.](image)
**Time-Averaged Quantities**

The instantaneous velocity was time-averaged over a period from 4.5 to 7.1 seconds. Figure 5.14 shows the time-averaged velocity magnitude at the z/d=0 plane. The steady state RANS equations also produce a time-averaged solution. Careful examination of the time-averaged flowfield from the LES results shows that the jets that make up the core of the channel are symmetric about a xz plane which runs through the centre of each grid. Therefore, the geometry and subsequent computational requirements could be reduced significantly if symmetry planes are invoked along the two xz planes that run along the two central grids. This simplified geometry with boundary conditions was given in Figure 4.3 of Chapter 4. These simulations involved solving the RANS equations. The results are given in sections 5.1.2 and 5.1.3.
Figure 5.15 shows a comparison of the normalized mean streamwise velocity vs. x/d for the LES and experimental data of D'Incau (1983). A RANS solution is also shown for the case of $U_b=0.45$ m/s. The appearance of the local maxima at $x/d=13.5$ is likely a result of the two very large re-circulation zones that appear behind the grids at the side walls. The RANS solution does not show this maxima because it was obtained using symmetry boundary conditions at the centre planes of the adjacent grids. Hence, the jet acts as a free jet uninfluenced by the two re-circulation zones.

A closer examination of the LES results shows the re-circulation zones have their maximum y-direction width at $x/d=13.5$. The width of the re-circulation zones is significant when compared to the total cross-sectional flow area (See Figure 5.14). It appears that the reduction in the cross-sectional flow area causes the flow to accelerate,

![Figure 5.15: Normalized mean streamwise velocity vs. x/d. Comparison between models and experiment.](image_url)
and this is seen as an increase in the mean streamwise velocity. In fact, the normalized mean velocity at $x/d=13.5$ can be estimated by multiplying the normalized mean velocity obtained from the RANS solution by the ratio of the channel area to that of the reduced channel area due to the re-circulation,

$$\left(\frac{U}{U_b}\right)_{LES} = \left(\frac{U}{U_b}\right)_{RANS} \frac{A_{channel}}{A_{reduced}} = 1.16 \frac{10.6}{8.0} = 1.537 \text{ m/s}$$ (5.1)

The normalized mean velocity predicted by the LES at $x/d=13.5$ is 1.52 m/s. The close agreement suggests that it is the re-circulation zones which cause the local maximum.

The discrepancy with the experimental data can be explained as follows. The experimental data was obtained using a 0.45% consistency fibre suspension whereas the LES and RANS simulations were run using material properties of water only. Qualitative observations of the fibre flow in the grid-generated turbulence flow cell show that the size of the re-circulation zones is reduced substantially in the presence of the fibres. As was discussed in Chapter 3, the fibres alter the momentum of the fluid near the exit of the grids. This translates into a smaller re-circulation zone and hence, the influence on the centre-line streamwise velocity is reduced. In fact, the deviation of the RANS results from the experimental data in the region $7<x/d<25$ indicate that the re-circulation zones may still be affecting the streamwise velocity in the fibre suspension flow.

It is apparent that the two re-circulation zones affect the entire flow field downstream of the grids. The flow does not reattach to the side walls until $x/d=23.5$. Figure 5.16 shows the instantaneous $z$-velocity at the $z/d=0$ plane. Although the maximum magnitude of the $z$-velocity is only 13.2 % of the bulk velocity, it is significant enough to indicate that the two re-circulation zones are fully three-dimensional.
Figure 5.16: Instantaneous contours of z-velocity on z/d=0 plane at 6.9988 seconds.

Furthermore, it would appear that flocs are not destroyed inside these regions, since these are slow moving large eddies. However, flocs that get trapped along the shear layer that bounds the re-circulation zones are shredded apart and completely dispersed.
5.1.2 Sensitivity of RANS solution to numerical parameters

As mentioned in the last section, the LES time-averaged velocity vectors show that the jets that emerge from the channels between the grids appear to be symmetric about a plane which coincides with the centre plane of the each grid. The computational requirements could be reduced substantially if the geometry could be simplified by using symmetry boundary conditions. This simplified geometry was shown in Figure 4.3. The RANS equations were solved using this geometry to produce a steady time-averaged solution. This section, and section 5.1.3, give the results for the RANS simulations.

Because the RANS simulations are less computationally restrictive than the LES computations, a more systematic parametric study can be performed. This involves analyzing the effects of mesh size on the solution as well as achieving full convergence. In order to minimize the discretization and iterative errors as much as possible, it is necessary to perform a grid independence test and a full convergence test. The grid independence test consists of evaluating the solution on successively finer meshes until the differences between the results computed on the latest two meshes do not differ substantially. For the RANS simulations, three different mesh sizes were used: 14,630 cells, 46,000 cells, and 72,400 cells. Figure 5.17 shows a comparison of the turbulence intensity (the most relevant quantity), computed on all three grids using the RNG $k-\varepsilon$ turbulence model, as a function of $x/d$. It appears that there is a negligible difference between the results computed on the 46,000 cell mesh and the 72,400 cell mesh. Therefore, for all subsequent simulations, the 46,000 cell mesh was used exclusively.

