INFORMATION TO USERS

This manuscript has been reproduced from the microfilm master. UMI films the text directly from the original or copy submitted. Thus, some thesis and dissertation copies are in typewriter face, while others may be from any type of computer printer.

The quality of this reproduction is dependent upon the quality of the copy submitted. Broken or indistinct print, colored or poor quality illustrations and photographs, print bleedthrough, substandard margins, and improper alignment can adversely affect reproduction.

In the unlikely event that the author did not send UMI a complete manuscript and there are missing pages, these will be noted. Also, if unauthorized copyright material had to be removed, a note will indicate the deletion.

Oversize materials (e.g., maps, drawings, charts) are reproduced by sectioning the original, beginning at the upper left-hand corner and continuing from left to right in equal sections with small overlaps. Each original is also photographed in one exposure and is included in reduced form at the back of the book.

Photographs included in the original manuscript have been reproduced xerographically in this copy. Higher quality 6" x 9" black and white photographic prints are available for any photographs or illustrations appearing in this copy for an additional charge. Contact UMI directly to order.
Fluid mechanics and particle transport in a channel with one porous wall: Application to membrane filtration

Chellam, Shankararaman, M.S.
Rice University, 1991
RICE UNIVERSITY

FLUID MECHANICS AND PARTICLE TRANSPORT IN A CHANNEL WITH ONE POROUS WALL: APPLICATION TO MEMBRANE FILTRATION

by

SHANKARARAMAN CHELLAM

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE MASTER OF SCIENCE

APPROVED, THESIS COMMITTEE

Mark R. Wiesner, Assistant Professor, Dept. of Environmental Science and Engineering, Chair

Mason B. Tomson, Professor, Dept. of Environmental Science and Engineering

David J. Hellums, Professor, Dept. of Chemical Engineering

Clint Dawson, Assistant Professor, Dept. of Mathematical Sciences

Houston, Texas
April, 1991
Abstract

Fluid Mechanics and Particle Transport in a Channel with One Porous Wall: Application to Membrane Filtration

Shankararaman Chellam

Fluid mechanics of a channel with one porous wall was studied from first principles as the initial step towards understanding polarization phenomena in membrane modules. A regular perturbation method was used to solve the steady-state Navier-Stokes equations for an incompressible, constant property fluid in two dimensions with uniform suction and slip at the permeable boundary. The effects of solute and hydrodynamic parameters on concentration polarization during potable water treatment applications are investigated numerically. Inertia dominated and permeation drag dominated particle transport is discussed. Experimentally determined residence time distributions of particles in a microporous channel are interpreted in the light of inertial and permeation forces. Inertial lift theory is shown to predict initial particle transport. Experimentally observed long trailing edges in particle residence time distributions indicate the importance of other transport mechanisms even in dilute suspension mechanics. It is seen that inertial effects are negligible under conditions typical of microfiltration.
Acknowledgements

markwiesner for believing that I am capable of any research, for all his guidance and
the freedom that he has given me, Dr. Hellums for actually making me like fluid mechanics (it was a real pleasure to learn from him), Masontomson for all his peptalks and for trying to tell me what research is about (and for his sense of humor), Clint Dawson for helping me with boundary conditions and helpful hintson computer programming. Hope I will continue to learn from these people in the future also. My really nice colleagues (in random order) Vasukarefatendraha and Bart Simpson. These guys put up with all the crap (quite literally) I gave them. George Robinson for times, places (munchies, Tacobell ...) and friendship. Luncheons and nightlife in the basement will be different without him. James "The almost physycist" Robinson for oyysters, Neilyoung, valhala, Molly rice (will he ever make it with her?) Blue oyster cult, Βλαυεοψτερχυλτ, etc. Rei and Swati for spending time with me and taking my mind away from my work. The lack of much female influence (except for six month aberration), Dansch Melling for the night at the "axiom", my parents for their support, love and letting me have the family name, cheeri, for thinking that I could never do wrong, Kannan, for auseheislearningwhat is important in life and what is not. Ravi, Asmyoldebrothera nd cricket coach, for making sure I will do exactly as I please. Afive member band with heric, Buck, Allen, Joe and Albert for keeping me going on long hard nights and days. They are actually gving me graduation concert!! Rockefeller for bringing them toh ouston twice with a span of six months. Shinerbock for costing only thirty five cents. My old bosses shared sweet memories supported and encouraged me through alcohol, opium and serious hardship work. Radhakrishnan for all his didactic zeal in mathematics and kps for teaching me inorganic chemistry.

This work was supported by the National Science Foundation, Grant BCS-8909722 and the Department of Environmental Science and Engineering at Rice University.
# Table of Contents

1. **Introduction** .......................................................... 1  
   1.1 General concepts, background and motivation .......... 1  
   1.2 Objectives ....................................................... 3  
   1.3 Limitations of this study .................................. 5  

2. **Literature Review** ................................................. 7  
   2.1 Fluid Mechanics in Porous Ducts ......................... 7  
      2.1.1 Boundary conditions at a porous surface ........ 11  
   2.2 Transport of solutes in porous ducts ................. 14  
      2.2.1 Numerical Solutions ................................. 15  
      2.2.2 Analytical solutions ................................. 17  
   2.3 Membrane filtration of colloidal suspensions .......... 19  
      2.3.1 The role of fluid inertia ............................ 20  
      2.3.2 Orthokinetic effects ................................. 30  
      2.3.2.1 Convective flow models ......................... 30  
      2.3.2.2 Shear-induced back-transport models .......... 31  

3. **Theoretical Analysis** ........................................... 35  
   3.1 Mathematical Modeling of Fluid Flow ................. 35  
      3.1.1 Problem formulation ................................. 35  
      3.1.2 Perturbation Solution ............................... 37  
      3.1.3 Discussion on fluid mechanics .................... 42  
   3.2 Mass transfer of Brownian components ................. 48  
      3.2.1 Set-up of the governing equations ................. 48  
      3.2.2. Finite difference solution ....................... 51  
      3.2.3 Discussion on concentration polarization ........ 55
3.2.3.1 Effect of the diffusion coefficient ............ 55
3.2.3.2 Effect of the slip coefficient .......... 62
3.2.3.3 Effect of hydrodynamic parameters ......... 63
3.2.4 Computational aspects ................................. 65
3.3 Particle transport in porous channels ................. 66
  3.3.1 Problem formulation ............................. 66
  3.3.2 Inertial lift and particle trajectories ........... 73
  3.3.3 Engineering Significance ....................... 76
  3.3.4 Asymptotic Solution near the Membrane surface . 87
  3.3.5 Steady-State Concentration Profiles ............. 90
  3.3.6 Computational aspects ......................... 92
4. Experimental work ........................................... 94
  4.1 Materials and procedures ............................ 94
    4.1.1 Water ........................................... 94
    4.1.2 Tracer .......................................... 94
    4.1.3 Particles ....................................... 95
    4.1.4 Feed water pump .................................. 95
    4.1.5 Flow meter ...................................... 96
    4.1.6 Injection system ................................ 97
    4.1.7 Detection system ................................ 98
    4.1.8 Weighing system ................................ 99
    4.1.9 Pressure measurement ......................... 100
    4.1.10 Tubing and fittings ............................ 101
    4.1.11 Data acquisition system ..................... 101
    4.1.12 Membrane filtration unit ..................... 104
List of Figures

2.3.1 Dimensionless lateral force as calculated by Ho and Leal .......... 25

2.3.2 Concentration distributions of neutrally buoyant suspensions subject to a lift force and simultaneous Brownian motion. ............... 27

2.3.3 Comparison of solutions for a freely rotating neutrally buoyant sphere in 2-D vertical Poiseuille flow ........................................ 29

3.1.1 The coordinate system used in the solution of the 2-D, steady state Navier-Stokes equations. .......................................................... 35

3.1.2 Comparison of the zero and first order solutions of the axial velocity at mid-channel ................................................................. 43

3.1.3 Comparison of the zero and first order solutions of the transverse velocity at mid-channel ......................................................... 43

3.1.4 Influence of the slip coefficient on the mid-channel axial velocity profile that might exist in a parallel plate microfilter .......... 44

3.1.5 Effect of axial slip velocity on the mid-channel transverse velocity profile ................................................................. 45

3.1.6 Streamlines for laminar flow in the channel (σ=0). ............... 47

3.1.7 Streamlines for laminar flow in the channel (σ=0.2) ............. 48

3.2.1 The square grid scheme used for the finite difference solution .. 52

3.2.2 Influence of solute diffusivity on mid-channel concentration profiles ................................................................. 57

3.2.3 Removal of NaCl and CaSO4 from a brackish water using reverse osmosis................................................................. 58

3.2.4 Concentration profiles at mid-channel during the UF of a 50K - 100K fraction of humic acid with a high background ionic strength.. 60

3.2.5 Mid-channel concentration profiles for the UF of a 50K-100K humic acid fraction at a low background ionic strength .................. 61
3.2.6 Mid-channel concentration profiles illustrating the effect of the slip velocity .............................................. ................................. .. 62

3.2.7 Influence of permeation rate on concentration polarization....... 64

3.2.8 Mid-Channel concentration profiles at varying crossflow velocities .......................................................... ................................. .... 64

3.3.1 Spherical particle undergoing plane flow in a channel with one porous wall.......................................................... ................................. .. 67

3.3.2 Variation of permeation drag and inertial lift forces in a channel with one porous wall.......................................................... ................................. 74

3.3.3 Simulated position trajectories of a particle of radius 10 \( \mu \text{m} \) (like PAC) in an ultrafilter .......................................................... ................................. 77

3.3.4 Simulated position trajectories of a particle of radius 3 \( \mu \text{m} \) (like bacteria) in an ultrafilter .......................................................... ................................. 78

3.3.5 Simulated time trajectories of large PAC particles \((a_p = 10 \mu \text{m})\) in an ultrafilter .......................................................... ................................. 81

3.3.6 Position trajectories of particles \((a_p = 17.5 \mu \text{m})\) in a microfilter when inertial effects are important.......................................................... ................................. 82

3.3.7 Residence times for inertia dominated and permeation drag dominated particles in an ultrafilter as a function of initial lateral position .......................................................... ................................. 83

3.3.8 Predicted residence time distribution of large, neutrally buoyant PAC particles \((a_p = 10 \mu \text{m})\) in an ultrafilter .......................................................... ................................. 86

3.3.9 Predicted residence time distributions of small, spherical bacteria \((a_p = 3 \mu \text{m})\) in a ultrafilter .......................................................... ................................. 86

3.3.10 Change in \( \gamma_{\text{crit}} \) as a function of axial position in the channel for particle capture on the membrane surface for fixed values of \( \beta \) ........................................ 88

3.3.11 Effect of \( \gamma_{\text{crit}} \) on the limiting value of \( \beta \) when the particle just touches the membrane surface.......................................................... ................................. 89
3.3.12 Effect of permeation drag on the steady-state distribution of particles in a channel with one porous wall .......................... 91
3.3.13 Steady-state distribution of particles in a channel with one porous wall illustrating the effect of the diffusion coefficient.............. 92
4.1.1 Flow meter calibration curve ..................................... 97
4.1.2 Flow diagram for the impulse input macro.......................... 103
4.1.3 The RC circuit for filtering any noise in the incoming weight signal ......................................................... 104
4.1.4 Plan view of the filter top piece .................................... 104
4.1.5 Front view of a sampling port........................................ 105
4.1.6 Machine drawing for the Teflon flow channel ..................... 105
4.1.7 Schematic of the experimental set-up used for measuring the RTD of both tracer solutions and particle suspensions ................... 108
4.2.1 Experimental data from one tracer injection experiment showing the RTD and reject water accumulation ......................... 110
4.2.2 Correlating the mathematically calculated first response with the experimental observations by conducting a tracer study ............... 113
4.2.3 Residence time distribution of particles of radius 0.24 μm in the membrane filter.................................................. 116
4.2.4 Computer simulation of the RTD of 0.24 μm radius particles ... 117
4.2.5 Experimental observations and predicted values of the first response as a function of influent flow rate for particles of radius, \( a_p = 0.25 \ \mu m \) .................................................. 119
4.2.6 Comparison of theoretical predictions of first passage time and experimental observations for particles of radius 0.24 μm .......... 120
4.2.7 Residence time distribution of particles of radius 0.47 μm in the membrane filter.................................................. 124
4.2.8 Residence time distribution of particles of radius 1.6 μm in the membrane filter ........................................ 125

4.2.9 Residence time distribution of particles of radius 3.5 μm in the membrane filter ........................................ 126

4.2.10 Computer generated RTD for particles of radius 0.47 μm .... 127

4.2.11 Computer generated RTD for particles of radius 1.6 μm .... 128

4.2.12 Computer generated RTD for particles of radius 3.5 μm .... 129

4.2.13 Experimental observations and predicted values of the first response as a function of influent flow rate for particles of radius, $a_p = 0.47 \mu m$ ........................................ 134

4.2.14 Experimental observations and predicted values of the first response as a function of influent flow rate for particles of radius, $a_p = 1.6 \mu m$ ........................................ 134

4.2.15 Experimental observations and predicted values of the first response as a function of the influent flow rate for particles of radius, $a_p = 3.5 \mu m$ ........................................ 135

4.2.16 Comparison of theoretical predictions of the first passage time and experimental observations for particles of radius 0.47 μm ... 136

4.2.17 Comparison of theoretical predictions of the first passage time and experimental observations for particles of radius 1.6 μm .... 137

4.2.18 Comparison of theoretical predictions of the first passage time and experimental observations for particles of radius 3.5 μm .... 137

4.2.19 Summary of all first response data ........................................ 138

A1.1 The cartesian coordinate system for both the boundary layer and potential flow problems ........................................ 143

A1.2 Momentum boundary layer during a typical reverse osmosis application ........................................ 149

A1.3 Momentum boundary layer during an ultrafiltration application ........................................ 149
A1.4 Momentum boundary layer during an ultrafiltration application .................................................. 150

A1.5 Development of the momentum boundary layer during a typical experiment. .................................. 150
## List of Tables

2.3.1 General forms for the lift velocity derived by Vasseur and Cox ........................................ 28

3.1.1 Estimates of the slip velocity in membrane systems .............. 45

4.1.1 Rotameter Calibration Data .......................................... 96

4.1.2 Tubing used in the experimental apparatus ...................... 101

4.1.3 Information on membrane filters used in experiments ............ 106

4.2.1 Results of a tracer study on the porous channel using the Durapore membrane ................... 112

4.2.2 Results of pulse inputs of 0.24 μm radius particles in the porous channel using the Durapore membrane .................. 115

4.2.3 Order of magnitude analysis of lateral forces on a $a_p=0.24$ μm particle in a channel of height 762 μm .................. 119

4.2.4 Results of pulse inputs of 0.47 μm radius particles in the porous channel using the Track-etch membrane .................. 121

4.2.5 Results of pulse inputs of 1.6 μm radius particles in the porous channel using the Track-etch membrane .................. 122

4.2.6 Results of pulse inputs of 3.5 μm radius particles in the porous channel using the Track-etch membrane .................. 123

4.2.7 Order of magnitude analysis of lateral forces for a $a_p=0.47$ μm particle in a channel of height 762 μm .................. 131

4.2.8 Order of magnitude analysis of lateral forces for a $a_p=1.6$ μm particle in a channel of height 762 μm .................. 132

4.2.9 Order of magnitude analysis of lateral forces for a $a_p=3.5$ μm particle in a channel of height 762 μm .................. 132
Chapter 1

Introduction

1.1 General concepts, background and motivation: There has been a change in the regulatory environment and perception of the public towards the quality of the drinking water in the United States. Congress amended the original Safe Drinking Water Act (SDWA) in 1986 to establish regulations for eighty-three new contaminants. The SDWA amendments focus on microbiological, organic and inorganic quality of water. The recently finalized Surface Water Treatment Rule (SWTR) dictates minimum requirements for the removal/inactivation of Giardia cysts as 99.9\% (3 log removal) and enteric viruses as 99.99\% (4 log removal). These removals can be achieved through a combination of physical (filtration) and chemical (disinfection) practices. Reduced maximum contaminant limits (MCLs) for disinfection by-products (DBPs), many of which are suspected carcinogens, are the primary foci in the organic purity of water. Increased disinfectant dosage and/or contact time is likely to result in greater amounts of DBPs in the water thus making filtration an important "polishing" step in potable water treatment.

Pressures to provide potable water of higher quality occur at a time when the sources of renewable high raw waters are increasingly in short supply. In arid and semi-arid parts of the world, desalination of sea and brackish waters may be the most important means for providing drinking water. Some communities are investigating strategies for water re-use
and/or the use of contaminated ground/surface waters. Membrane processes may play a role in aiding water treatment and supply professionals in meeting future demands on water quality and quantity.

A membrane can be thought of as a barrier that restricts the passage of various chemical species in a very specific manner. Separation of the constituents of a feed stream using membranes is possible because of differences in the transport rates of species through the membrane interface. Volume flux and separation of constituents is possible by the application of a hydrostatic pressure differential between the two phases separated by the membrane when the hydrodynamic permeability is different for different species (Strathmann, 1981). Thus, the driving force for the flux is a gradient in the pressure. Membrane processes that depend on this principle are classified as pressure-driven. Other driving forces can also lead to separation. These include gradients in concentration, temperature, electrical potential etc. This thesis addresses the theory of mass transport in pressure-driven membrane processes.

Pressure-driven membrane processes include reverse osmosis (RO), nanofiltration (NF), ultrafiltration (UF) and microfiltration (MF). These processes differ mainly in the size range of the permeable species, the relative magnitude of the pressure differential and the possible permeate flux. RO membranes retain ionic constituents, operate under very high pressure differentials and produce small permeate fluxes. In contrast, MF membranes are permeable to species up to $\approx 0.1 \ \mu m$ and produce high
fluxes under small pressure differentials relative to RO. NF and UF have characteristics intermediate to RO and MF.

Desalination by reverse osmosis (RO) was the first large scale application of membranes in potable water treatment and is still the most energy-efficient process for this purpose. In 1988, the worldwide capacity for desalination using RO was estimated to be 2.25 billion gallons per day (Haggin, 1990). RO is also used for pretreating boiler feed water and in deionizing water for the semi-conductor industry. Ultrafiltration and microfiltration have potential for use in removing DBPs and DBP precursors along with bacteria and particles from water. This has led to wide spread interest in the application of membrane processes in the potable water treatment industry in the context of the SWTR and the forthcoming DBP regulations.

Inherent in any membrane separation process is the accumulation of rejected components on the membrane surface. This phenomenon, called concentration polarization often results in an increased resistance to the transport of solvent thereby decreasing the permeate flux. Understanding concentration polarization will aid in the design, selection and operation of pressure driven membrane processes.

1.2 Objectives: This study focuses on developing a fundamental understanding of physical processes that govern the transport of solutes and particulate matter in membrane modules. The principal objectives of the research were:
1. To model mass transport in membrane filtration units as a function of the size of the materials present in the feed stream.

2. To compare experimental observations of particle transport in the size range of interest in potable water treatment with the values obtained from a previously developed model for the particle trajectory in porous channels.

The salient features of this research effort are summarized below.

1. All investigations were made on a simple system: a rectangular channel with one porous wall. Fluid flow was assumed to be steady, incompressible and laminar without any external forces. Also, only dilute suspensions of spherical particles were used so that particle-particle interactions could be neglected.

2. The effects of axial and transverse velocity components and solute diffusivity on concentration polarization were examined.

3. Particle trajectories incorporating non-linear inertial effects were simulated for some cases of interest in UF and MF and the role of particle size in relation to channel geometry and hydrodynamics in determining transport was examined.

4. For a given flow field, the time required for a particle to cross a given length of porous boundary was determined as a function of the initial lateral position and size.
5. Experiments were performed to obtain the residence time distribution for a pulse input of particles on the fluid entering the channel. The observed first response (associated with the particle spending the least time in the channel) was compared to the mathematically computed first passage time (related to the fastest moving trajectory).

1.3 Limitations of this study:

1. In determining concentration profiles, the field equations representing momentum and mass transfer were decoupled. In reality, polarization of mass on the membrane will affect permeation thereby making the wall permeation rate non-uniform with axial distance.

2. The very interesting dynamic (time variant) behavior in membrane modules have not been analyzed.

3. Many membrane systems operate in the turbulent flow regime providing mixing in the transverse direction thereby reducing concentration differences between the bulk liquid and the membrane surface and alleviating the effects of concentration polarization. Effects of fluid turbulence have not been considered in this work.
4. Membrane filters work on continuous feeds. In the analysis of such an input, interactions between the rejected species and the membrane may change their physical and chemical properties (e.g. diffusivity, density, viscosity, etc.) and have to be considered along with any non-Newtonian behavior due to the deposited mass. For the most part, experimental and modeling work presented in this thesis do not account for these interactions.

5. In analyzing colloidal fouling of membranes, theories of dense suspension rheology will prove useful. Electrokinetic effects will be another interesting area for analysis, considering the large differences in ionic environments that exist within a very small area in membrane filtration units. These factors have not been explicitly accounted for in this work.
Chapter 2

Literature Review

The fundamental physical phenomena determining clean solvent recovery and concentration polarization in a membrane filter are the underlying fluid mechanics and mass transfer processes in the system. In this chapter a review of pertinent published literature is presented.