A full convergence test involves monitoring the residual level for each variable to ensure that the solution has converged. In Fluent\textsuperscript{TM}, the residual is defined as the absolute
value of the remainder left over for each discretized equation for each variable, summed over all the computational cells. This value is also scaled by some appropriate parameter, in Fluent™, this is the flux at each cell. Normally, a solution is considered converged if this scaled residual falls below $10^{-3}$, however, for the RANS simulations, this was not the case. Figure 5.18 shows the convergence history for a RANS simulation at $U_b=0.45$ m/s. The residuals do not converge monotonically to $10^{-3}$, implying that the solution is not fully converged at the $10^{-3}$ residual level. The computations were continued until the residuals fell below $10^{-6}$. The convergence from $10^{-4}$ to $10^{-6}$ is monotonic. An analysis of the solution at $10^{-3}$ residual level and $10^{-6}$ residual level showed that there were some considerable differences. For example, there was a 0.31% increase in drag coefficient.

![Graph](image_url)

Figure 5.17: Turbulence Intensity vs. $x/d$. RNG $k-\varepsilon$ model. $U_b=0.45$ m/s
from $10^{-3}$ to $10^{-6}$. Convergence was also tested to $10^{-9}$. In this case, there was only a 0.0012% increase in the drag coefficient from the solution at the $10^{-6}$ residual level. Therefore, in all subsequent simulations, the computations were terminated when the residuals fell below $10^{-6}$.

![Convergence History](image)

Figure 5.18: Convergence history for RANS simulation. $U_0=0.45$ m/s.

Another important parametric study was to determine the sensitivity of the solution to the specified value of turbulence intensity and length scale at the inlet boundary condition. It was found that the solution downstream of grids, especially in the decay portion ($x/d>10$), did not differ appreciably for different values of turbulence intensity and length scale set at the inlet. This suggests that the history of the flow upstream of the grids is not particularly important. This should be expected, since the turbulence energy generated by the grids is far more intensive than the turbulence energy present in the flow upstream of the grids. Therefore, for the simulations at 0.45 m/s, the
turbulence intensity was set at 5% and the length scale was equal to 0.07L, where L is a relevant dimension of the channel. For this study, L was set equal to the height of the channel, 0.011 m. For the simulations at 0.26 m/s, the turbulence intensity was set as 2.5%, and the length scale was again equal to 0.07L.

5.1.3 Mean flow and turbulence quantities

It is often assumed that the turbulent flow downstream of grids is fairly isotropic and homogeneous in the spanwise directions. Experiment shows that this is indeed the case, see Roach (1986) and Mohamed and LaRue (1990). The assumption that a turbulent flow is isotropic and homogeneous reduces the complexities involved in describing the turbulence and aids in the development of the fibre suspension model. Since the flow cell was approximated using the simplified geometry and its associated symmetry boundary conditions, it was necessary to validate the turbulent flowfield produced by the solution of the RANS equations.

Figure 5.19 shows a comparison of the predicted and experimentally obtained normalized axial velocity vs. the normalized axial distance along the centreline of the channel. The experimental data is taken from D'Incau's (1983) experiments done on the exact same geometry using Laser Doppler Velocimetry. The time-averaged velocity agrees very well with the data. Figure 5.20 shows a comparison of the predicted and experimentally obtained turbulence intensity along the centreline of the channel. In the experiments, the turbulence intensity was defined as: \( \text{Tu} = \sqrt{\text{u}^2} / \text{U}_b \), while in the computations, it is defined as: \( \text{Tu} = \sqrt{2k/3} / \text{U}_b \). Note that in both the experiment and
Figure 5.19: Comparison between predicted and experimental values of normalized Axial velocity vs. \( x/d \). \( U_b = 0.45 \text{ m/s} \)

Figure 5.20: Comparison between predicted and experimental values of turbulence Intensity vs. \( x/d \). \( U_b = 0.45 \text{ m/s} \).
the numerical simulation, the turbulence intensity is based on a fluctuating velocity obtained by subtracting the *time-averaged* velocity from the instantaneous velocity. This assumes that any deviation from the time-averaged mean is due to turbulence. It was shown in section 5.1.1 that the transient behaviour is mostly associated with the mean rather than with the turbulence. However, for the comparison with this experimental data, it is valid to use the time-averaged results from the RANS predictions. As shown in Figure 5.20, the agreement appears to be satisfactory especially in the decay portion of the flow ($x/d>10$). Therefore, it was concluded that the RNG $k-\varepsilon$ model is capable of capturing the relevant turbulence quantities necessary for the fibre model development.

The contours of the velocity magnitude along the centre plane ($z/d=0$) are shown in Figure 5.21 for the case of $U_b=0.45$ m/s. It can be seen that the steady state solution produces a jet that is asymmetric with respect to the centreline of the channel even at full convergence ($10^{-6}$ residual level). This phenomenon is commonly referred to as the "Coanda" effect (Durst et al., 1993).

This is an interesting feature of flows through sudden expansions. An asymmetric velocity profile is produced which has often been observed experimentally (see Fearn et al., 1990). Although most of the investigations have been done on laminar flows through sudden expansions, the effect has also been observed in turbulent flow experiments (Restivo & Whitelaw 1978).
Figure 5.21: Contours of Velocity magnitude at the centre plane, z/d=0, U₀=0.45 m/s.

It has been suggested by Restivo and Whitelaw that the asymmetry is a result of the amplification of disturbances along the shear layers and the subsequent antisymmetric nature of the shedding vortices. The direction in which the jet sways is believed to be a result of small imperfections in the experimental apparatus (Durst et. al., 1993). Numerically, the asymmetry is produced because truncation or discretization errors prevent a zero transverse (y-direction) velocity at the centre plane of the channel (Durst et. al., 1993). It is likely that the direction in which the jet sways depends on the sign of the error. The asymmetric profile is less pronounced at a bulk velocity of U₀=0.26 m/s, as seen in Figure 5.22. For the present study, the relatively good agreement of the velocity and turbulence intensity profiles shown in Figures 5.19 and 5.20 respectively.
suggest that this asymmetric profile has a small impact on the mean flow quantities, and therefore is of no concern with regards to developing the fibre suspension model.
5.2 Validation of fibre suspension model

Section 5.1 described the results obtained for the turbulent flow predictions only. This section gives the numerical predictions of the fibre suspension model. As mentioned previously, the fibre model was used together with the RANS predictions of the turbulence.

To develop a numerical model that is consistent with the experimental results, the RANS equations and the associated turbulence models needed to be employed. The experimentally obtained floculation intensity results are based on time-averaged consistencies (See section 2.2 for details). This means that the conservation equation for floculation intensity describes the transport of a time-averaged floculation intensity, which can only be obtained by solving it in conjunction with the RANS equations.

5.2.1 Sensitivity of solution to numerical parameters

As was done in section 5.1.2, a parametric study was performed in an attempt to minimize the numerical errors. Since the transport equation for floculation intensity is de-coupled from the RANS equations, it was solved separately. In all the simulations, the equation was solved until the residual level fell below $10^{-6}$. There was a negligible difference between the results at the $10^{-6}$ and $10^{-9}$ residual levels.

Figure 5.23 shows the sensitivity of the solution to the value of floculation intensity specified at the inlet boundary condition. The results appear to be insensitive in the decay portion of the flow ($x/d>10$). There is some variation in $f_l$ immediately downstream of the grids. In an attempt to remedy this, the value of $f_l$ at the inlet was set approximately equal to the predicted value far downstream of the grids ($x/d=70$). This
Figure 5.23: Flocculation intensity vs. \( x/d \) for various inlet values of fl. \( U_b=0.45 \) m/s, \( C_m=0.54\% \).

Figure 5.24: Flocculation intensity vs. \( x/d \). Comparison of results computed on two different mesh sizes. \( U_b=0.45 \) m/s, \( C_m=0.54\% \)
varied for the different Reynolds numbers and mean consistencies. As was mentioned in chapter 4, this was an iterative process.

Figure 5.24 shows a comparison of the predicted value of $f_l$ along the centreline of the channel computed on two separate mesh sizes. It is apparent that at these mesh sizes, there is no influence of mesh size on the solution and the results are grid independent.
5.2.2 Flocculation Intensity results

The numerical model for the fibre suspension was calibrated with the experimental data of Raghem Moayed (1999). The predicted values of flocculation intensity were compared against the experimentally obtained values for several sections downstream of the grids. As mentioned in Chapter 2, the experiments were run at the following consistencies and bulk velocities: 0.37%, 0.42%, 0.50%, & 0.54%, and 0.26 m/s and 0.45 m/s. Simulations were run for all these cases. Figures 5.25 to 5.31 show the predictions of $f_l$ and the experimental data along the centreline of the channel, i.e., versus $x/d$ at $y/d=0$, for all seven cases considered.

![Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.45$ m/s, $C_m=0.37\%$.](image-url)

Figure 5.25: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.45$ m/s, $C_m=0.37\%$. 
Figure 5.26: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.45$ m/s, $C_m=0.42\%$.

Figure 5.27: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.45$ m/s, $C_m=0.50\%$. 
Figure 5.28: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.45$ m/s, $C_m=0.54\%$.

Figure 5.29: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.26$ m/s, $C_m=0.42\%$. 
Figure 5.30: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.26$ m/s, $C_m=0.50\%$.

Figure 5.31: Flocculation intensity vs. $x/d$ at $y/d=0$. $U_b=0.26$ m/s, $C_m=0.54\%$
The results show that the model is able to predict the flocculation intensity, in particular, the location of the minimum in \( f_l \), which occurs around \( x/d = 11 \). The agreement is best in the decay portion of the flow, \( x/d > 10 \), where the turbulence is assumed isotropic and homogeneous. In the anisotropic region immediately downstream of the grids, \( x/d < 10 \), there appear to be some discrepancies with the experimental data. It is likely that fibres suppress the turbulence in this region. The model did not take into account this attenuation of the turbulence. The correlations used in the model were based on the fibre free turbulence quantities, which have large spatial variations in the flow. However, due to the attenuation of the turbulence by the fibres, the spatial variations of the turbulence quantities in a fibre suspension are less pronounced. The greater sensitivity of the model to the turbulence quantities is what causes the discrepancies in the immediate downstream section of the grids.