2.1 Fluid Mechanics in Porous Ducts:

A complete mathematical analysis of the fluid mechanics of a system is performed by solving the governing differential equations for the transfer of momentum together with the continuity equation subject to the appropriate boundary conditions. The form of Newton’s law that describes the conservation of momentum for a stationary control volume in a flowing incompressible fluid with density $\rho$ and local velocity $\mathbf{v}$ is (Happel and Brenner, 1965):

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = \nabla \cdot \mathbf{\Pi} + \rho \mathbf{F} \quad (2.1.1)$$

<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{\partial}{\partial t}(\rho \mathbf{v})$</td>
<td>rate of increase of momentum</td>
</tr>
<tr>
<td>$\nabla \cdot (\rho \mathbf{v} \mathbf{v})$</td>
<td>rate of momentum loss by convection</td>
</tr>
<tr>
<td>$\nabla \cdot \mathbf{\Pi}$</td>
<td>surface stress (pressure)</td>
</tr>
<tr>
<td>$\rho \mathbf{F}$</td>
<td>body forces (gravity)</td>
</tr>
</tbody>
</table>

The stress tensor $\mathbf{\Pi}$ is defined such that if $\mathbf{n}$ is an outer drawn unit normal to a surface, $\mathbf{\Pi} \cdot \mathbf{n}$ gives the force exerted per unit area on the surface by the surrounding fluid. For a Newtonian, incompressible fluid the stress tensor is
\[ \Pi = 2\mu \mathbf{D} - p\mathbf{I} \quad (2.1.2) \]

where \( \mathbf{I} \) is the unit tensor, \( p \) is the hydrostatic fluid pressure and \( \mathbf{D} \) is the rate of deformation tensor defined as,

\[ \mathbf{D} = \frac{1}{2} \left[ \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right] \quad (2.1.3) \]

Substituting the expression for \( \Pi \) in Eq. (2-1.1) gives the general form of the Navier-Stokes equations. The continuity equation is an expression of the conservation of mass and is written in vector form as,

\[ \frac{\partial p}{\partial t} = - \nabla \cdot (\rho \mathbf{v}) \quad (2.1.4) \]

All applications considered in this report are for incompressible fluids (constant \( \rho \)). The continuity equation therefore reduces to

\[ \nabla \cdot \mathbf{v} = 0 \quad (2.1.5) \]

For incompressible fluids with constant viscosity, \( \mu \), the Navier-Stokes equations are,

\[ \rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = - \nabla p + \mu \nabla^2 \mathbf{v} + \rho \mathbf{F} \quad (2.1.6) \]

Subject to the appropriate boundary condition it constitutes a complete description of fluid motion. Exact solutions are available only under certain simplifications and for specified geometries. Wang (1989; 1991) recently gave a comprehensive review of exact solutions for both steady and unsteady flows. For two-dimensional, isothermal flow of a constant property viscous fluid in a porous slit, the transfer of momentum in the
axial and transverse directions can be described in cartesian coordinates as (Kleinsteuerer, 1984)

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + v \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \tag{2.1.7}
\]

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial P}{\partial y} + v \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \tag{2.1.8}
\]

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{2.1.9}
\]

subject to the following boundary conditions

\[ u = v = 0 \quad \text{at a solid wall (no-slip)} \tag{2.1.10} \]

\[ u = 0 \text{ and } v = v_y \quad \text{at the porous wall} \tag{2.1.11} \]

and the initial condition

\[ u \text{ and } v \text{ are known throughout the domain of interest at } t = 0. \]

Approximate solutions are obtained by both analytical and numerical methods. Berman (1953) first obtained a steady-state solution for fluid flow in a rectangular channel with two equally porous walls using a regular perturbation method for low wall permeabilities. He expressed the velocity profiles as a series expansion in the perturbation parameter \( \text{Re}_w \) and derived the zero (leading order) and first order solutions in the perturbation series expansion. Yuan and Finkelstein (1956) in their studies on jet motor cooling and boundary-layer control derived the expressions for the steady laminar fluid flow in circular pipes using cylindrical
coordinates. Both these results were obtained assuming uniform suction at the walls, i.e.

\[ v_y = v_w \quad \text{along the porous boundary} \quad (2.1.12) \]

The velocity profiles for steady, creeping flows with variable wall suction for both channel and tube flow was obtained by Kozinski et al. (1970) by neglecting the non-linear inertial terms. They assumed an exponential decrease in the wall permeation rate with axial distance as the boundary condition for the normal velocity at the porous walls, i.e.

\[ v_y = v_o e^{-\alpha x} \quad \text{along the porous boundary} \quad (2.1.13) \]

Galowin and DeSantis (1971) analyzed steady, axisymmetric, laminar flow in an open-ended porous tube using the von-Kármán integral technique. In this method, the momentum transfer equation is integrated using the continuity equation and an appropriate form of the velocity profile is postulated that satisfies the physically meaningful boundary conditions. Galowin and DeSantis proposed a quadratic profile for the axial velocity as

\[ \hat{u} = \frac{u}{u_{\text{max}}} = \left[ 1 + f(x) \right] (1 - r^2) \quad (2.1.14) \]

The unknown function \( f(x) \) describes the change in the axial velocity from Poiseuille flow at the entrance, \( x \) is the axial distance coordinate and \( r \) is the radial distance from the tube axis. Galowin and co-workers (1974) later also presented a similar analysis for a porous tube with an impermeable end-wall which is of interest in some heat transfer applications as in the
condenser section of a heat pipe. The solution for steady, laminar, axisymmetric, fully developed flow in a porous tube with variable suction or injection was obtained by Terrill (1983) by superimposing potential flow on Poiseuille flow. Terrill developed solutions of the form

\[ u = u_0(r) + \frac{\partial}{\partial z} \Phi(r,z) \]  \hspace{1cm} (2.1.15)

\[ v = \frac{\partial}{\partial r} \Phi(r,z) \]  \hspace{1cm} (2.1.16)

where \( z \) is the coordinate along the tube axis, \( u_0(r) \) represents Poiseuille flow in a pipe and \( \Phi \) satisfies the continuity equation provided it is harmonic, i.e. it satisfies Laplace’s equation

\[ \nabla^2 \Phi = 0 \]  \hspace{1cm} (2.1.17)

Green (1979) obtained expressions for the velocity components and pressure variation for the two dimensional flow of fluid in a slit with one porous wall using a perturbation method under the assumption of low wall permeability \( (Re_w \ll 1) \).

2.1.1 Boundary conditions at a porous surface

While modeling the flow of a viscous fluid, the tangential and normal velocity components are usually assumed to vanish at a solid surface because of friction between the fluid and the surface (no-slip). Beavers and Joseph (1967) first investigated the effect of tangential migration of fluid at a permeable surface. They confined oil to flow in a narrow channel of height \( h \), and measured mass efflux in this gap by
having both permeable and impermeable lower boundaries. Their results showed greatly enhanced mass efflux values when the flow is bounded by a permeable surface than in the case of an impermeable surface indicating the presence of a momentum boundary layer within the porous boundary within which the velocity changed from the "slip" value to the mean velocity within the porous block, Q (volumetric flow rate per unit cross-sectional area). Darcy's law was applied for flow in the bulk of the porous medium. i.e.

\[ Q = - \frac{k}{\mu} \frac{dP}{dx} \]  \hspace{1cm} (2.1.18)

Also, they assumed that the slip velocity for the free fluid on the porous surface is proportional to the shear rate at the permeable boundary. Thus the slip velocity was empirically expressed as:

\[ \frac{\partial u}{\partial y} = \frac{\alpha}{\sqrt{k}} (u_{\text{slip}} - Q) \]  \hspace{1cm} (2.1.19)

where \( \alpha \) is a dimensionless quantity thought to be related only to the nature of the permeable surface, its structure and porosity (and independent of the channel geometry). In their experiments with Foametal and Aloxite, \( \alpha \) varied in the range 0.1 \( \leq \alpha \leq 4.0 \). Taylor (1971) fabricated a model of an ideal porous material consisting of accurately machined grooves in a Perspex disk for which the permeability could be calculated from its geometry. Above this disk, at an accurately measured distance, a solid brass disk was placed. The whole system was immersed in oil and the lower grooved disk was rotated using a motor. The torque exerted on the
upper disk was measured experimentally. In this system the Darcy velocity, $Q$, is zero. Therefore Equation (2.1.19) can be written as

$$\alpha = \frac{\sqrt{k}}{u_{\text{slip}}} \frac{\partial u}{\partial y}$$  \hspace{1cm} (2.1.20)

In an accompanying paper, Richardson (1971) derived expressions for the shear stress on the top disk relating it to the torque and the gap between the lower and upper disks. Thus, values for $\alpha$ can be calculated for different gaps. Taylor reported an initial rapid decrease in $\alpha$ as the gap increased which later reached an asymptotic value indicating that the dimensionless constant, $\alpha$, may be dependant on the channel geometry as well. Saffman (1971) analyzed flow in a channel with one porous boundary as a particular case of flow through a non-homogenous porous medium and theoretically derived the form of the boundary condition. Mathematically, the system was described as a discontinuous step function:

\[
\begin{align*}
\text{porosity} &= 1 \text{ and permeability} = \infty \quad \text{in the gap} \\
\text{porosity} &= n \text{ and permeability} = k \quad \text{in the porous material}
\end{align*}
\]  \hspace{1cm} (2.1.21)

Darcy's law was extended to a non-homogenous porous medium using a statistical approach and then analyzed by singular perturbation (boundary layer) techniques to arrive at the boundary condition at the porous wall:

$$u_{\text{slip}} = \frac{\sqrt{k}}{\alpha} \frac{\partial u}{\partial y} + O(k)$$  \hspace{1cm} (2.1.22)

The statistical approach used was also verified by using it to derive Einstein's law for the viscosity ($\mu^*$) of dilute suspensions of rigid spherical particles as a function of the volume fraction ($\phi$):
\[ \mu^* = \mu (1 + 2.5 \phi) \]  

(2.1.23)

Beavers et al. (1974) proved the existence of a slip velocity even for gas flows in porous-walled ducts but could not conclusively prove the earlier assertion of Beavers and Joseph that \( \alpha \) was a function of the permeable material only. Singh and Laurence used the form of the boundary condition derived by Saffman and presented expressions for the velocity profiles in channel flow bounded by two porous walls (1979a) as well as tube flow (1979b) as the first step in their investigations on the effect of slip velocity on concentration polarization.

2.2 Transport of solutes in porous ducts:

Convection and molecular diffusion are the two important phenomena that together determine the transport of dissolved components in membrane systems. Mass transfer in such systems is described by the convection-diffusion equation. In the absence of external forces, neglecting diffusion in the axial direction, the transport equation for an incompressible fluid at steady state in two dimensions is:

\[ u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2} \]  

(2.2.1)

In a particular geometry of flow, subject to the appropriate boundary conditions, both analytical and numerical solutions can be obtained. Equation (2.2.1) being second order in \( y \) and first order in \( x \), needs two boundary conditions at constant \( y \) and only one at constant \( x \). The usual boundary conditions on \( y \) employed are (Kleinstreuer, 1984):
\[ \frac{\partial c}{\partial y} = 0 \] no flux at solid wall \hspace{1cm} (2.2.2)

\[ D \frac{\partial c}{\partial y} = r v_w c_w \] at the membrane wall \hspace{1cm} (2.2.3)

where \( r \) is the solute rejection efficiency \((r=1\) for perfect retention). Equation (2.2.3) is the statement that at steady-state the convective flux of solute towards the membrane is balanced by the diffusive back transport towards the bulk solution and is the basis of the gel-polarization model (also known as the film-theory model). In such a modeling approach it is thought that the entire resistance to mass transfer occurs in a stagnant film of thickness \( \delta \) (the concentration boundary layer). For flows with symmetry, the following boundary condition should be imposed

\[ \frac{\partial c}{\partial y} = 0 \] at the centerline of the duct \hspace{1cm} (2.2.4)

The boundary condition at constant \( x \) is like an initial condition

\[ c(x=0, y) = c_o \] (uniform inlet concentration profile) \hspace{1cm} (2.2.5)

The solution technique often involves separating the treatment of momentum and mass transfer. In this method, the velocity profiles are first determined and then inserted in the convection-diffusion equation to solve for the concentration profile.

2.2.1 Numerical Solutions: Numerical solutions usually involve a finite difference scheme. Brian (1965) published a numerical analysis of laminar flow in a parallel plate reverse osmosis membrane module with decreasing water flux as solute accumulates on the membrane surface for incomplete
rejection. He used the expressions derived by Berman for the velocity profiles at any cross-section, along with the phenomenological expression for the permeation flux as a function of the pressure drop across the membrane ($\Delta P$) and the osmotic pressure difference between the saline solution at the membrane surface and the product water ($\Delta \pi$) derived by Merten (1963), $K$ being the membrane permeability constant.

$$v_w = K (\Delta P - \Delta \pi) \quad (2.2.6)$$

Brian thus solved Equation (2.2.1) subject to the boundary conditions given by Equations (2.2.3), (2.2.4) and (2.2.5) coupled with (2.2.6). He reported that the average polarization for the constant flux case is very nearly equal to the variable flux case even under conditions where the polarized layer caused the permeation flux to decrease by a factor of five from the channel entrance to the channel exit. Kleinstreuer and Paller (1983) simultaneously solved the coupled momentum and mass transport equations (coupled via the wall permeation rate and the wall concentration) in a plate and frame ultrafiltration system with one porous wall. They divided the semipermeable membrane into $n$ segments and modeled the normal wall velocity as a discrete function varying between each subdivision (but as a constant within each segment). The authors also reported favorable agreement between their computer simulations and experimental results published by Madsen (1977). Singh and Laurence (1979a; 1979b) investigated the effect of the slip velocity on mass transfer in ultrafiltration and reverse osmosis in both channel and tube flows. They used the form of the boundary condition derived by Saffman (Equation
2.1.21) of the order \( \sqrt{k} \) for the axial velocity at the membrane surface and derived expressions for the axial and transverse velocity distributions using a procedure similar to the one followed by Berman (1953). In their analysis, momentum and mass transfer were treated independently by decoupling the governing equations. The slip velocity was found to decrease solute accumulation on the membrane surface and a slip-velocity induced back transport mechanism was proposed.

**2.2.2 Analytical solutions:** Analytical solutions for solute buildup at the surface of a reverse osmosis membrane in both tubular and parallel plate systems exist but are usually cumbersome and difficult to use except for the approximate solution of Dresner (1964) who expressed concentration polarization \( \Gamma (= \frac{c_w}{c_{avg}} - 1) \) for laminar flow between two parallel plates as

\[
\Gamma = 1.536^{\frac{3}{\xi}} \quad \xi < 0.02
\]

\[
\Gamma = \xi + 5(1 - \exp(\frac{\xi}{3})) \quad \xi > 0.02 \tag{2.2.7}
\]

where \( \xi = \frac{v_whx}{3D^2u_o} \) for parallel flow.

Sherwood et al. (1965) analyzed the filtration of an isothermal, incompressible solution of only one salt with constant diffusivity using a perfectly retentive membrane in laminar flow (channel and tube flow) as well as in turbulent flow (tube flow only). They described the velocity field using the zero order solution of Berman for parallel flow and the result obtained by Yuan and Finkelstein for tube flow. Concentration
profiles were expressed as an infinite series expansion. They compared their laminar channel flow results to the approximate solution of Dresner and found good correlation. Concentration polarization in laminar flow between two parallel membranes was shown to be substantially less in constant pressure reverse osmosis systems than that calculated for the constant permeation case by Gill et al. (1965). Unlike Brian's (1965) work they used the initial permeation rate $v_{wo}$ rather than a length averaged value in their comparisons. Johnson and McCutchan (1972) presented data collected from a reverse osmosis system treating sea water using a 1" diameter tubular asymmetric membranes made of cellulose acetate. Their data showed that product water quality and quantity were more sensitive to changes in the flow parameters in the laminar regime than in the turbulent regime. Kozinski and Lightfoot (1972) worked on the ultrafiltration of Bovine Serum Albumin (BSA) using a rotating disk membrane and developed correlations for the non-Newtonian behavior of concentrated solutions of BSA at a pH of 6.7. They also reported that an average value for the viscosity was sufficient in many cases for modeling mass transfer in ultrafiltration processes. The von-Kármán integral method (Schlichting, 1968) was used by Leung and Probstein (1979) while solving the concentration polarization problem for 2-D steady, laminar flow between two prefectly rejecting membranes. In this method the convection-diffusion equation is integrated across the boundary layer and the inner and outer boundary conditions are implemented. Appropriate profiles for the concentration and velocity have to be assumed first and later solved for. They assumed a non-linear dependence of the osmotic pressure with concentration and also a concentration-dependent diffusion coefficient but
neglected the concentration dependence of viscosity based on the results of Kozinski and Lightfoot (1972). They used BSA as a model compound for their ultrafiltration experiments and reported very good correspondence between the model predictions of the permeate flux and the experimental observations over a wide range of pressure differentials.

2.3 Membrane filtration of colloidal suspensions: Mass transfer and subsequent flux decline in the filtration of dissolved solutes has been well described by the gel polarization model discussed in the earlier section (Equation 2.2.3). A diffusivity for spherical particles of radius \( a_p \), in a medium of viscosity \( \mu \), at an absolute temperature \( T \), can be calculated from the Stokes-Einstein relationship:

\[
D = \frac{kT}{6\pi\mu a_p} \tag{2.3.1}
\]

\( k \) being the Boltzmann's constant \((=1.3805 \times 10^{-23}\) J/K). Using a Stokes-Einstein diffusion coefficient, however, grossly underpredicts the flux behavior in the membrane filtration of particulate matter. Thus Blatt et al. (1970) concluded:

1. Particle back-transport to the bulk feed stream is augmented by fluid mechanical effects over that expected from just Brownian diffusion, or

2. The hydraulic resistance of the deposited mass does not limit the transmembrane flow of solvent.

Blatt et al. (1970) favored the latter explanation and proposed that the steady-state cake thickness is determined by a tangential convection of
the deposited particles (the resultant of the fluid shear and non-Newtonian cake rheology) and not by diffusive back-transport. Porter (1972) reported permeate flux data from ultrafiltration experiments with colloidal feeds. Similar permeate fluxes were obtained in the filtration of whole blood (including 8 \( \mu \text{m} \) erythrocytes) and plasma. Observed flux data from the filtration of polystyrene latex \( (a_p = 0.095 \ \mu \text{m}) \) were 38 times higher than that calculated from the gel polarization model \( (c_g = 75\%) \) using a Stokes-Einstein diffusivity of 2.3x10^{-8} \text{cm}^2/\text{sec}. Porter suggested enhanced back-transport to explain these large fluxes and invoked the tubular pinch effect to qualitatively explain this observations. Green and Belfort (1980) termed this the "flux-paradox". In an attempt to resolve the flux-paradox, Green and Belfort invoked an inertial lift mechanism as a means of enhancing diffusive transport of materials away from the membrane surface. Another explanation of this flux-paradox is the concept of a shear-induced diffusion of particles in a concentrated suspension to supplement back transport. These theories are reviewed later in this chapter.

2.3.1 The role of fluid inertia: There have been many excellent reviews on this subject in the past, (Brenner, 1966b; Cox and Mason, 1971; Leal, 1980). The purpose of this section is not to give an exhaustive review of published literature on inertial effects but only to build a background for the particle trajectory model which will be discussed later.

Poiseuille (1836) first observed that blood corpuscles migrated away from the capillary walls. Jeffery (1922) analyzed the motion of ellipsoidal particles in a viscous fluid. He determined the forces acting on the particle, and extended Einstein's work to describe the effect of ellipsoidal particles
on the rheology of the suspending fluid medium. His analysis was restricted to creeping flow. Jeffery solved the approximate linearized equations of motion

\[ \mu \nabla^2 \mathbf{u} - \nabla p = 0 \quad (2.3.2) \]

\[ \nabla \cdot \mathbf{u} = 0 \quad (2.3.3) \]

along with the boundary conditions

\[ \mathbf{u} = \Omega \times \mathbf{r} \text{ at the surface of the ellipsoid} \quad (2.3.4) \]

where \( \mathbf{r} \) is the position vector in an inertial coordinate system with the origin at the center of the ellipsoid and \( \Omega \) is the unknown angular velocity of the particle. Following his solution, Jeffery hypothesized that the ellipsoids move in a fashion so as to minimize the dissipation of energy. The suspension viscosity, \( \mu^* \), was expressed as a function of the volume fraction of the ellipsoids, \( \varnothing_{\text{vol}} \), undergoing laminar motion as

\[ \mu^* = \mu (1 + n \varnothing_{\text{vol}}) \quad (2.3.5) \]

The coefficient, \( n \), was left in an indeterminate form but upper and lower bounds were specified for both oblate and prolate spheroids. Saffman (1956) and later Bretherton (1962) established that the linearity of Equations (2.3.2) - (2.3.4) does not predict a transverse force on a rigid particle translating in one direction. Weak non-linear effects arising from the effects of fluid inertia, non-Newtonian rheology or deformable shape are necessary for the existence of lateral force. The non-uniform radial concentration of rigid spheres in suspensions undergoing Poiseuille flow in
tubes was first reported by Segré and Silberberg (1961). They reported observations from experiments with dilute suspensions ($\varphi \leq 0.4\%$) of monodisperse neutrally buoyant polymethyl methacrylate spheres ($0.4 \text{ mm} \leq a_p \leq 0.8 \text{ mm}$) suspended in a viscous fluid undergoing vertical flow in a straight tube. Spheres were introduced uniformly but were found to migrate in the radial direction and collect in a thin annular region (tubular pinch effect). Karnis et al. (1963) extended this work and reported that the tubular pinch effect is also exhibited by neutrally buoyant, rigid rods and disks. Using singular perturbation techniques Saffman† (1965) calculated the lift force ($F_L$) on a rigid sphere in unbounded simple shear flow with velocity gradient $G$, when its translation velocity ($V$) is parallel to the fluid streamlines as:

$$F_L = \frac{81.2}{4\pi} V a_p^2 \sqrt{\frac{G}{V}}$$  \hspace{1cm} (2.3.6)

When the Stokesian drag ($-6\pi \mu a_p V_{\text{lift}}$) is vectorially added and the total force set to zero an effective lift velocity in unbounded flow is:

$$V_{\text{lift}} = \frac{81.2}{24\pi^2} \frac{V a_p}{\mu} \left(\frac{G \rho}{\mu}\right)^{1/2}$$  \hspace{1cm} (2.3.7)

Karnis et al. (1966) made experiments in both Couette and Poiseuille flow and measured rotation and spin on rigid particles, orbital drifts, radial migration of rigid and deformable particles and also the effect of a concentrated suspension of rigid spheres undergoing tube flow on the

---

† In the original derivation the factor $4\pi$ was omitted. Chang and Harper (1966) corrected the formula.
velocity profile and pressure drop. They verified the results of Segré and Silberberg and reported that deformable particles, regardless of their initial position, migrated towards the tube axis. The development of a particle free layer during Poiseuille flow of a concentrated suspension of rigid spheres was found to result in a blunt velocity profile near the tube axis (zero shear) and also to decrease the apparent viscosity of the suspension. This effect might reduce the energy requirement for the pumping of suspensions through pipes. Brandt and Bugliarello (1966a) made spectacular direct photographic observations of concentrated suspensions \(1.5\% \leq \alpha_{vol} \leq 5\%) of neutrally buoyant, rigid spheres in a long rectangular channel. They reported four regimes of behavior as the suspension flows through the channel:

1. Uniform (random) distribution of spheres at the inlet section.

2. Depletion of particles from a region close to the wall resulting in the formation of a particle free layer adjacent to it. Adjacent to this region is a peak in the particle concentration while in the central core the concentration has increased only slightly over the initial value.