Figures 5.32 to 5.37 show the same comparisons taken at \( y/d = 0.5 \). This location is halfway between the centre of a grid and the centreline of the channel, i.e., aligned with the side of the grid. The magnitude of both the mean and turbulent strain is the highest at this position, and diminishes as \( x/d \) increases. Although the model predicts the trends, the values of flocculation intensity differ considerably. The most notable difference is in the immediate wake of the grids (\( x/d < 10 \)). The model tends to under-predict \( f_l \) in this region. Again, the model is sensitive to the turbulence quantities, which were obtained using a fibre-free simulation. An over-prediction of turbulent kinetic energy will cause an under-prediction of flocculation intensity. This effect is augmented by the fact that the two-equation turbulence model tends to over-predict the values of turbulent kinetic energy and turbulent viscosity in the anisotropic portion of the flow.
Figure 5.32: Flocculation intensity vs. $x/d$ at $y/d=0.5$. $U_b=0.45$ m/s, $C_m=0.42\%$.

Figure 5.33: Flocculation intensity vs. $x/d$ at $y/d=0.5$. $U_b=0.45$ m/s, $C_m=0.50\%$. 
Figure 5.34: Flocculation intensity vs. $x/d$ at $y/d=0.5$. $U_b=0.45 \text{ m/s}$, $C_m=0.54\%$.

Figure 5.35: Flocculation intensity vs. $x/d$ at $y/d=0.5$. $U_b=0.26 \text{ m/s}$, $C_m=0.42\%$. 
Figure 5.36: Flocculation intensity vs. $x/d$ at $y/d=0.5$. $U_b=0.26$ m/s, $C_m=0.50\%$.

Figure 5.37: Flocculation intensity vs. $x/d$ at $y/d=0.5$. $U_b=0.26$ m/s, $C_m=0.54\%$. 
Figures 5.38 to 5.40 show the comparison of fl along the transverse direction (y/d) at a fixed x/d position. Note that these comparisons are taken at x/d=0.12 and x/d=0.21, which are just downstream of the grids. It is clear that the model appears to under-predict the values of fl, especially along the shear layer at y/d=+/-0.5. This is primarily due to the over-prediction of turbulent kinetic energy in this anisotropic portion of the flow. The over-prediction is caused by the isotropic turbulence model, but as well from the fact that the model was derived based on a one-way coupling technique. The effects of the fibres on the continuous phase were ignored. As was discussed in Chapter 3, the modulation of the turbulence by the fibres may be significant, particularly in the region just downstream of the grids. In spite of the quantitative disagreement, the model predicts the general trend in flocculation intensity.

![Graph showing flocculation intensity vs. y/d at x/d=0.21. U_b=0.45 m/s, C_m=0.50%.](image)

Figure 5.38: Flocculation intensity vs. y/d at x/d=0.21. U_b=0.45 m/s, C_m=0.50%.
Figure 5.39: Flocculation intensity vs. y/d at x/d=0.21. \(U_b=0.26\) m/s, \(C_m=0.50\%\).

Figure 5.40: Flocculation intensity vs. y/d at x/d=0.12. \(U_b=0.45\) m/s, \(C_m=0.37\%\).
Figures 5.41 to 5.43 show the values of the production and destruction terms in the equation for flocculation intensity as a function of x/d for three different cases. Near the exit of the grids, the destruction term has its highest magnitude and decreases further downstream. The production term has its minimum value at approximately x/d=8. These two terms dominate the equation for flocculation intensity. Turbulent diffusion is very small compared to these terms because the spatial variations of fl are small. Note that far from the grids, the magnitude of the destruction approaches that of the production. This is what causes the value of fl downstream to level off to a value that is no longer dependent on x/d.

Figure 5.41: Production and destruction of fl versus x/d. U₀=0.45 m/s, C_m=0.50%.
Figure 5.42: Production and destruction of $f_l$ versus $x/d$. $U_b=0.45$ m/s, $C_m=0.37\%$.

Figure 5.43: Production and destruction versus $x/d$. $U_b=0.26$ m/s. $C_m=0.50\%$. 
5.2.3 Qualitative results

In this section some qualitative results for flocculation intensity will be given. These are intended to illustrate the capability of the model to predict relevant features of the flow. Figure 5.44 shows a direct comparison between an optical image of the suspension at the exit of the grids and the predicted value of turbulent strain rate. The turbulent strain rate was the predominant variable appearing in the destruction term in the equation for flocculation intensity. The darker areas in the optical image indicate regions of high fibre flocculation. Note that along the shear layer, where the turbulent strain rate is the highest, the suspension is almost completely dispersed. This corroborates the hypothesis that the destruction of fibre flocs is dependent of the turbulent strain rate.

Figure 5.45 shows the contours of flocculation intensity along the plane at z/d=0. Notice that the flocculation intensity drops considerably in the wake of each grid where the turbulent kinetic energy is a maximum. Figure 5.46 shows cross-sectional contours of
Figure 5.45: Contours of Flocculation intensity along the xy plane at \(z/d=0\). \(U_o=0.45\) m/s, \(C_m=0.50\%\).