3. Widening of the particle free layer and the formation of a concentrated central core of nearly uniform concentration.

4. Development of instabilities finally resulting in the breakup of the core.

Unfortunately, they were unable to explain their results theoretically.

Goldsmith and Mason (1967) presented an exhaustive review of both theoretical and experimental results pertaining to the rheology of
suspensions. They mainly considered non-Brownian systems and related macroscopic rheological properties to the microscopic properties of both dilute and concentrated suspensions. The first completely general description of the tubular pinch effect was developed by Cox and Brenner (1968). They considered three dimensional Poiseuille flow in the presence of walls and the non-uniformity of fluid shear. Using singular perturbation methods they expressed the force and couple on a particle placed in an arbitrary bounded flow as an expansion in the particle Reynolds number and obtained the general form of the radial migration velocity. The only restriction in their theory is that the body should not be too close to the walls. Owing to their complex structure, some of the numerical coefficients were not evaluated. A more detailed description of their theory is postponed to a later section (section 3.3.3). Cox and Mason (1971) reviewed the behavior of rigid and deformable particles of various cross sections in both steady and unsteady flow through tubes of circular cross section. Lateral migration of neutrally buoyant rigid spheres in simple shear and two dimensional Poiseuille flow was studied theoretically by Ho and Leal (1974). The lateral force was expressed in terms of the lateral position s, fluid density ρ, the particle radius a_p, the non-dimensional particle size κ (=a_p/h, h is the distance between the parallel walls) and the mean velocity V_{mean} as:

\[ F_{\text{lift}} = \rho V_{\text{mean}}^2 a_p^2 \kappa^2 G(s) \] (2.3.8)

where the function
\[ G(s) = \begin{cases} 
4G_1(s) & \text{for simple shear} \\
36(1-s)^2 G_1(s) - 36(1-2s)G_2(s) & \text{for 2-D Poiseuille flow} 
\end{cases} \] (2.3.9)

The functions \( G_1(s) \) and \( G_2(s) \) were tabulated by Ho and Leal. \( G(s) \) is depicted below in graphical form in Figure 2.3.1. It is seen that for simple shear \( G(s)=0 \) at the channel axis and for the case of 2-D Poiseuille flow \( G(s)=0 \) at \( s=0.2, 0.5 \) and 0.8. The mid-channel is an unstable equilibrium point while \( s=0.2 \) and 0.8 are stable lateral positions. These agree well with the observations of Halow and Wills (1970a; 1970b) in their Couette flow studies where they found stable equilibrium at \( 0.5 \leq s \leq 0.55 \). Surprisingly, this theory also predicts the equilibrium positions observed by Segré and Silberberg who had done experiments with a circular tube.

![Graph of \( G(s) \) for simple shear and 2-D Poiseuille flow](image)

Figure 2.3.1 Dimensionless lateral force as calculated by Ho and Leal. The dotted line is for the case of simple shear flow and the full line is for the case of 2-D channel Poiseuille flow.
In addition to calculating lift forces on single spheres they also
derived expressions for the dimensionless steady state concentration
distributions \( \varphi(s)/\varphi_m \) for small particles under the opposing forces of
inertia (which tends to crowd them in a preferred axial position) and
Brownian motion (which tends to smoothen out any concentration
gradients). Equation 2.3.10 is the expression derived by Ho and Leal for
the steady state concentration distribution. The form shown here is a slight
adaptation of the original expression where the lower limit of integration
was set to 0.5. \( \varphi(s) \) represents the particle concentration at a dimensionless
distance, \( s \), from the wall and \( \varphi(m) \) is a mean concentration as defined in
Equation (2.3.11).

\[
\varphi(s) = \varphi_m \frac{\exp \left( \int_{0}^{s} K G(s') ds' \right)}{1 \int_{0}^{1} \exp \left( \int_{0}^{s''} K G(s') ds' \right) ds''}
\]

(2.3.10)

where the mean concentration \( \varphi_m = \int_{0}^{1} \varphi(s') ds' \)

(2.3.11)

and \( K \) is a parameter describing the relative importance of inertial lift to
Brownian diffusion.

\[
K = \frac{\text{Inertial lift}}{\text{Brownian diffusion}} = \frac{\text{Re_p} \kappa^2 U_m h}{\text{D}}
\]

(2.3.12)

Figure 2.3.2 shows steady state concentration distributions for
suspensions undergoing Poiseuille flow in a rectangular channel. For large
values of $K$, sharp concentration peaks are observed at the stable preferred lateral positions (inertia controlled), smaller values of $K$ tend to smooth out any preferred positions (diffusion controlled). Vasseur and Cox (1976) studied the migration of a sphere bounded by two parallel vertical plane walls. Their results are thus applicable to both Couette flow and plane Poiseuille flow. They analyzed both neutrally buoyant and non-neutrally buoyant spheres as well as freely rotating and non-rotating particles. They expressed the lateral migration velocities in terms of triple integrals involving the Green's function for creeping flow in the presence of the given boundaries.

Figure 2.3.2 Concentration distributions of neutrally buoyant suspensions subject to a lift force and simultaneous Brownian motion. $K$ is the ratio of the effect of inertial lift and Brownian diffusion. Large $K$ indicates an inertia controlled system leading to preferred positions. Increasing the importance of diffusion blurs any concentration gradients. In generating this plot, the polynomial fit for the function developed by Vasseur and Cox (See table 2.3.1) was used instead of $G(s)$ from Equation 2.3.9.
The important assumptions under which Vasseur and Cox derived the expressions for the lateral velocity are:

1. The sphere is not too close to the wall.

2. The dimensionless particle size $\kappa$ is small so that the particle can be approximated by a point force.

3. $\text{Re}_p/\kappa \ll 1$, so that only the inner expansion needs to be considered for calculating the inertia induced velocity.

Table 2.3.1 shows the expressions derived by Vasseur and Cox for the lift velocity on particles in the rectangular channel in terms of the volume integrals.

Table 2.3.1 General forms for the lift velocity derived by Vasseur and Cox

<table>
<thead>
<tr>
<th>Expression†</th>
<th>Validity</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{\text{lift}} = \frac{\kappa^2 a_p U_m^2}{V} h_1(\beta)$</td>
<td>Neutrally buoyant sphere in simple shear or Poiseuille flow, either freely rotating or purely translating particle.</td>
</tr>
<tr>
<td>$V_{\text{lift}} = \text{Re}_p U_m h_2(\beta)$</td>
<td>Non-neutrally buoyant sphere in simple shear or Poiseuille flow, either freely rotating or purely translating particle.</td>
</tr>
</tbody>
</table>

† $h_1(\beta)$ and $h_2(\beta)$ are volume integrals

$\text{Re}_p$ defined for a non-neutrally buoyant sphere as $a_p V/V$; where $V$ is the upward velocity due to gravity in an quiescent unbounded fluid.

The volume integral for the case of a neutrally buoyant sphere allowed to rotate in plane Poiseuille flow was evaluated by Otis (1986) and a sixth order polynomial fit was obtained (see section 3.3.2). Cox and Hsu (1977) obtained a solution for the lift velocity for a neutrally buoyant sphere
suspended in Poiseuille flow in the presence of a plane wall. For a freely rotating particle their solution is:

\[ V_{\text{lift}} = \frac{\kappa^2 a_p U_m^2}{v} \times \frac{5}{72} (1 - 2\beta) (22 - 146\beta) \]  \hspace{1cm} (2.3.13)

This result is compared to the functional form, \( G(s) \), obtained by Ho and Leal (Equation 2.3.9. for plane Poiseuille flow) and to the corresponding volume integral of Vasseur and Cox in Figure 2.3.3. The divergence of the solution obtained by Ho and Leal near the plane wall was thought to be arise from poor numerical convergence.

Figure 2.3.3 Comparison of solutions for a freely rotating neutrally buoyant sphere in 2-D vertical Poiseuille flow given by Ho and Leal and Vasseur and Cox. The solution given by Cox and Hsu for the lift velocity for a freely rotating neutrally buoyant sphere in the presence of a single plane wall is also given as the asymptotic solution valid near the plane boundaries.
2.3.2 Orthokinetic effects:

2.3.2.1 Convective flow models: The approach favored by Blatt et al. (1970) to explain steady state concentration polarization did not receive much attention until the work of Leonard and Vassilieff (1984). They divided the membrane module in two distinct regions:

1. The bulk feed, where the concentration was assumed to be uniformly equal to \( c_b \).
2. The deposited layer on the membrane surface where the concentration was set at the wall value based on closest possible packing, \( c_w \).

By proposing a shear-induced convective flow mechanism for the removal of accumulated material (i.e. completely neglecting back diffusion and inertial lift) they were able to solve for the boundary that separates the two regions (the concentration boundary layer) at steady state. In a later work (Vassilieff et al., 1985) they expressed the flux, \( J \), that would occur under pressure independent conditions as a function of the wall shear rate, \( \gamma_w \):

\[
J = \left( \frac{c_w}{c_b} - 1 \right) \frac{\gamma_w}{2L} H^2 \quad (2.3.14)
\]

where \( H \) is a function describing the thickness of the resisting particle layer.

\[
H = \begin{cases} 
\text{constant} & \text{for } H < H_{\text{critical}} = 25 \, \mu m \\
\infty & \text{for } H > H_{\text{critical}} = 25 \, \mu m 
\end{cases} \quad (2.3.15)
\]
Davis and Birdsell (1987a) adopted a similar approach of a flowing cake to explain the results of their experiments at high shear rates with neutrally buoyant acrylic latex particles that were 150 to 212 \( \mu \)m in diameter. They treated the flowing cake as Newtonian and used a constant volume fraction (\( \varphi = 0.45 \)) for the cake layer.

2.3.2.2 Shear-induced back-transport models: Eckstein et al. (1977) experimentally determined correlations for the self-diffusion coefficient arising from particle-particle interactions for concentrated suspensions in simple shear flow. Particles suspended in simple shear have both translational and rotary motion. Every particle therefore has a viscous boundary layer associated with it which causes a drag force on neighboring particles. Particles associated with different streamlines have different velocities. Interactions of the velocity fields associated with the viscous layer between particles when overtaking are irreversible and a net lateral migration occurs. By directly viewing the lateral position of labeled particles in a Couette device (with a gap width \( W \)) at a fixed spatial position and measuring the time for consecutive observations, Eckstein and coworkers were able to correlate the self-diffusion coefficient for neutrally buoyant spheres (of radius \( a_p \)) in concentrated suspensions with volume fraction \( \varphi_{\text{vol}} \) and the shear rate (\( du/dy \)). Assuming an unbounded flow (for small values of \( a_p/W \) and \( a_p/y \)) they correlated the diffusion coefficient \( D \) as

\[
D = \begin{cases} 
0.02 \frac{a_p^2}{dy} \varphi_{\text{vol}} & 0 < \varphi_{\text{vol}} < 0.2 \\
0.025 \frac{a_p^2}{dy} & 0.2 < \varphi_{\text{vol}} < 0.5 
\end{cases} \tag{2.3.16}
\]
Zydney and Colton (1986) in trying to explain plasmapheresis of concentrated plasma (40% erythrocytes) used Eckstein’s correlation for a shear-enhanced particle diffusivity (rather than just a Brownian diffusivity) and Leveque’s correlation for the boundary layer thickness to obtain the following expression (derived from film theory) for the length averaged permeate flux, $J$, in microfiltration:

$$J = 0.078 \left( \frac{a_p^4}{L} \right)^{1/3} \gamma_w \ln \left( \frac{c_w}{c_b} \right)$$  \hspace{1cm} (2.3.17)

They reported good agreement between the predictions of Equation (2.3.17) and experimental plasmapheresis data but correspondence was poor for the microfiltration of other colloidal suspensions like clay and latex.

Leighton and Acrivos (1987a) developed a technique to measure the shear-induced self diffusivity of a particle in concentrated suspensions at low Reynolds numbers. Their procedure did not involve a measurement of the exact lateral position of the labeled particle but only involved measuring the variations in the transit time to complete successive circuits in the Couette device. They showed that the assumption of unbounded flow was violated in the earlier work of Eckstein and that wall effects lead to an underestimation of the diffusion coefficient. Their results for the shear-enhanced particle diffusivity can be expressed as (1987b)

$$D \approx \left| \frac{d u}{d y} \right| a_p^2 0.33 \varphi^2 \left( 1 + 0.5 e^{8.8 \varphi} \right) \quad 0 \leq \varphi \leq 0.5$$  \hspace{1cm} (2.3.18)
For small volume fractions, $\phi$, there was a considerable spread in the experimental data (25 - 50%) and this expression was considered to be only a rough approximation that probably underestimates particle diffusivity. The diffusivities calculated from Equation 2.3.18 can be compared with those calculated from the Stokes-Einstein relationship (see Equation 2.3.1). For a particle in a concentrated suspension ($\phi=0.4$) with $a_p = 1.0 \, \mu m$ in a shear field of 1000 sec$^{-1}$, the shear-induced diffusivity is $1.8 \times 10^{-5}$ cm$^2$/sec; which is $10^4$ times greater than the Stokes-Einstein prediction of $2 \times 10^{-9}$ cm$^2$/sec. Also, at a shear rate of 24 sec$^{-1}$, Leighton and Acrivos correlated the suspension viscosity of 46 $\mu m$ spheres as

$$\mu(\phi) = \left[1 + 1.5 \frac{\phi}{1 - \phi / 0.58}\right]^2 \quad \phi \leq 0.5 \quad (2.3.19)$$

Using these correlations Leighton and Acrivos (1986) were able to describe the resuspension of a previously settled layer of negatively buoyant particles. They found that even under conditions of small Reynolds numbers, viscous effects (not associated with turbulence) play an important role in particle transport. It was shown that when a shear stress was applied, the settled layer expanded in height, was entrained in the bulk flow and was convected away. At equilibrium, they equated the downward flux of particles to the shear-induced diffusive flux and were able to predict the height of the settled layer in their experiments quite well. Davis and Leighton (1987b) developed a "local" model (valid at a specified axial coordinate) for the crossflow microfiltration of particle suspensions using this concept of viscous resuspension (due to the shear-induced diffusivity) and also considering the convective transport of the cake along the
membrane surface. The diffusive transport in this case is balanced by a convective flux rather than a gravity flux (the case in the original paper). In this work they considered non-uniform particle concentration and non-linear velocity profiles in the cake. The viscosity was modeled using Equation 2.3.19 as a function of the particle volume fraction rather than as a constant in the earlier work. This local model was generalized into a global model by Romero and Davis (1988) to predict the permeate flux as a function of the axial coordinate and the thickness of the cake layer. This model also predicts the existence of a stagnant particle layer underneath the flowing layer that provides the major resistance to permeate flow.
Chapter 3

Theoretical Analysis

3.1 Mathematical Modeling of Fluid Flow:

3.1.1 Problem formulation: Consider the laminar flow of an incompressible fluid of density ρ and kinematic viscosity ν in a channel of rectangular cross section having one permeable boundary; the other boundary is solid. One side of the cross section (the width) is much greater than the other side (the height) so that the flow can be treated as effectively being two dimensional. The coordinate system used for the description of the problem is given in Figure 3.1.1. The channel is of length L and height h. The axial distance coordinate, measured from the channel entrance, is denoted by x. y represents the coordinate axis orthogonal to the channel walls measured from the non-porous wall. u and v represent the velocity components in the x and y directions respectively.

![Diagram](image)

Figure 3.1.1 The coordinate system used in the solution of the 2-D, steady state Navier-Stokes equations.
If there are no external forces acting on the fluid, at steady state we can write the Navier-Stokes equations for this system as:

\[
\begin{align*}
\mathbf{u} \frac{\partial \mathbf{u}}{\partial x} + v \frac{\partial \mathbf{u}}{\partial y} &= -\frac{1}{\rho} \frac{\partial P}{\partial x} + v \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \quad (3.1.1) \\
\mathbf{u} \frac{\partial \mathbf{v}}{\partial x} + v \frac{\partial \mathbf{v}}{\partial y} &= -\frac{1}{\rho} \frac{\partial P}{\partial y} + v \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) \quad (3.1.2)
\end{align*}
\]

Equation (3.1.1) and (3.1.2) express the transfer of momentum in the x and y directions respectively. The continuity equation is:

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (3.1.3)
\]

Let \( \lambda (= y/h) \) be the non-dimensional variable in the y direction. Equations (3.1.1), (3.1.2) and (3.1.3) transform into:

\[
\begin{align*}
\mathbf{u} \frac{\partial \mathbf{u}}{\partial x} + \frac{v}{h} \frac{\partial \mathbf{u}}{\partial \lambda} &= -\frac{1}{\rho} \frac{\partial P}{\partial x} + v \left( \frac{\partial^2 u}{\partial x^2} + \frac{1}{h^2} \frac{\partial^2 u}{\partial \lambda^2} \right) \quad (3.1.4) \\
\mathbf{u} \frac{\partial \mathbf{v}}{\partial x} + \frac{v}{h} \frac{\partial \mathbf{v}}{\partial \lambda} &= -\frac{1}{\rho h} \frac{\partial P}{\partial \lambda} + v \left( \frac{\partial^2 v}{\partial x^2} + \frac{1}{h^2} \frac{\partial^2 v}{\partial \lambda^2} \right) \quad (3.1.5) \\
\frac{\partial \mathbf{u}}{\partial x} + \frac{1}{h} \frac{\partial \mathbf{v}}{\partial \lambda} &= 0 \quad (3.1.6)
\end{align*}
\]

The following physically meaningful boundary conditions complete the mathematical description of the problem.

\[
\begin{align*}
u(\lambda=0) &= 0 \quad (3.1.7) \\
v(\lambda=0) &= 0 \quad (3.1.8) \\
v(\lambda=1) &= v_w \quad (3.1.9) \\
u(\lambda=1) &= u_{\text{slip}} \quad (3.1.10)
\end{align*}
\]
Equations (3.1.7) and (3.1.8) are the no-slip (adherence) criteria for the flow of a viscous fluid past a solid surface. Equation (3.1.9) mathematically describes the assumption of constant permeation rate, \( v_w \). In a real membrane module there exists a pressure drop across the length of the duct. Thus if the membrane is cast with a constant permeability then we can expect the permeation rate to decrease along the length of the duct. We can get a constant permeation rate if the permeability of the membrane increases along the length of the duct. However, all real membranes are cast with uniform permeability and so the assumption of uniform permeation rate is only an approximation. In describing the slip velocity that may exist when a fluid flows past a permeable surface the model proposed by Saffman (1971) will be used (Equation 2.1.22), neglecting the \( O(k) \) term. We therefore describe the slip velocity as being proportional to the shear rate.

\[
\begin{align*}
 u (\lambda=1) &= u_{\text{slip}} = -\frac{\sqrt{k}}{\alpha h} \frac{\partial u}{\partial \lambda} \\
&= 3.1.11
\end{align*}
\]

3.1.2 Perturbation Solution: Berman (1953) described a solution technique for the similar problem of flow between two equally permeable walls. His technique will be used to derive velocity profiles for the flow geometry under consideration. For incompressible flows, the velocity vector \( \mathbf{v} \) can be expressed in terms of a vector potential \( \Psi \) as:

\[
\mathbf{v} = \nabla \times \Psi
\]

(3.1.12)

In two dimensions, in terms of the scalar stream function \( \psi \), we write:
\[ u = \frac{\partial \psi}{\partial y} = \frac{1}{h} \frac{\partial \psi}{\partial \lambda} \quad (3.1.13) \]
\[ v = -\frac{\partial \psi}{\partial x} \quad (3.1.14) \]

Let \( u_o \) represent the uniform inlet velocity. We introduce a stream function from a mass balance on the fluid in the channel as:
\[ \psi = [h u_o - v_w x] f(\lambda) \quad (3.1.15) \]

where \( f(\lambda) \) is an unknown function of the distance coordinate \( \lambda \).

Substituting Equation (3.1.15) into Equations (3.1.13) and (3.1.14) expressions are obtained for the velocity components as:
\[ u = \left( u_o - \frac{v_w x}{h} \right) f'(\lambda) \quad (3.1.16) \]
\[ v = v_w f(\lambda) \quad (3.1.17) \]

When Equations 3.1.16 and 3.1.17 are substituted into Equations (3.1.4) and (3.1.5) we obtain:
\[ \left( u_o - \frac{v_w x}{h} \right) \left\{- \frac{v_w}{h} \left[ (f')^2 - ff' \right] - \frac{v}{h^2} f'' \right\} = -\frac{1}{\rho} \frac{\partial P}{\partial x} \quad (3.1.18) \]
\[ \frac{v_w^2}{h} f f' - \frac{v v_w}{h^2} f''' = -\frac{1}{\rho h} \frac{\partial P}{\partial \lambda} \quad (3.1.19) \]

We note that the left hand side of Equation (3.1.19) is a function of \( \lambda \) only (i.e. independent of \( x \)). Assuming the pressure is twice differentiable we can differentiate Equation (3.1.19) w.r.t. \( x \) to get:
\[ \frac{\partial^2 P}{\partial x \partial \lambda} = 0 \quad (3.1.20) \]
or \( \frac{\partial^2 p}{\partial \lambda \partial x} = 0 \) \hspace{1cm} (3.1.21)

Using this result we obtain Equation 3.1.22 upon differentiating Equation (3.1.18):

\[
\left( u_o - \frac{v_w}{h} \frac{x}{h} \right) \frac{\partial}{\partial \lambda} \left[ \frac{v_w}{h} \left[ (f')^2 - f f'' \right] + \frac{v}{h^2} f''' \right] = 0
\]

(3.1.22)

This equality should be valid for all values of \( x \) and thus,

\[
\frac{\partial}{\partial \lambda} \left[ \frac{v_w}{h} \left[ (f')^2 - f f'' \right] + \frac{v}{h^2} f''' \right] = 0
\]

(3.1.23)

Integrating Equation (3.1.23) and multiplying by \( \frac{h^2}{v} \) we get the ordinary differential equation:

\[
\frac{v_w h}{v} \left[ (f')^2 - f f' \right] + f''' = C
\]

(3.1.24)

where \( C \) is the constant of integration.

Defining a wall Reynolds number \( Re_w = \frac{v_w h}{v} \), we can rewrite Equation (3.1.24) as,

\[
Re_w \left[ (f')^2 - f f' \right] + f''' = C
\]

(3.1.25)

Equation (3.1.25) is a third order, non-linear ordinary differential equation with an unknown constant \( C \). Therefore we still need four boundary conditions to correctly pose the problem. Boundary conditions (3.1.7) - (3.1.9) are now expressed in terms of \( f(\lambda) \):

\[
f'(\lambda = 0) = 0
\]

(3.1.26)
\begin{align*}
f(\lambda=0) &= 0 \\
f(\lambda=1) &= 1 \tag{3.1.27} \\
\text{Transforming (3.1.11) in terms of } f(\lambda) \text{ we get} \\
f'(\lambda=1) &= -\frac{\sqrt{k}}{\alpha h} f''(\lambda=1) \tag{3.1.29} \\
\text{We define the slip coefficient } \vartheta = \frac{\sqrt{k}}{\alpha h}, \text{ and rewrite Equation (3.1.29) as} \\
f'(\lambda=1) &= -\vartheta f''(\lambda=1) \tag{3.1.30} \\
\text{Equation (3.1.25) with the associated boundary conditions (3.1.26) - (3.1.29) constitute a solution to the fluid flow problem as constructed. For small values of } Re_w, \text{ an approximate solution can be obtained using regular perturbation theory (Logan, 1987) using } Re_w \text{ as the perturbation parameter. As the first step in such a solution technique we express the unknowns in the form of a perturbation series in the parameter } Re_w \text{ of the form:} \\
f(\lambda) &= f_o(\lambda) + Re_w f_1(\lambda) + Re_w^2 f_2(\lambda) + \ldots + Re_w^n f_n(\lambda) + \ldots \tag{3.1.31} \\
C &= C_o + Re_w C_1 + Re_w^2 C_2 + \ldots + Re_w^n C_n + \ldots \tag{3.1.32} \\
\text{where } f_i \text{ and } C_i \text{ are independent of } Re_w. \text{ Substituting (3.1.31) and (3.1.32) into Equation (3.1.25) and collecting the corresponding powers of } Re_w, \\
f_o''' &= C_o \tag{3.1.33} \\
f_1''' &= C_1 + f_o f_o'' - (f_o')^2 \tag{3.1.34} \end{align*}
\[ f_2''' = C_2 - 2f'_0 f'_1 + f''_0 f'_1 + f''_1 f_1 \] (3.1.35)

Equation (3.1.33) is the unperturbed problem and its solution gives the leading order term in the perturbation series expansion. Subsequent equations have information on the correction terms of order \( \text{Re}_w \) and \( \text{Re}_w^2 \) respectively. We now express the "lumped" boundary conditions (3.1.26) - (3.1.30) in terms of each term in the series expansion.

\[ f'(0) = 0 \quad \Rightarrow \quad f'_i(0) = 0 \quad \forall \ i \] (3.1.36)
\[ f(0) = 0 \quad \Rightarrow \quad f_i = 0 \quad \forall \ i \] (3.1.37)
\[ f(1) = 1 \quad \Rightarrow \quad f_0 = 0 \text{ and } f_i = 0 \quad \text{for } i \geq 1 \] (3.1.38)
\[ f'(1) = -\varnothing f''(1) \quad \Rightarrow \quad f'_i = -\varnothing f''_i \quad \forall \ i \] (3.1.39)

Equations (3.1.33), (3.1.34) and (3.1.35) along with the boundary conditions given by (3.1.36) - (3.1.39) can be readily solved to give the approximate solution to any degree of accuracy. The solution to the unperturbed problem is (i.e. \( f'_0 \) is the leading order term):

\[ f'_0 = -\frac{2(1 + \varnothing)}{(1 + 4\varnothing)} \lambda^3 + \frac{3(1 + 2\varnothing)}{(1 + 4\varnothing)} \lambda^2 \] (3.1.40)

The first correction term (the first order solution) is obtained knowing the leading order term and is given below as Equation (3.1.41).

\[ f_1 = K_1 \frac{\lambda^3}{6} + K_2 \frac{\lambda^2}{2} - \frac{12(1 + \varnothing)^2}{210(1 + 4\varnothing)^2} \lambda^7 + \frac{(1 + \varnothing)(1 + 2\varnothing)}{5(1 + 4\varnothing)^2} \lambda^6 - \frac{3(1 + 2\varnothing)^2}{10(1 + 4\varnothing)^2} \lambda^5 \]

where \( K_1 \) and \( K_2 \) are constants that depend only on the slip coefficient.
\[ K_1 = \frac{-1}{(1 + 4\omega)^3} \left\{ \frac{24(1+\omega)^3}{35} - \frac{12(1+\omega)^2(1+2\omega)}{5} + \frac{36(1+\omega)(1+2\omega)^2}{10} - \frac{12(1+\omega)^2(1+6\omega)}{5} + \frac{36(1+\omega)(1+2\omega)(1+5\omega)}{5} - 9(1+4\omega)(1+2\omega)^2 \right\} \quad (3.1.42) \]

\[ K_2 = \frac{1}{(1 + 4\omega)^3} \left\{ \frac{12(1+2\omega)(1+\omega)^2}{35} - \frac{4(1+\omega)^2(1+5\omega)}{5} - \frac{6(1+\omega)(1+2\omega)^2}{5} + \frac{9(1+2\omega)^3}{5} - \frac{12(1+\omega)(1+2\omega)(1+5\omega)}{5} - 3(1+4\omega)(1+2\omega)^2 \right\} \quad (3.1.43) \]

The velocity profiles can now be written as:

\[ u(x, \lambda) = \left( u_o - \frac{v_w x}{h} \right) \left( f_o + Re_w f_1 \right) \quad \text{and} \quad (3.1.44) \]

\[ v(\lambda) = v_w \left( f_o + Re_w f_1 \right) \quad (3.1.45) \]

3.1.3 Discussion on fluid mechanics: We shall now inspect the change in the solution brought about by the inclusion of the first correction term. The zero and first order solutions for the mid-channel axial and transverse velocity profiles as described by this model are graphically presented in Figures 3.1.2 and 3.1.3 respectively for conditions that might be encountered in the ultrafiltration of a water \( (u_o = 40 \text{ cm/sec}, v_w = 0.01 \text{ cm/sec}, \omega = 0, \text{height} = 760 \mu\text{m}, v = 0.01 \text{ cm}^2/\text{sec}) \). This corresponds to a wall Reynolds number (perturbation parameter) of 0.076.
Figure 3.1.2 Comparison of the zero and first order solutions of the axial velocity at mid-channel. Note that the two curves overlap indicating that convergence is attained even by the inclusion of only the first order correction term of $O(Re_w)$.

Figure 3.1.3 Comparison of the zero and first order solutions of the transverse velocity at mid-channel. Inclusion of only the first order correction term of $O(Re_w)$ is justified by the convergence observed.

The velocities have been normalized using the local maximum values. There is very good convergence and the two solutions are practically
identical. On this basis we can truncate the solution to include only two terms in the series expansion.

The effect of the slip coefficient on the velocity profiles is illustrated in Figures 3.1.4 and 3.1.5. Values used for the mean inlet velocity \( u_o = 150 \text{ cm/sec} \) and average permeation rate \( v_w = 0.06 \text{ cm/sec} \) are typical of microfiltration. The no-slip case corresponds to \( \varphi = 0 \). Increasing slip leads to flatter profiles and reduced wall shear stresses. Also, it is seen that the slip velocity is more sensitive to changes in the slip coefficient for small values and seems to approach an asymptotic value for large slip coefficients (Singh and Laurence, 1979a).

![Graph showing influence of slip coefficient on velocity profile](image)

**Figure 3.1.4** Influence of the slip coefficient on the mid-channel axial velocity profile that might exist in a parallel plate microfilter. Increasing slip reduces velocity gradients near the porous wall.
Figure 3.1.5 Effect of axial slip velocity on the mid-channel transverse velocity profile

Table 3.1.1 Estimates of the slip velocity in membrane systems.

<table>
<thead>
<tr>
<th>Conditions</th>
<th>Process</th>
<th>( v_w ) (m/sec)</th>
<th>( \Delta P ) (Pa)</th>
<th>( \Delta x ) (m)</th>
<th>( k ) (m²)</th>
<th>( \varnothing ) (k¹/² cm)</th>
<th>( u_{\text{max}} ) (m/sec)</th>
<th>( u_{\text{slip}} ) (m/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>RO</td>
<td>10⁻⁵</td>
<td>3x10⁶</td>
<td>0.2x10⁻⁶</td>
<td>6.7x10⁻²²</td>
<td>5x10⁻⁸</td>
<td>0.15</td>
<td>1.5x10⁻⁸</td>
</tr>
<tr>
<td></td>
<td>UF</td>
<td>10⁻⁴</td>
<td>3.5x10⁵</td>
<td>1x10⁻⁶</td>
<td>2.9x10⁻¹⁹</td>
<td>10⁻⁶</td>
<td>1</td>
<td>2x10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>MF</td>
<td>6x10⁻⁴</td>
<td>10⁵</td>
<td>10⁻⁶</td>
<td>6x10⁻¹⁸</td>
<td>5x10⁻⁶</td>
<td>2</td>
<td>2x10⁻⁶</td>
</tr>
<tr>
<td></td>
<td>MF with</td>
<td>6x10⁻⁴</td>
<td>10⁵</td>
<td>5x10⁻⁶</td>
<td>3x10⁻¹⁷</td>
<td>1x10⁻⁵</td>
<td>2</td>
<td>4x10⁻⁵</td>
</tr>
</tbody>
</table>

channel height = 5x10⁻³ m  
\( \alpha = 0.1 \)  
\( \mu_{\text{water}} = 10^{-3} \text{ N.s/m}^2 \)

Table 3.1 shows calculations on the slip velocity in typical membrane filtration applications. It is important to note that the slip velocity plays a negligible role at the free membrane surface. However, in
a membrane system with mass transfer, the slip velocity may play a role in determining subsequent deposition at the surface of a loosely packed concentration polarization layer where the permeability may be high.

To help in flow visualization streamlines for laminar flow can be plotted. Define the dimensionless stream function $\Psi (x, \lambda)$ as:

$$\Psi (x, \lambda) = \frac{\psi (x, \lambda)}{hu_o} = \left(1 - \frac{v_w x}{hu_o}\right)[f_o(\lambda) + Re_w f_1(\lambda)]$$  

(3.1.46)

Define an entrance Reynolds number based on the average influent velocity

$$Re_{ent} = \frac{u_o h}{v}$$  

(3.1.47)

The non-dimensional stream function is expressed in terms of the entrance and wall Reynolds numbers as:

$$\Psi (x, \lambda) = \left(1 - \frac{Re_w}{Re_{ent}} \frac{x}{h}\right)[f_o(\lambda) + Re_w f_1(\lambda)]$$  

(3.1.48)

Non-dimensional streamlines are plotted in Figure 3.1.6 for a microfiltration apparatus with the no-slip boundary condition. ($U_o=75$ cm/sec, $v_w=0.06$ cm/sec, $\theta=0$, height=760 $\mu$m, $v=0.01$ cm$^2$/sec).
Figure 3.1.6 Streamlines for laminar flow in the channel ($\sigma=0$). Fluid flow parameters typical of microfiltration ($U_o=75$ cm/sec, $V_w=0.06$ cm/sec, height=760 $\mu$m, length=50 cm). No-slip condition at the porous wall. Note that the streamlines are orthogonal to the porous boundary.

Figure 3.1.7 is a similar plot using the same parameters used in generating Figure 3.1.6 except the no-slip assumption has been relaxed. A value of the slip coefficient, $\sigma=0.2$ was used. We note that in this case the streamlines are no longer orthogonal to the membrane surface. This is an essential result because the tangential velocity at the membrane surface is the normal derivative of the streamline. Skewness results in a non-zero normal derivative resulting in a finite slip velocity.
Figure 3.1.7 Streamlines for laminar flow in the channel (\( \sigma = 0.2 \)). Fluid flow parameters typical of microfiltration (\( U_o = 75 \) cm/sec, \( V_w = 0.06 \) cm/sec, height=760 \( \mu \)m length=50 cms). Slip boundary condition at the porous wall (\( \sigma = 0.2 \)). Note that the streamlines are skewed to the porous boundary indicating the existence of a tangential velocity component.

3.2 Mass transfer of Brownian components:

3.2.1 Set-up of the governing equations: Consider the steady flow of an incompressible fluid between two infinite parallel boundaries one of which is porous. Let the width of the channel be much larger than the height. Under these conditions, when there are no external forces acting on the fluid, the convection-diffusion equation that governs mass transfer can be written in two dimensions as:

\[
u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = D \left( \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right)
\]  

(3.2.1)

Define the dimensionless variables
\[ u = \frac{u}{u_o}, \quad v = \frac{v}{v_w}, \quad c = \frac{c}{c_o}, \quad x = \frac{x}{x_o} \text{ and } \lambda = \frac{v}{h} \quad (3.2.2) \]

where \( c_o \) is the uniform inlet concentration. \( u_o \) and \( v_w \) have been defined before. \( x_o \) is an unspecified reference parameter used for non-dimensionalizing the axial distance coordinate. We shall first try to express \( x_o \) in terms of all other physical parameters in the problem. Introducing (3.2.2) in Equation (3.2.1)

\[ \left( \frac{u u_o c_o}{x_o} \right) \frac{\partial c}{\partial x} + \left( \frac{v v_w c_o}{h} \right) \frac{\partial c}{\partial \lambda} = D \left[ \frac{c_o}{x_o^2} \frac{\partial^2 c}{\partial x^2} + \frac{c_o}{h^2} \frac{\partial^2 c}{\partial \lambda^2} \right] \quad (3.2.3) \]

multiply Equation (3.2.3) by \( \frac{x_o}{u_o c_o} \) to get

\[ u \frac{\partial c}{\partial x} + \frac{x_o v_w}{hu_o} v \frac{\partial c}{\partial \lambda} = D \left[ \frac{1}{u_o x_o} \frac{\partial^2 c}{\partial x^2} + \frac{x_o}{h^2 u_o} \frac{\partial^2 c}{\partial \lambda^2} \right] \quad (3.2.4) \]

Note that we have now put the convection-diffusion equation in a non-dimensional form. To eliminate the unknown reference quantity, \( x_o \), we set the dimensionless group \( \frac{x_o v_w}{hu_o} \) to equal unity. Hence, in terms of the known (specified) parameters in the problem, \( x_o \), is written as:

\[ x_o = \frac{hu_o}{v_w} \quad (3.2.5) \]

Substitute Equation (3.2.5) in Equation (3.2.4) and rearranging:

\[ u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial \lambda} = \frac{D v_w}{v_w h} \left[ \frac{v_w^2}{u_o^2} \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial \lambda^2} \right] \quad (3.2.6) \]
Typically, $v_w = u_o$ in membrane systems with tangential-flow. Hence $(v_w^2/u_o^2) \ll 1$ and therefore the term $\frac{v_w^2}{u_o^2} \frac{\partial^2c}{\partial x^2}$ is much smaller than $\frac{\partial^2c}{\partial \lambda^2}$ in Equation (3.2.6). We therefore can neglect diffusion in the axial direction compared to diffusion in the transverse direction. Thus, the simplified form of the convection-diffusion equation becomes:

$$u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial \lambda} = \frac{D}{v_w h} \frac{\partial^2 c}{\partial \lambda^2} \tag{3.2.7}$$

In operating parallel plate membrane modules, there exists a characteristic distance dimension in the axial direction; the channel length, $L$. We therefore non-dimensionalize the $x$ coordinate by this reference quantity in subsequent analysis. We now establish a finite difference scheme for solving the two-dimensional mass transfer problem under steady state conditions where we neglect axial diffusion.

Consider the convection-diffusion equation in dimensional form,

$$u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2} \tag{3.2.8}$$

subject to the boundary conditions

$$\frac{\partial c}{\partial y} = 0 \quad y = 0 \quad \forall x \tag{3.2.9}$$

$$D \frac{\partial c}{\partial y} = v_w c_w \quad y = h \quad \forall x \tag{3.2.10}$$

$$c = c_o \quad x = 0, \forall y \tag{3.2.11}$$

Equation (3.2.9) specifies that there is no-flux through the solid wall. At steady state, when concentration profiles are established and invariant,
mass transport to and from the boundary layer are equal thus effectively maintaining a dynamic balance. Convective transport up to the membrane surface \( (=v_w c_w) \) is balanced by diffusive back transport \( (=D \frac{\partial c}{\partial y}) \). Equation (3.2.10) mathematically expresses the equality of these two transport mechanisms. A uniform inlet concentration, \( c_o \), is assumed as the boundary condition at constant \( x \). This serves as an initial condition in the proposed finite difference scheme.

3.2.2. Finite difference solution: Introducing the non-dimensional variables in Equation (3.2.8)

\[
\frac{u}{u_o}, \quad \frac{v}{v_w}, \quad \frac{c}{c_o}, \quad \frac{x}{L} \quad \text{and} \quad \frac{\lambda}{h}
\]

(3.2.12)

and rearranging we get in dimensionless form,

\[
\frac{u}{u_o} \frac{\partial c}{\partial x} + \left( \frac{v}{v_w} \frac{L}{u_o h} \right) \frac{v}{u_o h^2} \frac{\partial c}{\partial \lambda} = \frac{D L}{u_o h^2} \frac{\partial^2 c}{\partial \lambda^2}
\]

(3.2.13)

The boundary conditions are also expressed in dimensionless form as

\[
c = 1 \quad x=0, \quad \forall \lambda
\]

(3.2.14)

\[
\frac{\partial c}{\partial \lambda} = 0 \quad \lambda = 0 \quad \forall \lambda
\]

(3.2.15)

\[
\frac{\partial c}{\partial \lambda} = \frac{v}{c_o} \frac{c_w v_w h}{D} \quad \lambda = 1 \quad \forall \lambda
\]

(3.2.16)

Figure 3.2.1 shows the gridding scheme for developing the finite difference equations. Introduce the finite difference approximations

\[
\frac{\partial c}{\partial x} = \frac{c(x) - c(x - \Delta x)}{\Delta x} = \frac{c_{i,m} - c_{i,m-1}}{\Delta x}
\]

(3.2.17)
\[ \frac{\partial c}{\partial \lambda} = \frac{c(\lambda) - c(\lambda - \Delta\lambda)}{\Delta\lambda} = \frac{c_{j \cdot m} - c_{j-1 \cdot m}}{\Delta\lambda} \]  \hspace{1cm} (3.2.18)

\[ \frac{\partial^2 c}{\partial \lambda^2} = \frac{c(\lambda + \Delta\lambda) - 2c(\lambda) + c(\lambda - \Delta\lambda)}{\Delta\lambda} = \frac{c_{j+1 \cdot m} - 2c_{j \cdot m} + c_{j-1 \cdot m}}{(\Delta\lambda)^2} \]  \hspace{1cm} (3.2.19)

---

Figure 3.2.1 The square grid scheme used for the finite difference solution of Equation 3.2.13. \( m \) is the subscript for the \( x \) direction and \( j \) is the subscript for the \( y \) direction.