Figure 5.46: Cross-sectional (yz plane) contours of flocculation intensity at various \(x/d\) positions downstream of grids. \(U_o=0.26\) m/s, \(C_m=0.50\%\).
fl at various $x/d$ positions downstream of the grids. At $x/d=1$, the flocculation intensity is very low in the separated flow region behind each grid. It remains high in the centre of the channel, however. When flocculation intensity is averaged over the entire cross-section, it has its lowest value at $x/d=10$. It is also fairly uniform over the entire cross-section. This is where the suspension is the best dispersed and represents the most favorable conditions for paper formation. As the turbulence energy decays downstream, the flocculation intensity begins to rise, as seen at $x/d=30$. It remains low near the walls at the top and bottom of the channel since the turbulent stresses reach a maximum in the boundary layer. Moving further downstream ($x/d=60$), fl rises to a value similar to what it had upstream of the grids. It continues to have a maximum at the core of the channel, and decreases somewhat near the walls.
Chapter 6
Practical Implications

The objectives of this study were to provide some insight into the mechanisms of fibre floc formation and destruction using computational fluid dynamics. A better understanding of the fundamental interactions between fluid turbulence and fibre dispersion can ultimately lead to the improved design of modern headboxes. With this in mind, the Large Eddy Simulation was performed to unravel some of the physics that may be responsible for fibre dispersion, while the fibre suspension model was developed to model the flow of a fibre suspension at papermaking consistencies under the same conditions used in operational headboxes.

The LES results revealed that fibre dispersion may be the result of strains imposed by mean motion rather than turbulent motion in a grid-generated turbulent flow. It is generally believed that it is the grid-generated turbulence that acts to destroy flocs and provide uniform dispersion. However, the current result shows that the minimum in fibre flocculation coincides with the greatest strain in the mean motion, and that the actual turbulence levels are low enough to assume a negligible role.
It has been suggested by Kerekes (1983) that flocs break apart due to elongational or tensile strain in the mean motion. The present LES results appear to support this idea, in part. Downstream of the grids, it is likely that both elongational and shear strain are acting to deform flocs. Regardless of whether it is elongational or shear, or both, it is difficult to assess whether it is the mean motion or the turbulent motion that is causing the floc breakup.

Turbulence generators are currently designed to produce small scale turbulence under the assumption that the small scales are necessary to break apart fibre flocs. At the same time, they produce regions of excessive hydrodynamic strain in the mean motion, as seen by the present result. In either case, both the turbulence intensity and the magnitude of the hydrodynamic strain decrease downstream of the generators, leading to an increase in floc formation prior to their arrival at the headbox exit.

The fibre suspension model is based on time-averaged quantities in turbulent flow and is consistent with the approach used to obtain the experimental data. It was developed under the assumptions of isotropic and homogeneous turbulence. The turbulence far downstream of the grids closely approximates this kind of idealization, which may explain the relatively good agreement between the model results and the experimental data. Although it does not directly predict the transient flow features shown by the LES result, it does appear to model the effects quite well. The model can be applied to the downstream section of turbulence generators, and in particular, it can provide a useful guide to determining the locations of minimum fibre flocculation. The extension of the model to other types of flows, however, remains uncertain at this time.
In addition, the results have revealed that the turbulence history of the flow upstream of the grids (or turbulence generators in headboxes) has little impact on the flow characteristics downstream of the grids. This would suggest that a complete model of the headbox could be obtained by modeling the turbulence generators and converging sections exclusively.
Chapter 7

Conclusions

In this thesis the objective was to gain a better understanding of fibre floc formation and dispersion using Computational Fluid Dynamics modeling. A Large Eddy Simulation of the entire flow-cell geometry predicted some of the relevant large scale flow patterns occurring in the grid-generated turbulent flow. In addition, a fibre suspension model was developed and applied to the same geometry that predicted bulk and time-averaged quantities, which are in good agreement with the experimental results.

7.1 Large Eddy Simulation

The principle conclusion from the LES result, obtained on the same geometry and at the same bulk velocity as that in the experiment, was that the minimum in fibre flocculation \( (x/d = 8.5) \) occurred approximately where the mean motion exhibited the maximum time dependence \( (x/d=7.61) \), and hence, the maximum strain. Furthermore, it was shown through Fourier analysis, that the turbulent kinetic energy at these locations made up a disproportionately small amount of the total kinetic energy. Note, however,
that LES is incapable of resolving the smallest scales of turbulence, and hence, unable to predict the turbulence energy at these small scales.

The LES result would appear to imply that it is the stresses imposed by the mean motion, rather than by the turbulent, which cause the floc breakup. The mean motion variation in the region from $x/d=5$ to $x/d=15$ was observed visually in the experiments conducted by Raghem Moayed (1999) at the same bulk velocity. Furthermore, the simulation was able to capture the two large three-dimensional re-circulation zones near the end walls, also observed experimentally. Further work is necessary to generalize this conclusion to other flow conditions.

The LES also provided validation of the RANS solution. A comparison of the normalized mean axial velocity predicted the RANS simulation showed good agreement with the corresponding LES result. There was a discrepancy between the RANS and LES results for the region between $x/d=7$ and $x/d=25$. The LES result showed a local maximum at $x/d=13.5$. This was attributed to the acceleration of the mean flow through the core of the channel caused by the reduction in flow area induced by the two large re-circulation zones at the end walls.