Substituting Equations (3.2.17) - (3.2.19) in Equation (3.2.13) and rearranging to get the finite difference equation for all interior nodes,

\[ A_{j-1} c_{j-1 \cdot m} + B_j c_{j \cdot m} + E_j c_{j+1 \cdot m} = F_j \quad \text{for } 2 \leq j \leq nj-1 \]  \hspace{1cm} (3.2.20)

\[ A_{j-1} = -v \left( \frac{v_w L}{u_0 h} \right) \frac{1}{\Delta \lambda} - \frac{DL}{u_0 h^2} \left( \frac{1}{(\Delta \lambda)^2} \right) \]  \hspace{1cm} (3.2.21)

\[ B_j = \frac{u}{\Delta x} + v \left( \frac{v_w L}{u_0 h} \right) \frac{1}{\Delta \lambda} + 2 \left( \frac{DL}{u_0 h^2} \right) \left( \frac{1}{(\Delta \lambda)^2} \right) \]  \hspace{1cm} (3.2.22)

\[ E_j = -\left( \frac{DL}{u_0 h^2} \right) \left( \frac{1}{(\Delta \lambda)^2} \right) \]  \hspace{1cm} (3.2.23)
\[ F_j = \frac{u_i}{\Delta x} c_{j,m-1} \]  \hspace{1cm} (3.2.24)

These coefficients are valid for all the interior points. At the porous and solid boundaries we use the boundary conditions (3.2.15) and (3.2.16) and simplify as given below.

At the non-porous boundary, \( j = 1 \). From Equation (3.2.15),

\[ \frac{\partial c}{\partial \lambda} = 0 \Rightarrow \frac{c_{i+1,m} - c_{i-1,m}}{2\Delta \lambda} = 0 \Rightarrow c_{2,m} - c_{0,m} = 0 \Rightarrow c_{2,m} = c_{0,m} \]  \hspace{1cm} (3.2.25)

Substituting Equation (3.2.25), \( u = 0 \) and \( j = 1 \) into Equation (3.2.20) we obtain the finite difference equation valid at the solid wall.

\[ B_1 \ c_{1,m} + E_1 \ c_{2,m} = 0 \hspace{0.5cm} \text{for} \hspace{0.5cm} j = 1 \]  \hspace{1cm} (3.2.26)

The coefficients \( B_1 \) and \( E_1 \) are:

\[ B_1 = v_1 \left( \frac{v_w L}{u_0 h} \right) \frac{1}{\Delta \lambda} + 2 \left( \frac{D L}{u_0 h^2} \right) \frac{1}{(\Delta \lambda)^2} \]  \hspace{1cm} (3.2.27)

\[ E_1 = -v_1 \left( \frac{v_w L}{u_0 h} \right) \frac{1}{\Delta \lambda} - 2 \left( \frac{D L}{u_0 h^2} \right) \frac{1}{(\Delta \lambda)^2} \]  \hspace{1cm} (3.2.28)

The finite difference equation at the porous wall can be obtained similarly. Expressing equation (3.2.16) as a finite difference approximation:

\[ \frac{c_{n+1,i} - c_{n-1,i}}{2\Delta \lambda} = v_{nj,m} \ c_{nj,m} \left( \frac{v_w h}{D} \right) \]  \hspace{1cm} (3.2.29)

Rearranging, we obtain the result:
\[ c_{nj+1} = 2\Delta\lambda \cdot v_{nj} \cdot c_{nj} \cdot \left( \frac{v_w h}{D} \right) + c_{nj-1} \]  \quad \text{(3.2.30)}

Substitute Equation (3.2.30) and \( j = nj \) in Equation (3.2.20) to get the finite difference equation valid at the porous wall.

\[ A_{nj-1} \cdot c_{nj-1} + B_{nj} \cdot c_{nj} = F_{nj} \quad \text{for } j = nj \]  \quad \text{(3.2.31)}

The coefficients are as given below:

\[ A_{nj-1} = -v_{nj} \left( \frac{v_w L}{u_o h} \right) \frac{1}{\Delta\lambda} - 2 \left( \frac{DL}{u_o h^2} \right) \frac{1}{(\Delta\lambda)^2} \]  \quad \text{(3.2.32)}

\[ B_{nj} = \frac{u_{nj}}{\Delta x} + v_{nj} \left( \frac{v_w L}{u_o h} \right) \frac{1}{\Delta\lambda} + 2 \left( \frac{DL}{u_o h^2} \right) \frac{1}{(\Delta\lambda)^2} - 2 \frac{v_{nj} v_w L}{hu_o \Delta\lambda} \]  \quad \text{(3.2.33)}

\[ F_{nj} = \frac{u_{nj}}{\Delta x} \cdot c_{nj-1} \]  \quad \text{(3.2.34)}

The solution procedure is as follows:

**Step 1.** Start at \( m = 2 \) (\( m = 1 \) is the "initial" condition: \( c = 1 \)). Evaluate the axial and transverse velocity profiles and the coefficients \( A_j, B_j, E_j \) and \( F_j \) for \( 1 \leq j \leq nj \). These coefficients constitute a tridiagonal system of the form:

\[
\begin{bmatrix}
A_1 & B_1 & E_1 \\
A_2 & B_2 & E_2 \\
& \ddots & \ddots \\
& & A_{i-1} & B_i & E_i \\
& & & A_{n-2} & B_{n-1} & E_{n-1} \\
& & & A_{n-1} & B_n & E_n \\
\end{bmatrix}
\begin{bmatrix}
c_1 \\
c_2 \\
\vdots \\
\vdots \\
c_i \\
\vdots \\
c_{n-1} \\
c_n \\
\end{bmatrix}
= \begin{bmatrix}
F_1 \\
F_2 \\
\vdots \\
\vdots \\
\vdots \\
F_{i} \\
\vdots \\
F_{n-1} \\
F_n \\
\end{bmatrix}
\]
Solve for the concentrations \( c_1, c_2, c_3 \ldots c_n \). The FORTRAN computer code for the tridiagonal matrix solver algorithm used is given in Appendix B (program name: TRIDIAG).

**Step 2.** Advance by \( \Delta x \) to step to next \( m \). Calculate the axial and transverse velocity profiles to compute the coefficients. Then evaluate the right hand side \( F \) matrix from concentrations computed at the previous step. Now, solve for the concentrations \( c_1, c_2, c_3 \ldots c_n \) at the new axial position.

**Step 3.** Repeat step 2 to advance into the channel until the desired axial position is reached.

### 3.2.3 Discussion on concentration polarization:

The velocity components coupled with the diffusivity of the retained species determine concentration polarization. Intuitively, we can expect to decrease solute build-up by either increasing diffusive back-transport or by decreasing convective transport up to the membrane surface. We shall examine the effect each of these parameters have on solute accumulation near the porous wall.

#### 3.2.3.1 Effect of the diffusion coefficient: Bovine Serum Albumin (BSA) is a globular protein very often used as a model compound in ultrafiltration studies. It has a molecular weight of 60,000 Daltons and a diffusion coefficient of \( 3.5 \times 10^{-6} \) cm\(^2\)/sec at its isoelectric point (pH 4.7). In these regards, BSA resembles a large molecular weight humic acid. The presence of specifically adsorbing cations will change the surface
chemistry of BSA and its size (thereby changing the diffusivity). Mass
transfer experiments with BSA at its isoelectric point were reported in a
parallel plate ultrafilter by Leung and Probstein (1979). Figure 3.2.2
shows the predicted concentration profiles for two diffusivities, D =
5.25×10⁻⁶ cm²/sec and D = 2.33×10⁻⁶ cm²/sec. The channel dimensions
were obtained from Leung and Probstein (1979). It is seen that the effect
of increasing the diffusion coefficient is a reduction in the wall
concentration. Also, it was computed that under the specified
hydrodynamic conditions, the accumulated mass increased approximately
by 50% for a 55% decrease in the diffusion coefficient. It is interesting to
note that while the wall concentration (and accumulated mass) decreased by
increasing the diffusion coefficient, the thickness of the polarized layer
increased by 30% (from a Δλ of 0.032 to 0.042). Thus, the effect of
decreasing the diffusion coefficient is to put more mass into a smaller
volume of liquid in the layers near the membrane.

Steady state concentration profiles are shown in Figure 3.2.3 for the
filtration of calcium sulfate and sodium chloride using a flat plate
composite DDS reverse osmosis membrane. These plots illustrate the large
differences in ionic environments that may exist between the membrane
surface and the bulk flow over the membrane.
Figure 3.2.2 Influence of solute diffusivity on mid-channel concentration profiles. Decreasing the solute diffusion coefficient increases the wall concentration and decreases the thickness of the polarized layer.

A NF membrane would be expected to retain divalent ions (Ca\(^{++}\) etc.) and not monovalent ions (Na\(^+\) etc.). No ionic species are expected to be retained by UF or MF membranes. In NF, a concentration gradient of the calcium salt is predicted to develop. The concentration of the sodium salt near the membrane is expected to be approximately equal to the mean concentration in the permeate. Constant diffusivity and no interaction between the different ionic species are assumed. It is seen that the concentration boundary layer occupies only a very small fraction of the channel height in both cases (about 2.5%). CaSO\(_4\) has a smaller diffusion coefficient than NaCl and therefore builds up more near the membrane surface and is predicted to contribute more to concentration polarization and flux reduction in commercial RO systems. Moreover, solutes such as
Ca\(^{++}\), Mg\(^{++}\) and other divalent metals may exceed their solubility limits and precipitate on the membrane thereby causing irreversible fouling.

![Figure 3.2.3 Removal of NaCl and CaSO\(_4\) from a brackish water using reverse osmosis. The concentration of Ca\(^{++}\) ions is thus expected to be higher near the membrane surface than in the bulk increasing the possibly of adsorptive interactions with other deposited solutes and the membrane itself.](image)

Larger species including macromolecular and colloidal materials will also be retained by RO, NF and to a lesser extent, UF membranes. Interaction between colloidal, macromolecular and ionic species may significantly change the physical and chemical properties of the suspended material and greatly alter the profiles calculated for independent species. Of particular interest in water treatment are interactions between dissolved or adsorbed natural polyelectrolytes (humic substances) and cations in these locally high ionic strength regions. Humic substances are the result of chemical and biological degradation of dead tissue and are the primary
source of organic matter in natural waters and have a wide range of molecular weights (Aiken et al., 1985). They cause undesirable color and influence the chemistry of metals by increasing their solubility through complexation (Perdue, 1989). Upon chlorination (during disinfection) of a water containing humic materials, chlorinated organic compounds including trihalomethanes (THMs) are formed. Some of these compounds are mutagens and/or suspected carcinogens. Removal of these humic precursors during water treatment is an important issue within the context of the anticipated regulations on DBPs. Cornel et al. (1986) investigated the effect of pH, ionic strength and molecular weight on the diffusion of humic acid in aquatic systems. For a given molecular weight, an increase in the ionic strength of the water was found to increase the diffusivity of humic acid. This was explained based on changes in hydrodynamic size that occur with changes in ionic strength. Humic materials are long molecules having ionizable carboxylic groups. At low ionic strengths, the mutual repulsion between these charged functional groups results in a large molecular size. This electrostatic repulsion is reduced by increasing the background ionic strength of the water thereby reducing the size and increasing the diffusivity. As illustrated in Figure 3.2.3, there are significant differences in the ionic composition of the water as a function of the transverse position within the flowpath over a membrane filter. There exists a high ionic strength region (due to solute accumulation) close to the membrane surface where the charges on the functional groups will be screened and the diffusivity of humic substances will be enhanced. Far away from this region, the chemical composition of the feed water is
expected to be relatively unchanged and we can expect lower diffusion coefficients. The predicted concentration profiles during the filtration of humic materials in a high ionic strength water and a low ionic strength water are plotted in Figures 3.2.4 and 3.2.5 respectively.

![Graph showing concentration profiles during UF](image)

Figure 3.2.4 Concentration profiles at mid-channel during the UF of a 50K - 100K fraction of humic acid with a high background ionic strength [NaCl]=100mM.

A three fold decrease in the diffusion coefficient (from $2 \times 10^{-6}$ cm$^2$/sec to $7 \times 10^{-7}$ cm$^2$/sec) results in a seven-fold increase in the dimensionless wall concentration (from 10.5 to 70). Again, it is observed that this increase in the wall concentration is accompanied by a decrease in the thickness of the polarized layer. The effect of decreasing the diffusion coefficient of the rejected species can be summarized as increasing the wall concentration and decreasing the thickness of the polarized layer. Qualitatively, this result can be understood by looking at diffusion as a "spreading-out" phenomenon.
Figure 3.2.5 Mid-channel concentration profiles for the UF of a 50K-100K humic acid fraction at a low background ionic strength [NaCl]=0mM. Note that the wall concentration is considerably higher than in Figure 3.2.4.

Higher diffusion coefficients will tend to spread out the mass accumulated in the boundary layer thus increasing its thickness. Thus not only does the polarized mass increase with decreasing diffusivity but this mass is packed tighter and may present an even greater resistance to the passage of solvent through the membrane. In addition, the driving force for adsorption of organic materials on the membrane surface and within the membrane pores will be enhanced and may lead to adsorptive fouling of the membrane. The effect is several-fold, since higher ionic strengths near the membrane surface are also likely to render the humic material more hydrophobic, which will again enhance adsorption. Finally, by decreasing the hydrodynamic radius of the polyelectrolytes, there may be increased potential for the penetration of this material into the membrane pores leading to clogging and irreversible fouling.
3.2.3.2 Effect of the slip coefficient: The mid-channel concentration profile during the ultrafiltration of humic acid is plotted as a function of the slip coefficient in Figure 3.2.6. It is noted that the presence of a slip velocity reduced concentration polarization. Singh and Laurence (1979a; 1979b) had obtained a similar result and they proposed a slip velocity-induced back transport mechanism based on their computer simulations of the effect of slip velocity on the concentration profiles in a parallel plate membrane filter with two equally porous walls and in a tubular membrane system.

![Graph showing the effect of slip coefficient on concentration profile](image)

Figure 3.2.6 Mid-channel concentration profiles illustrating the effect of the slip velocity; UF of a 50K - 100K fraction of humic acid with a high ionic strength background, [NaCl] = 100 mM. Increasing slip at the membrane surface decreases concentration polarization.

As shown earlier in Table 3.1, the slip velocity plays a negligible role at the free membrane surface. In any membrane filter with mass transfer, the accumulated cake layer presents a new boundary for the feed
stream. If sufficient shear is imposed on the system this cake will be fluidized and thus the permeability of this layer is not expected be constant (this is in contrast to a compacted cake which might present a uniformly high resistance to permeation). At the surface of this layer (where the permeability is very high) the effect of fluid slip may be important and is expected to be important in determining further convective transport of material from the bulk solution to the polarized layer.

3.2.3.3 Effect of hydrodynamic parameters: Convective transport is determined by the axial and transverse velocities. Increasing permeation rates result in greater transport up to the membrane causing more polarization. Figure 3.2.7 shows this effect very clearly. Here, the influence of the wall permeation rate on concentration polarization in the same BSA-UF system discussed earlier in section 3.2.3.1. The effect of a 50% increase in the permeation velocity is a 70% increase in the mass of the retained solute under the conditions specified.

During crossflow filtration, the shear force on the membrane wall provides a "sweeping" mechanism which tends to keep the filter clean. Figure 3.2.8 shows a family of mid-channel concentration profiles in the ultrafiltration of BSA at various axial velocities. As the tangential velocity increases both wall concentration and polarized layer thickness decrease indicating better filter performance.
Figure 3.2.7 Influence of permeation rate on concentration polarization in the UF of BSA at its isoelectric point. Convective transport up to the membrane surface is enhanced by increasing permeation rate thus aggravating concentration polarization.

Figure 3.2.8 Mid-Channel concentration profiles at varying crossflow velocities. Increasing shear on the deposited mass (by increasing tangential velocity) increases back-transport by a "sweeping" mechanism thereby reducing solute accumulation.
In all cases considered, it is seen that the concentration boundary layer occupies only a small fraction of the channel height. Thus, the approach of considering momentum and mass transfer separately appears to be reasonable. Calculations of laminar momentum boundary layers are given in Appendix A. It is noted that in all membrane solid-liquid separation systems, the momentum boundary layer is much greater in extent than the concentration boundary layer because of the high values for the Schmidt number, \( \text{Sc} = v/D \). For \( 10^{-5} \text{ cm}^2/\text{sec} \leq D \leq 2 \times 10^{-6} \text{ cm}^2/\text{sec} \), in the filtration of water \( (v=0.01 \text{ cm}^2/\text{sec}) \), \( 10^3 \leq \text{Sc} \leq 5 \times 10^3 \).

3.2.4 Computational aspects: Satisfactory numerical convergence is dependent on the grid size used in the finite difference algorithm. A square mesh was used in all model runs. All model runs were made on a Sun-Sparc 2 workstation using double precision arithmetic. The FORTRAN program DIFFUSION used for generating these concentration profiles is shown in Appendix B along with the tridiagonal matrix solver TRIDIAG. It was observed that the diffusion coefficient largely determined the grid spacing. Problems with small diffusion coefficients needed finer grid spacing than problems involving large diffusion coefficients. For example, in Figure 3.2.3 \( (D=10^{-5} \text{ cm}^2/\text{sec}) \) convergence was achieved even with a coarse grid \( (\Delta x = \Delta y = 5 \times 10^{-4}) \). This computer simulation required 15 minutes to generate the mid-channel concentration profiles. In contrast, generation of mid-channel concentration profiles with a smaller diffusion coefficient needed much finer grids. For \( D=7 \times 10^{-7} \text{ cm}^2/\text{sec} \) (see Figure 3.2.5) a grid size of \( \Delta x=\Delta y=1.25 \times 10^{-5} \) was necessary for convergence. Corresponding run time increased to more than eight hours.
3.3 Particle transport in porous channels:

Lateral migration of particles undergoing slow Poiseuille flow in non-porous ducts was analyzed theoretically by Cox and Brenner (1968). They formulated the general problem and also proposed the method of solution. The numerical coefficients involved in the solution were not evaluated because of their complex structure. Altena and Belfort (1984) adapted the theory developed by Cox and Brenner for flow in porous ducts. The following section has its basis on both these works, many equations and concepts given here have been taken directly from them. The case considered here is of a neutrally buoyant, freely rotating sphere undergoing Poiseuille flow in a channel with two parallel walls.

3.3.1 Problem formulation: Consider a sphere, $B$, of radius $a_p$ suspended in a fluid undergoing steady Poiseuille flow between two stationary parallel walls, $W$, separated by a distance $h$ (the height of the channel). One of the walls is porous while the other is solid. The problem is illustrated in Figure 3.3.1.

The absolute viscosity of the fluid is $\mu$, the density $\rho$ and the kinematic viscosity ($=\mu/\rho$) is $\nu$. Let the maximum (centerline) velocity of the undisturbed fluid velocity at the channel entrance, $u_{max}$ be the characteristic velocity associated with the flow. Two coordinate systems are defined; one with the center of the particle as the origin $r'=(r_1, r_2, r_3)$ and the other is a Cartesian coordinate system where $x$ denotes the axial distance from the channel entrance and $\beta$ is the dimensionless distance
from the porous wall. Define the dimensionless particle Reynolds number, $Re_p$, the dimensionless particle size, $\kappa$, and the dimensionless coordinate system with origin at the particle center, $r$ as:

$$Re_p = \frac{u_{\text{max}} a_p}{v}; \quad r = r'/a_p; \quad \kappa = a_p/\beta$$ \hspace{1cm} (3.3.1)

**Undisturbed flow:** The fluid flow in the absence of the particle is said to be undisturbed. The dimensional undisturbed velocity profile is denoted by $U'$ and the dimensional pressure by $P'$. The corresponding non-dimensional quantities are defined below.

$$U = \frac{U'}{u_{\text{max}}} \quad \text{and} \quad P = \frac{P'a_p}{\mu u_{\text{max}}}$$ \hspace{1cm} (3.3.2)
The undisturbed fluid flow satisfies the Navier-Stokes equations (Equations 3.1.1 and 3.1.2).

\[ \mathbf{U}^* \cdot \nabla \mathbf{U}^* = -\frac{1}{\rho} \nabla \mathbf{P}^* + \nu \nabla^2 \mathbf{U}^* \]  \hspace{1cm} (3.3.3)

Substituting the dimensionless variables defined in (3.3.2) and defining the dimensionless gradient operator as,

\[ \nabla = a_p \nabla \]  \hspace{1cm} (3.3.4)

the dimensionless Navier-Stokes equations are obtained.

\[ \text{Re}_p \mathbf{U} \cdot \nabla \mathbf{U} = -\nabla \mathbf{P} + \nabla^2 \mathbf{U} \]  \hspace{1cm} (3.3.5)

Equation (3.3.5) together with the continuity equation,

\[ \nabla \cdot \mathbf{U} = 0 \]  \hspace{1cm} (3.3.6)

and the boundary condition,

\[ \mathbf{U} = \left(0, 0, \frac{V_w}{u_{\text{max}}} \right) \text{ on the walls } W \]  \hspace{1cm} (3.3.7)

define the undisturbed flow problem completely.

**Complete fluid flow:** Let \( \mathbf{V}^* \) and \( \Omega^* \) be the translational (linear) and rotational (angular) velocities of the particle in the non-uniform shear field at a distance \( \beta \) from the porous wall. The fluid flow in the presence of the particle is said to be complete. The velocity and pressure of the complete fluid flow are represented by \( \mathbf{v}^* \) and \( \mathbf{p}^* \) respectively. Define the non-dimensional variables as follows:

\[ \mathbf{V} = \frac{\mathbf{V}^*}{u_{\text{max}}} ; \quad \Omega = \frac{\Omega^* a_p}{u_{\text{max}}} ; \quad \nu = \frac{\mathbf{v}^*}{u_{\text{max}}} ; \quad \mathbf{p} = \frac{\mathbf{p}^* a_p}{\mu u_{\text{max}}} \]  \hspace{1cm} (3.3.8)

The governing equations describing the complete fluid flow are:
\[ \text{Re}_p \mathbf{v} \cdot \nabla \mathbf{v} = - \nabla p + \nabla^2 \mathbf{v} \quad (3.3.9) \]

The complete fluid flow problem is described using Equation (3.3.9) together with the continuity equation,
\[ \nabla \cdot \mathbf{v} = 0 \quad (3.3.10) \]
and the boundary conditions,
\[ \mathbf{v} = \mathbf{U}(r) \quad \text{as } r \to \infty \quad \text{and} \]
\[ \mathbf{v} = \mathbf{\Omega} \times \mathbf{r} \quad \text{on the sphere, } \mathbf{B} . \quad (3.3.11) \]

**Disturbance flow:** The disturbance caused in the fluid flow because of the presence of the particle is called the disturbance flow. Let \( \mathbf{v}^* \) and \( p^* \) be the disturbances in the fluid velocity and pressure respectively. Hence:
\[ \mathbf{v}^* = \mathbf{v} - \mathbf{U} \quad (3.3.13) \]
\[ p^* = p - P \quad (3.3.14) \]

From Equations (3.3.5) and (3.3.9) we can write:
\[ \text{Re}_p \left( \mathbf{U} \cdot \nabla \mathbf{v}^* + \mathbf{v}^* \cdot \nabla \mathbf{v}^* + \mathbf{v}^* \cdot \nabla \mathbf{U} \right) = - \nabla p^* + \nabla^2 \mathbf{v}^* \quad (3.3.15) \]
Also,
\[ \nabla \cdot \mathbf{v}^* = 0 \quad \text{and} \]
\[ \mathbf{v}^* \to 0 \quad \text{as } r \to \infty \quad \text{and} \]
\[ \mathbf{v}^* = \mathbf{\Omega} \times \mathbf{r} - \mathbf{U}(r) \quad \text{on the particle } \mathbf{B} . \quad (3.3.16) \]

Under situations when \( \text{Re}_p \ll \kappa \ll 1 \) and \( \frac{V_w}{u_{\max}} \ll 1 \), we can obtain a perturbation series expansion for the velocity and pressure at a fixed \( \kappa \) as:
\[ \mathbf{U} = \mathbf{U}_0 + \text{Re}_p \mathbf{U}_1 + \ldots \quad (3.3.17) \]
\[ \mathbf{P} = \mathbf{P}_0 + \text{Re}_p \mathbf{P}_1 + \ldots \quad (3.3.18) \]
\[ \mathbf{v}^* = \mathbf{v}_0^* + \text{Re}_p \mathbf{v}_1^* + \ldots \quad (3.3.19) \]
\( p^* = p_0^* + R_e p_1^* + \ldots \) \hspace{1cm} (3.3.21)

Substituting Equations (3.3.18) and (3.3.19) into Equations (3.3.5) and (3.3.6) and equating the corresponding powers of \( R_e \) we obtain the zero order (terms without \( R_e \)) approximation.

\[ \nabla^2 U_0 - \nabla p_0 = 0 \] \hspace{1cm} (3.3.22)
\[ \nabla \cdot U_0 = 0 \] \hspace{1cm} (3.3.23)
with \( U_0 = 0 \) on the boundary \( W \) \hspace{1cm} (3.3.24)

We see that the zero order equations are the Stokes equations. The first order (terms with \( R_e \) raised to the first power) approximation is,

\[ U_0 \cdot \nabla U_0 = -\nabla p_1 + \nabla^2 U_1 \] \hspace{1cm} (3.3.25)
\[ \nabla \cdot U_1 = 0 \] \hspace{1cm} (3.3.26)
with \( U_1 = 0 \) on the boundary \( W \) \hspace{1cm} (3.3.27)

Similarly, substituting Equations (3.3.20) and (3.3.21) in Equations (3.3.15) and (3.3.16) and equating the corresponding powers of \( R_e \) we obtain the zero order approximation:

\[ \nabla^2 v_0^* - \nabla p_0^* = 0 \] \hspace{1cm} (3.3.28)
\[ \nabla \cdot v_0^* = 0 \] \hspace{1cm} (3.3.29)
with \( v_0^* = 0 \) on the boundary \( W \) \hspace{1cm} (3.3.30)
\( v_0^* \rightarrow 0 \) as \( r \rightarrow \infty \) \hspace{1cm} (3.3.31)
\[ v_0^* = \Omega \times r - U_0 \] on the particle B \hspace{1cm} (3.3.32)

The first order approximation is given as,
\[ \mathbf{U}_0 \cdot \nabla v_0^* + v_0^* \cdot \nabla v_0^* + v_0^* \cdot \nabla U_0 = - \nabla p_1^* + \nabla^2 v_1^* \]  
(3.3.33)

\[ \nabla \cdot v_1^* = 0 \]  
(3.3.34)

with \( v_1^* \) = 0 on the boundary \( W \)  
(3.3.35)

\( v_1^* \to 0 \) as \( r \to \infty \)  
(3.3.36)

\( v_1^* = - U_1 \) on the particle \( B \)  
(3.3.37)

Cox and Brenner (1968) divided the first order flow field \( (v_1^*, p_1^*) \) into two fields \( (v_1^*, p_1^*) \) and \( (v_1^*, p_1^*) \) for convenience in evaluation such that

\[ v_1^* = v_1^* + v_1^* \]

\[ p_1^* = p_1^* + p_1^* \]

The flow field \( (v_1^*, p_1^*) \) satisfies:

\[ \nabla^2 v_1^* - \nabla p_1^* = 0 \]  
(3.3.38)

\[ \nabla \cdot v_1^* = 0 \]  
(3.3.39)

\[ v_1^* = 0 \] on the walls, \( W \)  
(3.3.40)

\[ v_1^* \to 0 \] as \( r \to \infty \)  
(3.3.41)

\[ v_1^* = - U_1 \] on the particle, \( B \)  
(3.3.42)

The flow field \( (v_1^*, p_1^*) \) satisfies

\[ \nabla^2 v_1^* - \nabla p_1^* = - f \]  
(3.3.43)
\[ \nabla \cdot \mathbf{v}^* = 0 \] (3.3.44)

\[ \mathbf{v}^* = 0 \quad \text{on the walls, } W \] (3.3.45)

\[ \mathbf{v}^* \to 0 \quad \text{as } r \to \infty \] (3.3.46)

\[ \mathbf{v}^* = 0 \quad \text{on the particle, } B \] (3.3.47)

where \[ f = - ( \mathbf{U}_0 \cdot \nabla \mathbf{v}^* + \mathbf{v}_0^* \cdot \nabla \mathbf{v}_0^* + \mathbf{v}_0^* \cdot \nabla \mathbf{U}_0 ) \] (3.3.48)

Therefore we can write the expressions for the complete fluid flow (from Equations 3.3.13, 14, 18, 19, 20 and 21 as:

\[ \mathbf{v} = ( \mathbf{U}_0 + \mathbf{v}_0^* ) + \text{Re}_p ( \mathbf{U}_1 + \mathbf{v}_1^* + \mathbf{v}_1^* ) + \ldots \] (3.3.49)

\[ \mathbf{p} = ( \mathbf{P}_0 + \mathbf{p}_0^* ) + \text{Re}_p ( \mathbf{P}_1 + \mathbf{p}_1^* + \mathbf{p}_1^* ) + \ldots \] (3.3.50)

Now, we can express the force and couple acting on the particle, B as:

\[ \mathbf{F} = ( \hat{\mathbf{F}}_0 + \mathbf{F}_0^* ) + \text{Re}_p ( \hat{\mathbf{F}}_1 + \mathbf{F}_1^* + \mathbf{F}_1^* ) + \ldots \] (3.3.51)

\[ \mathbf{G} = ( \hat{\mathbf{G}}_0 + \mathbf{G}_0^* ) + \text{Re}_p ( \hat{\mathbf{G}}_1 + \mathbf{G}_1^* + \mathbf{G}_1^* ) + \ldots \] (3.3.52)

The flow field \((\mathbf{U}_0, \mathbf{P}_0)\) creates the force \(\hat{\mathbf{F}}_0\) and the couple \(\hat{\mathbf{G}}_0\) while the flow fields \((\mathbf{U}_1, \mathbf{P}_1), (\mathbf{v}_1^*, \mathbf{p}_1^*)\) and \((\mathbf{v}_1^*, \mathbf{p}_1^*)\) create \((\hat{\mathbf{F}}_1, \hat{\mathbf{G}}_1), (\mathbf{F}_1^*, \mathbf{G}_1^*), (\mathbf{F}_1^*, \mathbf{G}_1^*)\) respectively.

In general, problems involving expansions in \(\text{Re}_p\) are singular (Proudman and Pearson, 1957) and thus both inner and outer expansions are necessary along with a matching procedure. However, in many cases, for flow in closed ducts, Cox and Brenner (1968) showed, when \(\text{Re}_p \ll \kappa, \ldots\)
the force and couple on the particle can be calculated correct to $O(Re_p)$ by considering only the inner expansion.

3.3.2 Inertial lift and particle trajectories: Vasseur and Cox (1976) (see Table 2.3.1) solved for the velocity fields (Equation 3.3.49, 3.3.50) and the forces and couples (Equation 3.3.51, 3.3.52) for the specific case of plane Poiseuille flow. In the case of a neutrally buoyant sphere which is allowed to rotate the first expression in Table 2.3.1. is applicable. For low wall permeabilities, Altena and Belfort (1984) showed that the same expression derived by Vasseur and Cox can be used for flow in a porous channel. Thus, the expression for the inertial lift velocity is:

$$V_{\text{lift}} = \frac{\kappa^2 a_p U_m^*}{v} h_1(\beta) \tag{3.3.53}$$

where $U_m^*$ is the local maximum axial velocity and $\kappa$ is the dimensionless particle size ($= a_p/h$). Introducing the local particle Reynolds number $Re_p^* (= U_m^* a_p/v)$ we can rewrite Equation (3.3.53) as:

$$V_{\text{lift}} = Re_p^* \kappa^2 U_m^* h_1(\beta) \tag{3.3.54}$$

Otis (1986) evaluated the volume integral $h_1(\beta)$ and obtained a sixth order polynomial fit for the same. His result is shown below:

$$h_1(\beta) = 1.532139 - 12.182786 \beta + 21.652283 \beta^2 + 4.495068 \beta^3$$
$$- 28.176666 \beta^4 + 10.950694 \beta^5 + 0.198042 \beta^6 \tag{3.3.55}$$

The expression for the transverse component of the velocity has been derived in section 3.1.2. as a function of the dimensionless distance from
the non-porous wall. Expressing the result in terms of distance from the porous wall ($\beta$) for the no-slip case (slip coefficient, $\vartheta = 0$) we have:

$$v(\beta) = V_w \left(f_0(\beta) + \text{Re}_w f_1(\beta)\right)$$

where

$$f_0(\beta) = - (2\beta + 1)(1 - \beta)^2$$

$$f_1(\beta) = \frac{1}{70} (-16\beta^2 + 27\beta^3 - 21\beta^5 + 14\beta^6 - 4\beta^7 \ldots)$$

The axial velocity of the particle is given as:

$$u(x, \beta) = U_m^* \left(4\beta (1 - \beta) + O(\text{Re}_w)\right)$$

The functions $f_0(\beta)$ and $h_1(\beta)$ are shown below in Figure 3.3.2. We shall neglect terms of $O(\text{Re}_w)$.

Figure 3.3.2 Variation of the permeation drag (solid line) and the inertial lift (dotted line) forces in the channel. The thick line gives the algebraic sum of $f_0(\beta)$ and $h_1(\beta)$. The permeation drag is maximum at the porous wall but the inertial lift is symmetrical with respect to the channel axis (for low wall permeabilities). From Altena and Belfort, 1984.
The permeation drag is the primary driving force for particle transport towards the membrane while inertial lift tends to move particles away from the membrane surface. Vectorial addition of Equations (3.3.54) and (3.3.56) gives the particle velocity in the transverse (β) direction as:

\[
h \frac{d\beta}{dt} = V_w f_0(\beta) + Re_p^* \kappa^2 U_m^* h_1(\beta) \tag{3.3.60}\]

In the axial (x) direction, the particle moves with the fluid velocity. i.e.

\[
\frac{dx}{dt} = 4 U_m^* \beta (1 - \beta) \tag{3.3.61}\]

From a mass balance on the fluid we can relate the local maximum velocity, \(U_m^*\), to the maximum entrance velocity, \(U_m\), as:

\[
U_m^* = U_m - \frac{3 V_w x}{2 h} \tag{3.3.62}\]

Dividing Equation (3.3.60) by Equation (3.3.61) the position trajectory of the particle is obtained.

\[
\frac{d\beta}{dx} = \frac{V_w f_0(\beta) + Re_p^* \kappa^2 U_m^* h_1(\beta)}{4 h U_m^* \beta (1 - \beta)} \tag{3.3.63}\]

Let the particle enter the channel at an initial position \((x_0, \beta_0)\). The variation of its lateral position, \(\beta\), as a function of its axial position, \(x\), is described by Equation (3.3.63). This is an ordinary differential equation and has been solved using the Euler’s method. Equation 3.3.60 gives the time trajectory of a particle in the porous channel. Here \(\beta\) is an implicit function of \(x\) as specified by the position trajectory and the time value is obtained from the reciprocal of Equation 3.3.61.
3.3.3 Engineering Significance: Calculations of particle transport in membrane systems may give an indication of the fouling potential posed by different raw waters based on their particle size distributions. These particles may be found in the raw water itself or may have been introduced during the pretreatment process. For example membrane-adsorber reactors have been proposed as a potable water treatment technology (Anselme, 1991). In this treatment method, powdered activated carbon (PAC) is added to remove organic compounds such as those causing tastes and odors and/or DBP precursors. UF or MF membranes are used as solid-liquid separation devices to remove the PAC and adsorbed organics. One question which arises regarding this proposed treatment scheme is the potential for membrane fouling by the PAC and the size of PAC which should be utilized with the membrane. Commercially available PAC has a wide particle size distribution ranging from fines that are smaller than 3 \( \mu \text{m} \) to very coarse grains that are larger than 75 \( \mu \text{m} \) (Snoeyink, 1990). An average diameter of 20 \( \mu \text{m} \) is fairly typical of PAC. In Figure 3.3.3 computer simulations are shown of the position trajectories of particles of size \( a_p \) 10 \( \mu \text{m} \) in conditions that might exist in an ultrafilter \( (U_m = 50 \text{ cm/sec}, V_w = 0.015 \text{ cm/sec}, h = 762 \mu \text{m}, L = 46 \text{ cms}) \) used to separate PAC from feed water in a membrane-adsorber reactor. It is seen that inertial lift forces are important and counteract permeation drag forces leading to reduced deposition on the membrane. Due to significant inertial lift, particles in the membrane feed water in this size range are not predicted to contribute significantly to the fouling of UF membranes. The lift force scales as the cube of the particle size. Hence, small changes in
Figure 3.3.3 Position trajectories of large \( a_p = 10\mu m \), neutrally buoyant, freely rotating spherical particles in an ultrafiltration module. The flow field: \( U_m = 50\text{cm/sec} \), \( V_w = 0.015\text{cm/sec} \). The channel dimensions are \( h = 762\mu m \), \( L = 46\text{cms} \). This scenario may be representative of a membrane-adsorber unit used to filter PAC which had been added to remove organics from the raw water.
Figure 3.3.4 Position trajectories of small ($a_p = 3 \mu m$), neutrally buoyant, freely rotating spherical particles in an ultrafiltration module. The flow field: $U_m = 50 cm/sec$, $V_w = 0.015 cm/sec$. The channel dimensions are $h = 762 \mu m$, $L = 46 cm$. This scenario may be representative of bacterial transport in ultrafiltration systems where biofouling is a problem of considerable practical importance.
size lead to significantly different behaviors under same hydrodynamic conditions.

Other particles of interest in water treatment include bacteria. Bio-fouling of membranes is a problem of considerable practical importance (Ridgway et al. 1991). Bacteria have been reported to cause considerable fouling on membranes used for water treatment by the secretion of chemicals and polymers that form gel-layers on the surface. Spherical bacteria (known as cocci) are of the size range $0.25 \mu m \leq a_p \leq 2 \mu m$. In contrast to negligible deposition for a 10 $\mu m$ sphere, significant deposition is predicted for a suspension of 3 $\mu m$ microbes. This can be seen in Figure 3.3.4, where the position trajectories of such a particle are shown under the same flow field as in Figure 3.3.3. There is no migration across streamlines and the bacteria move along with the fluid leading to deposition and the possible formation of a bio-film on the membrane surface. About 35% of the bacteria in the feed stream are expected to be "captured" by the membrane (assuming a uniform concentration profile at the inlet) leading to significant fouling and concentration polarization. Increasing the pressure drop across the membrane (increased permeation rate) will lead to greater capture while increasing the crossflow velocity would decrease deposition. Such an analysis may be useful for modeling bio-fouling studies in membrane filters. Calculation of particle transport for smaller, bacteria-sized particles also raise questions regarding the use of PAC with continued recycling in the membrane-adsorber reactor. In such a scenario, PAC will be subject to attrition and wear resulting in the formation of smaller and smaller particles leading to a decrease in the lift
force resulting in increased deposition on the membrane surface. Once a particle is brought near the membrane surface chemical and physical forces play an important role in its transport which are not considered in this model; van der-Walls attractions, diffuse layer repulsion, hydrophobic and steric interactions should be considered in the "near-field" region. For an ultrafilter whose flowfield and geometry are as given above, an order of magnitude estimate of the lateral forces can be obtained as:

Estimate of permeation drag \( \frac{V_w}{U_m} = 3 \times 10^{-4} \) for both particle sizes.

Estimate of inertial lift \( \frac{\text{Re}_p^* \kappa^2}{2} = \begin{cases} 8.6 \times 10^{-4} & \text{for } a_p = 10 \ \mu m \\ 2.3 \times 10^{-5} & \text{for } a_p = 3 \ \mu m \end{cases} \)

It is seen therefore that in the case of the larger particle the inertial lift force is comparable to the permeation drag force making the particle migrate across the fluid streamlines while in the case of the smaller bacterium, inertial forces are dominated by the permeation drag of the fluid, making it move along with the fluid. This is seen in Figure 3.3.3 where under the existing flow field and channel geometry, inertial forces are important. Particle trajectories are not along the fluid streamlines and there is migration across the streamlines (tubular pinch effect). The corresponding time trajectories for Figure 3.3.3 are shown in Figure 3.3.5. It is seen that particles introduced near the porous wall spend more time in the channel than do particles that enter the channel near the solid wall. Particles starting near the solid wall are pushed to faster moving streamlines than are particles starting near the porous wall. This is due to the increased effect of permeation drag as these particles come closer to the membrane. Particles are kept from moving to lateral positions far removed
Figure 3.3.5 Time trajectories of large \(a_p=10\mu m\), neutrally buoyant, freely rotating spherical particles in an ultrafiltration module. The flow field: \(U_m=50\text{cm/sec},\)

\(V_w=0.015\text{cm/sec}.\) The channel dimensions are \(h=762\mu m, L=46\text{cms}.\) Trajectories originating near the mid-channel exit first. Particles initially near the porous wall experience greater permeation drag than particles starting from near the solid wall and hence spend most time in the channel.
Figure 3.3.6 Position trajectories in a microfiltration module. The flow field: \( U_m = 100 \text{cm/sec}, \ V_w = 0.06 \text{cm/sec} \). The channel dimensions are \( h = 0.26 \text{cms}, \ L = 46 \text{cms} \).
Figure 3.3.7 Residence times of different sized ($a_p = 10 \mu m$, $5 \mu m$ and $0.25 \mu m$), neutrally buoyant, freely rotating spherical particles in an ultrafiltration module. Particles are uniformly introduced at the channel entrance as a Dirac pulse at time 0. The flow field: $U_m = 50 cm/sec$, $V_w = 0.015 cm/sec$. The channel dimensions are $h = 762 \mu m$, $L = 46 cms$. Trajectories captured by the membrane have an infinite residence time and are not shown.
from the membrane surface with the result that these particles spend more time in the slower axial velocity fields. A particle trajectory plot is shown in Figure 3.3.6 for hydrodynamic conditions that are typical of microfiltration \((U_m = 100 \text{ cm/sec}, V_w = 0.06 \text{ cm/sec}, h = 0.26 \text{ cms}, L = 46 \text{ cms})\). It was observed that under these conditions inertial effects for \(a_p = 10 \mu m\) particle are negligible. Particle radius must be bigger than 17.5 \(\mu m\) for inertial effects to be comparable to permeation drag. The trajectories shown in Figure 3.3.6 are for a 17.5 \(\mu m\) neutrally buoyant sphere. The residence time for particles initially introduced uniformly as a Dirac pulse over the entire cross-section at the channel entrance is shown in Figure 3.3.7 for different particle sizes. Particles that are captured by the membrane have an infinite residence time. The undisturbed flow field is typical of ultrafiltration and has been used before for generating Figures 3.3.3 and 3.3.4. It is seen that the passage time for the fastest trajectory (trajectory needing the least time to cross the channel length) is independent of particle size. As noted earlier, the distribution is asymmetric and particles that are initially closer to the porous wall spend more time in the channel than do particles introduced at similar lateral distances from the solid wall. Large particles initially introduced as a plug undergo a redistribution across the cross-section, as determined by the effects of drag and inertial forces. All the mass passes through the channel in a short time span as evidenced by the relatively small range in the time needed for the fastest and slowest trajectories to emerge from the channel. Small particles are associated with very fast moving streamlines (near the centerline) as well as very slow moving streamlines (near the solid wall).
resulting in a wide range of residence times in the channel. Initially, a more concentrated plug of particles are predicted to emerge in the case of small particles compared to large particles because inertial effects have not carried them away from the faster moving streamlines near the channel axis to slower streamlines nearer the walls.

A computer simulation of the residence time distribution of the PAC particles are shown in Figure 3.3.8. The program RTD (see Appendix B) was used to generate this plot. Three distinct peaks are predicted due to the asymmetry of the system. First, the particles associated with the fastest streamlines close to the mid-channel are predicted to cross the channel. PAC particles starting from near the solid wall experience less permeation drag than do particles starting near the membrane surface. Therefore, these particles are moved to faster moving fluid elements earlier and constitute the second peak. Finally, those particles that started from lateral positions near the porous wall cross the channel.