Overall, the LES was capable of predicting the relevant large scale flow patterns occurring downstream of the grids. It appeared to capture much of the physics observed experimentally.

### 7.2 Fibre flocculation model

The fibre suspension model involved deriving an exact equation governing the transport of flocculation intensity, which is analogous to turbulence intensity. Modeling
assumptions regarding the production and destruction of flocculation were made to close
the equation. It was solved in conjunction with the Reynolds Averaged Navier-Stokes
equations for the turbulent flow field. The model results were validated and compared
against the experimental data of Raghem Moayed (1999) obtained on a grid-generated
turbulent flow cell.

The RNG $k-\varepsilon$ turbulence model was found capable of predicting the mean
turbulent flow field upon comparison with experimental data. Both the mean velocity and
turbulence intensity agreed well with the experimental results.

The fibre suspension model appeared to correctly predict the flocculation intensity
far downstream of the grids ($x/d>10$) where the turbulence is isotropic and homogeneous.
Near the grids ($x/d<10$), the model results deviate from the experimental data. Here, the
turbulence is non-isotropic and the suppression of turbulent energy by the fibres is not
taken into account in the model. In general, however, the model does appear to predict
the trends observed in the experimental data.

Of particular practical interest is the prediction of the minimum fibre flocculation.
The experiments of Raghem Moayed (1999) showed that this occurred around $x/d = 8.5$.
The fibre model predicts the minimum at $x/d = 11$. This minimum corresponds to the
position where fibre dispersion is a maximum, and represents the most favourable
conditions for paper formation. As $x/d$ is increased, the flocculation intensity was found
to increase, representing physically, the re-flocculation of fibres.

The fibre suspension model appears to model much of the relevant mechanisms
responsible for fibre flocculation and floc dispersion. It predicts the minimum in fibre
flocculation and the increase in flocculation intensity in the decay section of the grid-generated turbulent flow.

7.3 Recommendations for future work

It is recommended that more simulations be performed using Large Eddy Simulation at different Reynolds numbers. This will provide useful information regarding the relative magnitude of mean and turbulent kinetic energy, and the implications for fibre dispersion. Furthermore, the LES results should be validated against Particle Image Velocimetry (PIV) data to evaluate any modeling errors introduced by the subgrid-scale models.

The LES results can be used to further refine the fibre suspension model. It can provide more accurate descriptions of the destruction of flocculation intensity.

The PIV measurements will elucidate some the mechanisms behind turbulence modulation, which can then be incorporated into a model for attenuation of the turbulence by the fibres. This will provide a complete description of the fibre suspension flow.

Finally, an effort should be made to study the flow of a fibre suspension through a converging channel. Here, the action of the turbulence and mean motion on the fibre flocs is complex and not well understood.
References


Appendix

User defined functions (UDF) were used to implement the fibre suspension model in Fluent™. This involved writing C code to mathematically describe the source terms and diffusivity. To define a source term and diffusivity, the following variables defined in Fluent™ are used to call the functions that compute the source term and diffusivity:

```c
#define DEFINE_SOURCE(name, c, t, dS, i) real name(cell_t c, Thread *t, real dS[], int i)
#define DIFFUSIVITY(name, c, t, i) real name(cell_t c, Thread *t, int i)
```

The problem variables used in the simulations are given the following designations in Fluent™, all of which are the cell centered values:

- C_R(c,t)  
  density
- C_K(c,t)  
  turbulent kinetic energy
- C_D(c,t)  
  turbulent energy dissipation
- C_UDSI(c,t,i)  
  user defined scalar
- C_DUDY(c,t)  
  velocity derivative
- C_MU_T(c,t)  
  turbulent viscosity

The user defined variable declarations have the following designations:

- Cm  
  C_m  
  (mean consistency)
- Ub  
  U_b  
  (bulk velocity)
- D  
  D  
  (diffusion coefficient in transport equation for fl)
- C1fl  
  C_{1f}  
  (constant in transport equation for fl)
- C2fl  
  C_{2f}  
  (constant in transport equation for fl)
- Sigmafl  
  \( \sigma_f \)  
  (constant in transport equation for fl)
- kinlet  
  k_0  
  (inlet turbulent kinetic energy)
The user defined functions are given in the accompanying pages for all seven cases considered. They are executed in Fluent™ as interpreted UDF's.
Case: $U_b=0.45$ m/s, $C_m=0.37\%$

```c
#include "udf.h"

#define Cm 0.37
#define Ub 0.45
#define D 1.429e-7
#define Clfl 1.7e-4
#define C2fl 1.2
#define sigmaf 7.5
#define kinlet 0.000759
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(fl_source, cell, thread, dS, eqn)
{
    real x[3];
    double source, k, knorm, e, rho, pfl, dfl, fl;
    double bulkdudy, dudy, ratio;

    C_CENTROID(x, cell, thread);

    k = C_K(cell, thread);
    e = C_D(cell, thread);
    fl = C_UDSI(cell, thread, 0);
    rho = C_R(cell, thread);
    dudy = C_DUDY(cell, thread);

    dS[eqn] = -0.6 * rho * e / (C2fl * k);

    knorm = k / kinlet;
    bulkdudy = Ub / dgrid;
    ratio = fabs(dudy / bulkdudy);
    dudy = pow(ratio, n);
    pfl = Clfl * bulkdudy * dudy * rho / (Cm * Cm * pow(knorm, 0.19609));
    dfl = -0.6 * rho * e / (C2fl * k);
    source = pfl + dfl;
    return source;
}

DEFINE_DIFFUSIVITY(fl_diffusivity, cell, thread, i)
{
    real x[3];
    double diff_c, k, e, rho, mut;

    C_CENTROID(x, cell, thread);

    rho = C_R(cell, thread);
    mut = C_MU_T(cell, thread);

    diff_c = rho * D * mut / sigmaf;
    return diff_c;
}
```
Case: $U_b=0.45$ m/s, $C_m=0.42\%$

```c
#include "udf.h"

#define Cm 0.42
#define Ub 0.45
#define D 1.429e-7
#define C1fl 1.6e-4
#define C2fl 1.2
#define sigmef 7.5
#define kinlet 0.000759
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(fl_source, cell, thread, dS, eqn)
{
  real x[3];
  double source, k, knorm, e, rho, pfl, df1, fl;
  double bulkdudy, dudy, ratio;

  C_CENTROID(x, cell, thread);

  k = C_K(cell, thread);
  e = C_D(cell, thread);
  fl = C_UDSI(cell, thread, 0);
  rho = C_R(cell, thread);
  dudy = C_DUDY(cell, thread);

  dS[eqn] = -0.6 * rho * e / (C2fl * k);

  knorm = k / kinlet;
  bulkdudy = Ub / dgrid;
  ratio = fabs(dudy / bulkdudy);
  dudy = pow(ratio, n);
  pfl = C1fl * bulkdudy * dudy * e / (Cm * Cm * pow(knorm, 0.19609));
  df1 = -0.6 * rho * fl * e / (C2fl * k);
  source = pfl + df1;
  return source;
}

DEFINE_DIFFUSIVITY(fl_diffusivity, cell, thread, i)
{
  real x[3];
  double diff_c, k, e, rho, mut;

  C_CENTROID(x, cell, thread);

  rho = C_R(cell, thread);
  mut = C_MU_T(cell, thread);

  diff_c = rho * D + mut / sigmef;
  return diff_c;
}
```
Case: $U_b=0.45$ m/s, $C_m=0.50\%$

```c
#include "udf.h"

#define Cm 0.50
#define Ub 0.45
#define D 1.429e-7
#define Clfl 1.7e-4
#define C2fl 1.2
#define sigmaf 7.5
#define kinlet 0.000759
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(fl,source, cell, thread, dS, eqn)
{
    real x[3];
    double source, k, knorm, e, rho, pfl, df1, fl;
    double bulkdudy, dudy, ratio;

    C_CENTROID(x, cell, thread);

    k=C_K(cell, thread);
    e=C_J(cell, thread);
    fl=C_UDSI(cell, thread, 0);
    rho=C_R(cell, thread);
    dudy=C_DUDY(cell, thread);

    dS[eqn]=-0.6*rho*e/(C2fl*k);

    knorm=k/kinlet;
    bulkdudy=Ub/dgrid;
    ratio=fabs(dudy/bulkdudy);
    dudy=pow(ratio,n);
    pfl=Clfl*bulkduOUSudy*rho/(Cm*Cm*pow(knorm, 0.19609));
    df1=-0.6*rho*fl*e/(C2fl*k);
    source=pfl+df1;
    return source;
}

DEFINE_DIFFUSIVITY(fl_diffusivity, cell, thread, i)
{
    real x[3];
    double diff_c, k, e, rho, mut;

    C_CENTROID(x, cell, thread);

    rho=C_R(cell, thread);
    mut=C_MU_T(cell, thread);

    diff_c=rho*D+mut/sigmaf;
    return diff_c;
}
```
Case: $U_b = 0.45 \text{ m/s, } C_m = 0.54\%$

```
#include "udf.h"

#define Cm 0.54
#define Ub 0.45
#define D 1.429e-7
#define Clfl 1.5e-4
#define C2fl 1.15
#define sigmaf 7.5
#define kinlet 0.000759
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(fl_source, cell, thread, dS, eqn)
{