When inertial forces are not important (for smaller particle sizes), particles follow fluid streamlines and only one peak is predicted. This is seen in Figure 3.3.9 which shows the predicted residence time distribution for the particles representing spherical bacteria in an ultrafilter under same conditions as the larger PAC particles. Those bacteria starting from near the centerline are the first ones to traverse the length of the channel. Bacteria starting from lateral positions of less than $\beta \approx 0.35$ are expected to be captured by the membrane and thus are predicted to have an infinite residence time in the channel.
Figure 3.3.8 Predicted residence time distribution of large, neutrally buoyant PAC particles in an ultrafilter. Particles near mid-channel are the first to cross the channel followed by particles introduced near the solid wall. Particles starting from near the membrane are expected to have the longest residence times.

Figure 3.3.9 Predicted residence time distributions of smaller bacteria in a ultrafilter (when permeation drag controls particle transport). A mono-modal residence time distribution is predicted.
Other bacteria starting from near the solid wall take longer to exit the channel but due to a relatively uniform traversal they do not come out as a plug but only contribute to the long trailing edge.

3.3.4. Asymptotic Solution near the Membrane surface: The asymptotic solution presented by Cox and Hsu (Equation 2.3.13) for the inertial lift velocity of a sphere near a plane can be used to obtain the limiting case when the sphere just touches the membrane surface, i.e. the particle is captured by the membrane. Their result is:

\[ V_{\text{lift}} = \mathbf{Re}_p^* \kappa^2 U_m^* h_1(\beta) \]  \hspace{1cm} (3.3.64)

where \( h_1(\beta) = \frac{5}{12} (1 - 2\beta)(22 - 146\beta) \) \hspace{1cm} (3.3.65)

At steady state, with no lateral motion \( \frac{d\beta}{dt} = 0 \). Hence, from Equation (3.3.60) and (3.3.62) we obtain:

\[ \frac{V_w}{\mathbf{Re}_p^* \kappa^2 U_m^*} = -\frac{h_1(\beta)}{f_0(\beta)} \left( 1 - \frac{3 V_w x}{2 U_m h} \right) = \gamma \] \hspace{1cm} (3.3.66)

the ratio \( \gamma \) expresses the relative importance of permeation drag over inertial forces when the particle touches the wall \( (\beta = \kappa) \). Therefore the critical ratio of permeation drag to lift, \( \gamma_{\text{crit}} \), is obtained by substituting the value of \( \kappa \) for \( \beta \) in Equation (3.3.66). Figure 3.3.10 shows the variation of \( \gamma_{\text{crit}} \) along the channel length for three fixed values of \( \kappa \) in a channel of height 800 \( \mu \text{m} \) and a dimensionless ratio of the permeation rate to entrance maximum velocity of 0.001.
Figure 3.3.10 Change of the critical ratio of permeation drag to inertial lift forces as a function of axial position in the channel for particle capture on the membrane surface for fixed values of $\beta (=\kappa)$. $\gamma_{\text{crit}}$ should decrease with axial distance coordinate if particles are not captured early along the channel length.

For a given particle size, if permeation drag is much greater than inertial forces (large $\gamma_{\text{crit}}$) then capture takes place at the entrance itself (low values of $x$). If, on the other hand, capture takes place at increased distances from the entrance, permeation drag effects are reduced with respect to inertial forces (decreased $\gamma_{\text{crit}}$) allowing the particles to migrate down the channel until they are captured. Such a trend is observed in Figure 3.3.10 where, as one progresses down the channel (increasing $x$) $\gamma_{\text{crit}}$ decreases for any given $\kappa$. Also, increasing particle size (increasing $\beta$ or $\kappa$) increases the contribution of inertial effects on particle transport thereby decreasing $\gamma_{\text{crit}}$. This is seen in Figure 3.3.10 where curves associated with increasing particle size fall below one another. At any given axial position the capture of larger particles (i.e. greater inertial
effects) is associated with a decrease in $\nu_{\text{crit}}$. This is observed in Figure 3.3.11 where $\beta_{\text{limit}}(=\kappa)$ is plotted as a function of $\nu_{\text{crit}}$ at different axial positions. As expected each curve has a negative slope. Again, if capture takes place only at increased axial distances, the curves shift to the left indicating the increased importance of fluid inertia over permeation drag.

![Graph showing the effect of $\nu_{\text{crit}}$ on the limiting value of $\beta$](image)

Figure 3.3.11 Effect of $\nu_{\text{crit}}$ on the limiting value of $\beta$ when the particle just touches the membrane surface. Along each curve of constant $x$, $\nu_{\text{crit}}$ decreases as $\beta_{\text{limit}}$ increases because of the increasing effect of fluid inertia.

As discussed earlier in section 3.2.3, concentration polarization results in marked differences in the ionic environments between the bulk fluid flow and the membrane surface. In this "near-field" region, forces arising from physical and chemical interactions; diffuse double layer repulsion and steric hindrances for example, are likely to play a more

important role than fluid mechanics in determining particle transport. These effects have not been accounted for in the above discussion on $\gamma_{\text{crit}}$.

3.3.5 Steady-State Concentration Profiles: Altena and Belfort (1984) presented expressions for the steady state concentration profiles for Brownian suspensions undergoing flow in porous channels following a similar procedure followed by Ho and Leal (1974) (see section 2.3). They expressed the probability density function at steady-state as:

$$
\phi (\beta) = \phi_m \frac{\exp \left[ \frac{\beta}{K} \int_{0}^{\delta} g(\beta') d\beta' \right]}{\int_{0}^{1} \exp \left[ K \int_{0}^{\beta} g(\beta') d\beta' \right] d\beta'}
$$

(3.3.67)

where the mean concentration $\phi_m = \int_{0}^{1} \phi(\beta') d\beta'$

(3.3.68)

and $K$ is a parameter describing the relative importance of inertial lift to Brownian diffusion.

$$
K = \frac{\text{Inertial lift}}{\text{Brownian diffusion}} = \frac{\text{Re}_p \kappa^2 U_m h}{D}
$$

(3.3.69)

The function $G(\beta)$ is,

$$
G(\beta) = h_1(\beta) + \gamma f_0(\beta)
$$

(3.3.70)

Unlike the expression for $G(\beta)$ in non-porous ducts derived by Ho and Leal (see Equation 2.3.9) Equation (3.3.70) includes the effects of both inertial and permeation drag forces. The effect of $\gamma$ on the steady-state concentration profiles is illustrated in Figure 3.3.12. In the case of the
non-porous channel, the particles were distributed symmetrically around the longitudinal axis of the channel (see Figure 2.3.2). The effect of permeation at only one wall is to break this symmetry. Increasing the importance of permeation drag (increasing $\gamma$) results in the accumulation of particles near the porous wall while depleting the concentrations near the solid wall.

![Graph](image)

Figure 3.3.12 Effect of permeation drag on the steady-state distribution of particles in a channel with one porous wall. The concentration is non-dimensionalized using the mean concentration $\phi_m$ given in Equation 3.3.68. Particles assume steady-state lateral positions closer to the porous wall as the permeation drag is increased. $\gamma=0$ is the case for a non-porous channel.

Figure 3.3.13 is similar to Figure 2.3.2 and depicts the steady-state concentration profiles of Brownian particles at various values of the parameter $K$ defined in Equation 3.3.69. The effect of increasing the relative importance of Brownian diffusion over inertial effects (decreasing
values of K) is to transport particles from their preferred lateral positions resulting in a more uniform concentration profile at any channel cross-section. Again, the existence of permeation drag (γ=0.1) makes the concentration profiles asymmetric with respect to the channel axis.

![Graph](image)

Figure 3.3.13 Steady-state distribution of particles in a channel with one porous wall illustrating the effect of diffusion coefficient. Increasing D removes any preferred lateral positions that inertial forces try to maintain. The plot is generated using a value of 0.1 for γ. Permeation drag moves distributions closer to the permeable wall as seen earlier.

### 3.3.6 Computational aspects:
All trajectory plots shown were generated on a Sun-Sparc 2 workstation using double precision arithmetic. The trajectories were obtained using a simple Euler’s method. The total length of the channel was traversed in steps of 1/128 cms. The FORTRAN computer code, TIMETRAJ, used for determining the trajectories is shown in Appendix B. The function F(B) is the sixth order polynomial
approximation developed by Otis (1986). $G(S)$ gives the zero order approximation for the permeation drag. The right hand side of Equation (3.3.63) is represented by the function LATERAL(Z,B). The reciprocal of Equation (3.3.61) is given by the function TCROSS(Z,BETA). Computer run time for the generation of each trajectory was less than 15 seconds. The dimensionless steady-state concentrations were determined by evaluating Equation 3.3.67 using the composite Simpson's rule with equally spaced nodes. For each lateral position, $\beta$, the interval was divided into 200 nodes and the whole height of the channel ($0 \leq \beta \leq 1$) was traversed in 200 steps. Run time was around 5 minutes for generating the concentrations at each $\beta$. The program SCONC gives the code for the solution of Equation 3.3.67. Residence time distributions were obtained by running the program RTD. The number of trajectories crossing the channel at equal time intervals (0.1 seconds) were obtained using this program and the results plotted in Figures 3.3.8 and 3.3.9. Figure 3.3.7. was generated using the program PULSE.
Chapter 4

Experimental work

Experiments were designed to measure the residence time distributions (RTD) in a horizontal rectangular channel with one porous wall of dilute monodisperse suspensions comprised of spherical particles. A microporous membrane constituted the lower wall while the upper wall was solid. Details on the apparatus, materials and experimental procedures are presented in this chapter.

4.1 Materials and procedures:

4.1.1 Water: All suspensions and solutions were made using ultrapure water produced from a Milli-Q® water system (Millipore Corporation, Bedford, MA). The Milli-Q® unit treats deionized water by a four-stage purification process. DI water first passes through an activated carbon cartridge (Cat. No. CDFC 012 04) installed upstream of two mixed-bed ion exchange units (Cat. No. CPMB 012 02). Trace organics are removed using a Organex-Q cartridge (Cat. No. CDEX 012 01) composed of activated carbon, anion and cation exchange resins. A 0.22 μm point of use final filter (Cat. No. MPGL 04S K2) was utilized for particle and microbe removal. The pH of the final water is typically near 6.33 and has a resistivity near 18 mega-Ohm-cms.

4.1.2 Tracer: An aqueous solution of sodium dichromate (chemical formula-Na$_2$Cr$_2$O$_7$·2H$_2$O, formula weight-298, assay-99.8% as Na$_2$Cr$_2$O$_7$) was used for tracer studies on the filtration apparatus. The complete UV
spectrum was obtained and a peak observed at 258 nm which was then used as the detection wavelength in all experiments.

4.1.3 Particles: Dilute suspensions of monodisperse polystyrene latex microspheres (Seradyn inc., Indianapolis, IN) in the size range $0.25 \mu m \leq a_p \leq 3.5 \mu m$ were prepared for injection into the feed stream of the membrane unit. Four different particle diameters ($d_p$) viz. $0.482 \pm 0.0049 \mu m$, $0.944 \pm 0.013 \mu m$, $3.189 \pm 0.054 \mu m$ and $7.04 \pm 0.0641 \mu m$ were used in making up the suspensions. Stock solutions of 10% (w/w) solids were diluted in ultrapure water to produce an injection suspension of approximately 1% solids weight. The concentrations of latex in the feed stream was varied by changing the injection rate and duration. The specific gravity of the latices was reported as 1.05.

4.1.4 Feed water pump: Near pluse-free flow of ultrapure water was achieved using a micropump head (Cole-Palmer instrument company, Chicago, IL, Cat. No. 07002-27) fitted on a Ismatec digital variable speed drive (Cole-Palmer instrument company, Chicago, IL, Cat. No. 07617-70). This enables a maximum flow rate of 420 ml/min and a maximum system pressure of 50 psig. The wetted parts in the pumphead were the graphite pressure loaded spur gears; the Teflon O-ring and the SS 316 body. Graphite spur gears are subject to wear on prolonged operation. To prevent any graphitic particles that may result due to attrition from reaching the membrane filter, an in-line filter (Cole Palmer Instrument Company, Chicago, IL, Cat. No. 02909-60) was provided at the pump discharge end. These AAQ grade filters (Balston inc., Lexington, MA)
consisted of borosilicate glass microfiber filter tubes permanently sealed into a transparent nylon holder and had a 98% retention rating for 0.3 μm particles. Positive suction head was provided using a five gallon Nalgene low-density Polyethylene carboy (Fisher Scientific, Cat. No. 02-963BB). A spigot fitted with an adapter was used to accommodate the suction tube.

4.1.5 Flow meter: Feed water flow rate was monitored using a high resolution flow meter (±2% full scale accuracy) fitted with a 150 mm flow tube (Cole Palmer Instrument Company, Chicago, IL, Cat. No. 03227-32). The rotameter fittings were of aluminum and the float material was black glass. An acrylic tripod base with three leveling screws and a spirit level was used for mounting the flow meter vertically. A special magnifying window magnifies the scale in the flow tube for easier reading of the float position. Also, these rotameters had a 16-turn high precision metering valve for precise flow rate control. A similar flow meter was also installed at the reject end of the membrane filter and was used for controlling the system pressure by using the metering valve. The flow meter was calibrated and the results are given below.

<table>
<thead>
<tr>
<th>Rotameter setting</th>
<th>Mean flow rate (ml/sec)</th>
<th>Standard deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>2.036</td>
<td>0.0250</td>
</tr>
<tr>
<td>45</td>
<td>2.368</td>
<td>0.0081</td>
</tr>
<tr>
<td>50</td>
<td>2.725</td>
<td>0.0100</td>
</tr>
<tr>
<td>55</td>
<td>3.029</td>
<td>0.0225</td>
</tr>
<tr>
<td>60</td>
<td>3.380</td>
<td>0.0104</td>
</tr>
<tr>
<td>65</td>
<td>3.723</td>
<td>0.0195</td>
</tr>
<tr>
<td>70</td>
<td>4.055</td>
<td>0.0307</td>
</tr>
<tr>
<td>75</td>
<td>4.383</td>
<td>0.0414</td>
</tr>
<tr>
<td>80</td>
<td>4.681</td>
<td>0.0291</td>
</tr>
<tr>
<td>85</td>
<td>5.020</td>
<td>0.0029</td>
</tr>
<tr>
<td>90</td>
<td>5.378</td>
<td>0.0156</td>
</tr>
</tbody>
</table>
Figure 4.1.1 Flow meter calibration curve. Each measurement was repeated three times. The mean and standard deviation values are given in Table 4.1.1.

4.1.6 Injection system: Initially an attempt was made to affect pulse inputs using a flow through Rheodyne syringe loading sample injector (model 7125, 20 µl sample loop) fitted with a position sensing switch. However, the pressure drop in the connecting tubing (1/32" ID) and the sample loop was very high causing the feed water pump motor to decouple from the pump head. This system was later replaced with a model 22 syringe infusion pump (Harvard Apparatus inc., South Natick, MA) operated in the remote mode. The suspension/solution was injected into the bulk water flow using a luer lok Becton Dickinson plastic syringe. A 22 gauge non-reactive Teflon fluorocarbon resin flexible needle tubing (Fisher Scientific inc. O.D. 0.045", ID 0.027", Cat. No. 14-819-150R)
with a female hub for attachment to the luer tip on the syringe connected
the syringe to the main ultrapure water flow at the entrance to the channel.
The stepper motor which drives the pump is microprocessor controlled for
accurate flow rate control (±1% accuracy and ±0.1% reproducibility) and
remote operation. The pump was operated in the remote mode using
Transistor to Transistor Logic (TTL). Pin #7 is the TTL ground. Pin #17
is the active pin for the remote start/stop function. The logic is:

Pin #17
TTL High (2.5V - 5.0V) Normal running
TTL Low (0V - 0.5V) Pump stops

4.1.7 Detection system: A Spectra 100 flowthrough UV detector (Spectra
Physics inc., San Jose, CA) installed at the filter concentrate side
(membrane channel exit) was used as the detection system in experiments
with tracer and latex particles. The full scale voltage was set at 1.0 V. The
machine output was auto zeroed remotely before every injection using TTL
logic. The auto zero connection on the rear panel of the instrument works
on the following logic:

TTL High (momentary contact open) zeroing starts
TTL Low (momentary contact closure) recorder output set to zero volts

The TTL high state had to be maintained for at least thirty seconds for the
instrument to effectively zero the recorder output. UV data from the
recorder was recorded in a remote fashion. The recorder + and - terminals
were also located in the rear panel. The machine was equipped only with
the standard deuterium lamp. The inlet and exit fluid connections to the
flow cell were made using rigid 1/8" OD (1/16" I.D) Teflon tubing. A preparative flow cell (part number 9551-0070) fitted with sapphire windows formed the heart of the detection system. The path length was set at the maximum value of 3 mm to get an illuminated volume of 4.6 μl. This set-up could handle a maximum flow rate of 6000 ml/min. The detection wavelength was maintained at 258 nm for all tracer and particle experiments. The instrument output was linear for absorbance values up to three times the Absorbance Units Full Scale (AUFS) setting (the recorder output was clipped at 3.1 x the selected voltage range). To attain the maximum information, the AUFS was set at a value that was one-third of the value obtained from a trial injection before every experiment.

4.1.8 Weighing system: Reject flow rate was monitored using a FX-3000 precision electronic balance (A&D company Ltd, Milpitas, CA) coupled with a SER420 serial 4-20 mA converter (Rice Lake Weighing Systems, Rice Lake, WI) to ensure compatibility with the data acquisition system. The FX-3000 is a single range balance with a maximum capacity of 3100 grams and has a least count of 0.01 grams. The balance was set in the stream mode (C3-4) for continuous transmission of data from the RS-232 port. The filter was set for strong/bad environmental conditions (C2-2) because of the presence of an air conditioning vent which gave rise to a draft. The signal transmission rate of the balance had to be set at 1200 baud (C4-1) for the proper communication between the RS-232 output and the digital to analog converter. The balance has an external (N/O) auto zero capability. This point had to maintained at a high (5 V) state for the uninterrupted transmission of data. After every injection and data
acquisition, the balance was re-zeroed by changing the state of the external auto-zero pin to low (0 V). Data in the RS-232 format could not be acquired using the existing data acquisition system. Therefore digital data from the balance had to be converted to analog signals before acquisition. A programmable full scale converter (0 V - 5 V) was employed for this purpose. Using such an arrangement the resolution of the weighing apparatus was improved significantly. The converter was programmed at a positive slope and the full scale could be set as low as fifty grams. Thus, pulse experiments as short as thirty seconds could be run while acquiring sufficient information on the reject flow rate. The SER-420 analog outputs were digitally generated in 4096 discrete steps. Thus the 0 - 5 V output range is accurate to the nearest 0.00122 V. For a 50 g full scale setting this translates to 0.0122 grams which is least count of the balance. It will be seen later that the resolution of the data acquisition system was only 19.5 mV when the balance was set to read a maximum peak-to-peak voltage of 5.0 V. For a 50 g full scale this corresponds to 0.2 grams which is 20 x least count. Thus the limiting factor in measuring flux was not the weighing system but the data acquisition system.

4.1.9 Pressure measurement: A pocket test gauge with a 2.5" dial (Omega Engineering Company, Stamford, CT, Model No. PGT-25L-60) was used to determine the mid-channel pressure. This gauge had a full scale range of 0 - 60 psi. Accurate measurements were made by reading the knife-edge tip pointer moving against a mirrored background.
4.1.10 Tubing and fittings: Flexible Tygon as well as rigid, inert Teflon tubing were used. Quick-disconnect and Teflon fittings were used to connect tubing and transducers to the system. Teflon thread sealant tape was used to ensure water tight connections. A description of the tubing employed is given below in table 4.1.2. A turbulence promoter was installed upstream of the injection system to provide necessary mixing.