    real x[3];
    double source, k, knorm, e, rho, pfl, df1, fl;
    double bulkdudy, dudy, ratio;

    C_CENTROID(x, cell, thread);

    k = C_K(cell, thread);
    e = C_D(cell, thread);
    fl = C_UDSI(cell, thread, 0);
    rho = C_R(cell, thread);
    dudy = C_DUDY(cell, thread);

    dS[eqn] = -0.6*rho*e/(C2fl*k);

    knorm = k/kinlet;
    bulkdudy = Ub/dgrid;
    ratio = fabs(dudy/bulkdudy);
    dudy = pow(ratio, n);
    pfl = Clfl*bulkdudy*dudy*rho/(Cm*Cm*pow(kn0, 0.19609));
    df1 = -0.6*rho*fl*e/(C2fl*k);
    source = pfl + df1;
    return source;
}

DEFINE_DIFFUSIVITY(fl_diffusivity, cell, thread, i)
{
    real x[3];
    double diff_c, k, e, rho, mut;

    C_CENTROID(x, cell, thread);

    rho = C_R(cell, thread);
    mut = C_MU_T(cell, thread);

    diff_c = rho*D + mut/sigmaf;
    return diff_c;
}
```
Case: $U_h = 0.26$ m/s, $C_m = 0.42\%$

```c
#include "udf.h"

#define Cm 0.42
#define Ub 0.26
#define D 1.429e-7
#define C1f1 2.1e-4
#define C2f1 1.4
#define sigmaf 7.5
#define kinlet 0.0002535
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(fl_source, cell, thread, dS, eqn)
{
    real x[3];
    double source, k, knorm, e, rho, pf1, df1, fl;
    double bulkdudy, dudy, ratio;

    C_CENTROID(x, cell, thread);

    k = C_K(cell, thread);
    e = C_D(cell, thread);
    fl = C_UDSI(cell, thread, 0);
    rho = C_R(cell, thread);
    dudy = C_DUDY(cell, thread);

    dS[eqn] = -0.6*rho*e/(C2f1*k);

    knorm = k/kinlet;
    bulkdudy = Ub/dgrid;
    ratio = fabs(dudy/bulkdudy);
    dudy = pow(ratio, n);

    pf1 = C1f1*bulkdu*y*dudy*rho/(Cm*Cm*pow(knorm, 0.19609));
    df1 = 0.6*rho*fl*e/(C2f1*k);
    source = pf1 + df1;
    return source;
}

DEFINE_DIFFUSIVITY(fl_diffusivity, cell, thread, i)
{
    real x[3];
    double diff_c, k, e, rho, mut;

    C_CENTROID(x, cell, thread);

    rho = C_R(cell, thread);
    mut = C_MU_T(cell, thread);

    diff_c = rho*D+mut/sigmaf;
    return diff_c;
}
```
Case: \( U_b = 0.26 \text{ m/s}, C_m = 0.50\% \)

```c
#include "udf.h"

#define Cm 0.50
#define Ub 0.26
#define D 1.429e-7
#define Cifl 2.25e-4
#define C2fl 1.5
#define sigmaf 7.5
#define kinlet 0.0002535
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(f1_source, cell, thread, dS, eqn)
{
    real x[3];
    double source, k, knorm, e, rho, pfl, df1, f1;
    double bulkdudy, dudy, ratio;

    C_CENTROID(x, cell, thread);

    k=C_K(cell, thread);
    e=C_D(cell, thread);
    f1=C_UDSI(cell, thread, 0);
    rho=C_R(cell, thread);
    dudy=C_DUDY(cell, thread);

    dS[eqn]=-0.6*rho*e/(C2fl*k);

    knorm=k/kinlet;
    bulkdudy=Ub/dgrid;
    ratio=fabs(dudy/bulkdudy);
    dudy=pow(ratio, n);
    pfl=Cifl*bulkdu*duy*rho/(Cm*Cm*pow(knorm, 0.19609));
    df1=0.6*rho*f1*e/(C2fl*k);
    source=pfl+df1;
    return source;
}

DEFINE_DIFFUSIVITY(f1_diffusivity, cell, thread, i)
{
    real x[3];
    double diff_c, k, e, rho, mut;

    C_CENTROID(x, cell, thread);

    rho=C_R(cell, thread);
    mut=C_MU_T(cell, thread);

    diff_c=rho*D+mut/sigmaf;
    return diff_c;
}
```
Case: \( U_b = 0.26 \) m/s, \( C_m = 0.54\% \)

```c
#include "udf.h"

#define Cm 0.54
#define Ub 0.26
#define D 1.429e-7
#define C1fl 2.1e-4
#define C2fl 1.4
#define sigmaf 7.5
#define kinlet 0.0002535
#define dgrid 0.008
#define n 0.02

DEFINE_SOURCE(f1_source, cell, thread, dS, eqn)
{
    real x[3];
    double source, k, knorm, e, rho, pfl, df1, f1;
    double bulkdudy, dudy, ratio;

    C_CENTROID(x, cell, thread);

    k = C_K(cell, thread);
    e = C_D(cell, thread);
    f1 = C_UDSI(cell, thread, 0);
    rho = C_R(cell, thread);
    dudy = C_DUDY(cell, thread);

    dS[eqn] = -0.6*rho*e/(C2fl*k);

    knorm = k/kinlet;
    bulkdudy = Ub/dgrid;
    ratio = fabs(dudy/bulkdudy);
    dudy = pow(ratio, n);
    pfl = C1fl*bulkdudy*dudy*rho/(Cm*Cm*pow(knorm, 0.19609));
    df1 = -0.6*rho*f1*e/(C2fl*k);
    source = pfl + df1;
    return source;
}

DEFINE_DIFFUSIVITY(f1_diffusivity, cell, thread, i)
{
    real x[3];
    double diff_c, k, e, rho, mut;

    C_CENTROID(x, cell, thread);

    rho = C_R(cell, thread);
    mut = C_MU_T(cell, thread);

    diff_c = rho*D+mut/sigmaf;
    return diff_c;
}
```