Table 4.1.2 Tubing used in the experimental apparatus

<table>
<thead>
<tr>
<th>Section of the apparatus</th>
<th>Tubing material</th>
<th>Tubing size (ID x OD) (inches)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pump suction</td>
<td>Flexible Tygon</td>
<td>3/16 x 1/4</td>
</tr>
<tr>
<td>Pump discharge</td>
<td>Inert Teflon PFA</td>
<td>5/32 x 1/4</td>
</tr>
<tr>
<td>Flow meter inlet</td>
<td>Inert Teflon PFA</td>
<td>5/32 x 1/4</td>
</tr>
<tr>
<td>Flow meter outlet</td>
<td>Inert Teflon PFA</td>
<td>5/32 x 1/4</td>
</tr>
<tr>
<td>Turbulence promoter</td>
<td>Inert Teflon PFA</td>
<td>8 mm x 5.6 mm</td>
</tr>
<tr>
<td>Inlet to filtration unit</td>
<td>Inert Teflon PFA</td>
<td>5/32 x 1/4</td>
</tr>
<tr>
<td>Inlet to UV detector</td>
<td>Inert Teflon PFA</td>
<td>1/16 x 1/8</td>
</tr>
<tr>
<td>UV detector outlet</td>
<td>Inert Teflon PFA</td>
<td>1/16 x 1/8</td>
</tr>
<tr>
<td>Reject tubing</td>
<td>Flexible Tygon</td>
<td>3/16 x 9/16</td>
</tr>
</tbody>
</table>

4.1.11 Data acquisition system (DAS): PacqManager (version 1.05h) was the software used for interfacing between the Macpacq MP-10 hardware system (BIOPAC systems, Goleta, CA) and a Macintosh computer. Remote digital control of various equipment as well as data acquisition could be accomplished using this DAS. Two channels of analog data were utilized in the input mode for data acquisition viz. signal from the UV detector (channel 1) and signal from the weighing balance (channel 2). Three digital channels were used in the output mode for control purposes viz. auto-zeroing the UV detector (channel 2), re-zeroing the weighing balance (channel 1) and for remote operation of the syringe infusion pump (channel 0). All connectors marked ground or negative in
the external circuitry were connected to the GND A pin (because none of the incoming signals were expected to have a negative excursion) while the connectors marked positive in the external circuitry were connected to the corresponding channel pins. The macro written for making impulse inputs to the system and monitoring system outputs is given below (see user manual for Macpacq, 1989).

```
01  acquisition analog ; Only analog signals to acquire
02  triggermode immediate ; Start acquisition immediately
03  samplemode internal ; Use the 2 MHz internal clock
04  channels 1 2 ; Channels 1 and 2 for acquisition
06  bufferlength 4000 ; Number of samples to acquire
07  rate 100 ; Sampling rate (samples per second)
10  iodirection 15 ; Digital channels 0-3 are outputs
20  outputdata 6 ; Send 5V signal on channels 1 and 2
21  wait 30 ; Wait 30 milliseconds
22  outputdata 2 ; Make channel 1 high and 2 low
23  wait 3700 ; Wait 3.7 seconds
40  outputdata 3 ; Send 5V signal on channels 0 and 1
41  wait 200 ; Wait 200 milliseconds
42  outputdata 2 ; Make channel 1 high and 0 low
43  startacquisition ; Obtain data as specified in lines 1-7
45  halt ; Stop acquisition
```

The flow chart explaining the logic behind the macro commands is as follows:
Figure 4.1.2 Flow diagram for the impulse input macro.
When used as an oscilloscope, the DAS samples instantaneous signals and hence noisy weight data were acquired. To smooth any small variations in the incoming signal an RC circuit (see Figure 4.1.3) with a time constant of 0.1 seconds was installed at the input end of the DAS.

![RC Circuit Diagram](image)

Figure 4.1.3 The RC circuit for filtering any noise in the incoming weight signal.

### 4.1.12 Membrane filtration unit:

The filtration apparatus comprised of three parts: the top piece with the fittings for tubing and monitoring equipment, the bottom piece serving to support the flow channel in the middle. The top and bottom parts were machined from Plexi-glass blocks. Schematic diagrams of the top piece and a sampling port are given below.

![Plan View Diagram](image)

All dimensions in inches. Total 24 holes (12 on each side). Thickness 1 inch.

Figure 4.1.4 Plan view of the filter top piece.
Figure 4.1.5 Front view of a sampling port.

An accurately machined Teflon sheet (30 mils = 762 μm thick) was sandwiched between the top and bottom plexi-glass pieces and served as the flow channel. Two aluminum washers running along the length of the top piece served as washers. Twenty-four fasteners were each tightened to a torque of 30 inch-pounds and prevented any leaks. The plan view of the flow channel is given in Figure 4.1.6.

Figure 4.1.6 Machine drawing for the Teflon flow channel.
4.1.13 Membranes: Two types of hydrophilic membranes were used in the experiments: Durapore (modified polyvinylidene difluoride) and track-etch (bisphenol polycarbonate). The important characteristics are given below in Table 4.1.3.

Table 4.1.3 Information on membrane filters used in experiments.

<table>
<thead>
<tr>
<th>Type</th>
<th>Main Characteristics</th>
<th>Chemical composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Track-etch</td>
<td>Pore Size: 0.1 µm</td>
<td>bisphenol polycarbonate</td>
</tr>
<tr>
<td></td>
<td>Thickness: 10 µm±5%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Porosity: 10%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Supplier: Poretics, Corp.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Livemore, CA.</td>
<td></td>
</tr>
<tr>
<td>Durapore</td>
<td>Pore Size: 0.1 µm (nominal)</td>
<td>modified polyvinylidene difluoride</td>
</tr>
<tr>
<td></td>
<td>Thickness: 125 µm</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Porosity: 70%</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bubble point: 70 psi</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Supplier: Millipore Corp.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Bedford, MA.</td>
<td></td>
</tr>
</tbody>
</table>

Track-etch membranes have near-perfect cylindrical capillaric pores and thus have an absolute pore diameter. Other membrane types are characterized by a nominal pore size rating because the "pores" are tortuous and not well defined; water passes through a polymer mesh from one side of the membrane to the other. Track-etch membranes are very difficult to handle because of their small thicknesses. Durapore membranes are more than ten times thicker and hence are easier to handle (see Table 4.1.3). Initial experiments were conducted with the Track-etch membranes but owing to the great difficulty in changing membranes between experiments the Durapore membranes were substituted in later experiments. A special cut was ordered for both membranes. The Track-
etch membranes were purchased pre-cut to the required dimensions (20" long x 2" wide). The Durapore membrane was purchased as a sheet (1' long x 10" wide) and membranes of the required size were cut in the lab.

4.1.14 Experimental set-up: A schematic of the experimental apparatus showing the different sub-systems is depicted in Figure 4.1.7. Permeate flow is represented as being monitored whereas reject flow was actually measured. The permeate water was not recycled owing to the risk of contamination from the collection tank. Water was circulated for approximately five minutes at the desired flow rate before making injections. The UV detector was switched on at least fifteen minutes before running an experiment to allow the Deuterium lamp to reach steady operation. Particle suspensions were made immediately preceding experiments so as to decrease chances of flocculation/aggregation arising from contamination in dirty glass ware. Data acquisition started only after introducing the pulse in the main stream. Hence a time equal to half the pulse width was added to the time recorded in the data file. In experiments with the Track-etch membrane higher pressures were necessary for significant permeation. A silicone high vacuum grease (Dow corning corp, Midland, MI) was used to prevent any leakages from the filter unit. This was not necessary in experiments with the Durapore membrane owing to its higher permeability and greater thickness which helped form a better seal.
Figure 4.1.7 Schematic of the experimental set-up used for measuring the RTD of both tracer solutions and particle suspensions.
4.2 Experimental results and discussion:

4.2.1 Tracer study: Residence time distributions (RTD) of an ionic tracer (Na$_2$Cr$_2$O$_7$) were measured by injecting pulses using the apparatus shown in Figure 4.1.7. Dissolved molecules of tracer are assumed to follow fluid streamlines. Obtaining the RTD therefore aids in understanding the fluid mechanics of the experimental system. RTDs of pulse inputs of an aqueous dichromate solution were analyzed using the equations developed in section 3.1. In other words, the tracer study was done to calibrate the apparatus and to take into account any non-idealities that exist (dead spaces, entrance and exit effects, mixing in the inert tubing etc.). Figure 4.2.1 shows the data acquired during one tracer experiment.

Tracer injections were made at main flow rates in the range 2.368 ml/sec $\leq Q \leq 5.378$ ml/sec which correspond to average inlet linear velocities of 15.54 cm/sec $\leq$ $U_o$ $\leq$ 35.29 cm/sec (the channel cross-section dimensions are 2 cms wide x 762 $\mu$m high). Effluent curves obtained from the UV detector were analyzed to determine the first response of the detector to the presence of tracer in the channel effluent. The threshold for this first response was set at the resolution of the data acquisition system (20 mV). Residence time in the inert tubing at the channel inlet and exit was accounted for as follows. Influent flow was well mixed (because of the turbulence promoter just upstream of the injection point) and therefore the tracer was assumed to move at the average velocity of the flow between the point of injection and the entrance to the membrane channel. Fully developed parabolic profile was assumed at the channel exit (because of
Figure 4.2.1 Experimental data from one tracer injection experiment.
The monotonically increasing function gives information on the reject flux.
The pulse shown is the response of the UV detection system and gives the RTD.
longer tubing of smaller diameter). The flow rate measured by the weighing balance was used to calculate an average velocity. The maximum velocity for Poiseuille flow in tubes is twice the average value. Hence for first response studies, two times the average velocity was the value used for flow in the inert exit tubing from the channel exit to the detection system. Thus, the time spent in the channel (length = 46 cms) was obtained by subtracting the time spent in the inlet and outlet tubing from the experimentally observed first response. The mathematical prediction of the first response is obtained from running the program PULSE (see Appendix B) and substituting the corresponding flow parameters and channel dimensions. The "particle" size of the tracer molecules was taken as zero. The tracer study was performed using the Durapore membrane and the results are given in Table 4.2.1. The experimental data were correlated with the mathematical predictions and a linear fit was obtained (see Figure 4.2.2). This regression was used to adjust subsequent experimental observations of first responses obtained from injecting dilute suspensions of colloidal latex.
Table 4.2.1 Results of a tracer study on the porous channel using the Durapore membrane.

<table>
<thead>
<tr>
<th>Flow in (ml/sec)</th>
<th>Δp † (psi)</th>
<th>Reject flow (ml/sec)</th>
<th>A&amp;DFS § (grams)</th>
<th>AUFS ‡</th>
<th>Pulse width (ms)</th>
<th>Permeation rate † † ( V_w ) (cm/sec)</th>
<th>Expt first response ‡ ‡ (s)</th>
<th>Expt time spent in channel * (s)</th>
<th>Predicted time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.368</td>
<td>2.75</td>
<td>0.9338±0.0065</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0162±7.3x10⁻⁵</td>
<td>3.76±0.015</td>
<td>3.2494</td>
<td>3.2279</td>
</tr>
<tr>
<td>2.725</td>
<td>3.00</td>
<td>1.0213±0.0041</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0193±4.6x10⁻⁵</td>
<td>3.42±0.024</td>
<td>2.9616</td>
<td>2.8855</td>
</tr>
<tr>
<td>3.029</td>
<td>3.25</td>
<td>1.1132±0.0038</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0216±4.2x10⁻⁵</td>
<td>3.13±0.028</td>
<td>2.7065</td>
<td>2.6252</td>
</tr>
<tr>
<td>3.380</td>
<td>4.25</td>
<td>1.1878±0.008</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0248±9.1x10⁻⁵</td>
<td>2.91±0.033</td>
<td>2.5101</td>
<td>2.4104</td>
</tr>
<tr>
<td>4.055</td>
<td></td>
<td>1.35±0.0047</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0306±8.45x10⁻⁵</td>
<td>2.53±0.019</td>
<td>2.1931</td>
<td>2.0679</td>
</tr>
<tr>
<td>4.055</td>
<td>5.00</td>
<td>1.34±0.0075</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0306±5.3x10⁻⁵</td>
<td>2.54±0.007</td>
<td>2.1858</td>
<td>2.0694</td>
</tr>
<tr>
<td>4.681</td>
<td>6.00</td>
<td>1.4945±0.0067</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0360±7.6x10⁻⁵</td>
<td>2.26±0.024</td>
<td>1.9521</td>
<td>1.8329</td>
</tr>
<tr>
<td>5.378</td>
<td>6.75</td>
<td>1.6368±0.0067</td>
<td>50</td>
<td>0.02</td>
<td>200</td>
<td>0.0423±7.6x10⁻⁵</td>
<td>2.08±0.032</td>
<td>1.8009</td>
<td>1.6418</td>
</tr>
</tbody>
</table>

† Mid channel pressure; § A&D balance full scale; ‡ Spectra-100 UV full scale; † † membrane area for permeation 84.48 cm²
‡ pulse half width added to the observed time; * plug flow assumed at the inlet and parabolic profile at the exit tubing.
4.2.2 Particle studies: Pulse inputs similar to that described for the tracer were made using dilute particle suspensions and RTDs obtained. Particles smaller than the membrane pore diameter can potentially enter membrane passages and cause irreversible fouling thereby changing the permeability of the membrane during the experiment. To avoid this effect, only latex particles larger than the pore size of the membrane were studied. Particles of four different radii were studied: $a_p = 0.24 \, \mu\text{m}, 0.47 \, \mu\text{m}, 1.6 \, \mu\text{m}$ and $3.5 \, \mu\text{m}$. The mathematically predicted first responses were adjusted using the following regression equation derived from the tracer study:

$$\text{Time}_{\text{corrected}} = 0.92714 \times \text{Time}_{\text{predicted}} + 0.27068 \quad (4.2.1)$$
4.2.2.1 Study on \((a_p =) 0.24 \, \mu m\) particles:

White, spherical, polystyrene latex particles of radius \(0.241 \pm 0.0049 \, \mu m\) were used in experiments conducted with the Durapore membrane. Table 4.2.2 summarizes important instrument settings, the hydrodynamic parameters and the first response values obtained from both experiment and theory. The output of the detection system was sampled at the rate of 100 sec\(^{-1}\). Thus RTDs were obtained as volt - seconds plots. The area under such a curve gives information about the sampled mass (assuming linear concentration - volt behavior). A typical response of the UV detecting system to a pulse input of these particles, normalized by the encompassed area, is shown in Figure 4.2.3. As in the case of calculations for small, spherical bacteria sized particles (Figure 3.3.9) the transport of these latex particles is dominated by drag forces associated with the flux of permeate through the membrane. One sharp peak is observed. The simulated residence time distribution of the particles in the membrane filter introduced as a "Dirac" pulse under the given hydrodynamic conditions is given in Figure 4.2.4. Two interesting differences are seen between the experimentally observed response and the simulated RTD. The time needed for the signal to attenuate to 20% of the maximum value is close to 3.5 seconds in the idealized case while experimental observation gives a much higher value of around six seconds. This might be due the the finite pulse width of the particle inputs in the experiments. Impulse inputs of these particles were made in a span of 200 milliseconds. While the sharp leading edge is associated with the first front of fastest moving
Table 4.2.2 Results of pulse inputs of 0.24 μm radius particles in the porous channel using the Durapore membrane.

<table>
<thead>
<tr>
<th>Flow in (ml/sec)</th>
<th>ΔP† (psi)</th>
<th>Reject flow (ml/sec)</th>
<th>A&amp;DFS§ (grams)</th>
<th>AUFS£</th>
<th>Pulse width (ms)</th>
<th>Permeation rate†† $V_w$ (cm/sec)</th>
<th>Expt first response‡ (s)</th>
<th>Expt time spent in channel* (s)</th>
<th>Predicted time (s)</th>
<th>Correlated time* (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.380</td>
<td>3.5</td>
<td>1.392±0.011</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0225±1.3x10^{-4}</td>
<td>2.69±0.048</td>
<td>2.35±0.048</td>
<td>2.21</td>
<td>2.32</td>
</tr>
<tr>
<td>3.723</td>
<td>3.0</td>
<td>2.089±0.015</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0185±1.73x10^{-4}</td>
<td>2.19±0.024</td>
<td>1.95±0.024</td>
<td>1.70</td>
<td>1.85</td>
</tr>
<tr>
<td>3.723</td>
<td>4.5</td>
<td>1.187±0.007</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0287±8.4x10^{-5}</td>
<td>2.81±0.022</td>
<td>2.42±0.022</td>
<td>2.31</td>
<td>2.41</td>
</tr>
<tr>
<td>4.055</td>
<td>3.0</td>
<td>2.385±0.016</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0189±1.8x10^{-4}</td>
<td>1.98±0.021</td>
<td>1.77±0.021</td>
<td>1.52</td>
<td>1.68</td>
</tr>
<tr>
<td>4.055</td>
<td>5.0</td>
<td>1.263±0.006</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0316±7.2x10^{-5}</td>
<td>2.63±0.061</td>
<td>2.27±0.061</td>
<td>2.15</td>
<td>2.26</td>
</tr>
<tr>
<td>4.383</td>
<td>3.5</td>
<td>2.515±0.017</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0211±1.9x10^{-4}</td>
<td>1.88±0.033</td>
<td>1.69±0.033</td>
<td>1.43</td>
<td>1.59</td>
</tr>
<tr>
<td>4.383</td>
<td>5.0</td>
<td>1.727±0.016</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0300±1.9x10^{-4}</td>
<td>2.25±0.014</td>
<td>1.97±0.014</td>
<td>1.75</td>
<td>1.89</td>
</tr>
<tr>
<td>4.681</td>
<td>5.5</td>
<td>1.754±0.015</td>
<td>100</td>
<td>0.005</td>
<td>200</td>
<td>0.0331±1.7x10^{-4}</td>
<td>2.16±0.023</td>
<td>1.89±0.023</td>
<td>1.68</td>
<td>1.83</td>
</tr>
</tbody>
</table>

† Mid channel pressure; § A&D balance full scale; £ Spectra-100 UV full scale; †† membrane area for permeation 84.48 cm²
‡ pulse half width added to the observed time; * plug flow assumed at the inlet and parabolic profile at the exit tubing.
* The mathematical prediction was scaled using the regression obtained from the tracer study: $t_{corr} = t_{predict} \times 0.92714 + 0.27068$
Figure 4.2.3 Residence time distribution of particles of radius 0.24 µm in the membrane filter (the response of the UV detector is normalized by the area under the curve).
Fraction of particles in the influent

Time elapsed after particles entered the channel (sec)

Q_in = 4.055 ml/sec
U_m = 39.91 cm/sec
V_w = 0.032 cm/sec
Length = 46 cm
input: Dirac pulse
β_critical = 0.65
time(β = 0.99) = 38 sec
mid-channel shear rate: 667 1/sec

Figure 4.2.4 Computer simulation of the RTD of particles of radius 0.24 μm
trajectories, particles injected later in time will contribute to the observed pulse width. This makes the response of the UV detector to the non-ideal impulse input wider than the expected response for an ideal Dirac pulse. Another point of difference is in the long trailing edge observed in the experimental RTD. Theory predicts that by fifteen seconds almost all particles should have traversed the length of the channel and therefore no signal from the UV detector is expected. Experimental observation is counter to this expectation. At fifteen seconds, the UV detector shows a finite response. Once a particle is captured by the membrane due to permeation drag, theory assumes that it is removed from the flow. If this were indeed the case, the trailing edge would be expected to be shorter. The phenomenon that is responsible for this "delayed-response" is thought to be a shear-induced viscous resuspension of the layer of particles from the membrane surface to the bulk flow. In Figure 4.2.5, the experimental observations of the passage time corresponding to the fastest trajectory are plotted along with theoretically predicted values as a function of the influent flow rate. The wall permeation rate was different for each of the pairs of points. Reasonably good correspondence is observed between theory and experiment. From Table 4.2.3, we can see that permeation drag is four to five orders of magnitude greater than inertial effects and hence are expected to control the transport of these particles in the membrane filter. The theoretical predictions of the first passage time are compared to the experimental observations in Figure 4.2.6.
Figure 4.2.5 Experimental observations and predicted values of the first response in a porous channel as a function of influent flow rate for a suspension of particles of radius \( a_p = 0.25 \ \mu m \).

Table 4.2.3 Order of magnitude analysis of lateral forces on a \( a_p = 0.24 \ \mu m \) particle in a channel of height 762 \( \mu m \) under conditions listed below\(^\S\).

| \( Q \) (ml/min) | \( U_m \) (cm/sec) | \( V_w \) (cm/sec) | \( \Re_p \) \( (U_m a_p / \nu) \) | permeation drag \( (V_w / U_m) \) | inertial lift \( (\Re_p \kappa^2) \) | ratio of permeation drag to lift |
|-------------------|-------------------|-------------------|----------------|----------------|----------------|----------------|----------------|
| 3.380             | 33.27             | 0.0225            | 0.0798         | 6.76x10^-4     | 7.92x10^-9     | 85391.1        |
| 3.723             | 36.64             | 0.0185            | 0.0879         | 5.05x10^-4     | 8.72x10^-9     | 57869.4        |
| 3.723             | 36.64             | 0.0287            | 0.0879         | 7.83x10^-4     | 8.72x10^-9     | 89775.8        |
| 4.055             | 39.91             | 0.0189            | 0.0958         | 4.74x10^-4     | 9.50x10^-9     | 49836.1        |
| 4.055             | 39.91             | 0.0316            | 0.0958         | 7.92x10^-4     | 9.50x10^-9     | 83323.8        |
| 4.383             | 43.14             | 0.0211            | 0.1035         | 4.89x10^-4     | 1.03x10^-9     | 47621.5        |
| 4.383             | 43.14             | 0.0300            | 0.1035         | 6.95x10^-4     | 1.03x10^-9     | 67708.3        |
| 4.681             | 46.07             | 0.0331            | 0.1106         | 7.18x10^-4     | 1.10x10^-9     | 65495.9        |

\(^\S\kappa=0.0003\)
Figure 4.2.6 Comparison of theoretical predictions of first passage time and experimental observations for particles of radius 0.24 μm. The 95% confidence intervals of the true slope and intercept are given.

The experimental data are highly correlated with the theoretical predictions ($r^2 = 0.997$). However, the slope and the intercept of the straight line fit are statistically different from the anticipated values of one and zero respectively.

4.2.2.2 Study on ($a_p = $) 0.47, 1.6 and 3.5 μm particles:

Experiments were also performed using white, spherical, polystyrene latex particles of radius 0.472 ± 0.013 μm, 1.594 ± 0.054 μm and 3.52 ± 0.0641 μm. These experiments were conducted with a track-etch membrane having a pore size of 0.1 μm. Tables 4.2.4, 4.2.5 and 4.2.6 summaries important instrument settings, the hydrodynamic parameters and the first response values obtained from these experiments. Calculated first response times are also shown.
Table 4.2.4 Results of pulse inputs of 0.47 μm radius particles in the porous channel using the Track-etch membrane.

<table>
<thead>
<tr>
<th>Flow in (ml/sec)</th>
<th>ΔP † (psi)</th>
<th>Reject flow (ml/sec)</th>
<th>A&amp;DFS § (grams)</th>
<th>AUFS £</th>
<th>Pulse width (ms)</th>
<th>Permeation rate † † ( V_w ) (cm/sec)</th>
<th>Expt first response ‡ (s)</th>
<th>Expt time spent in channel * (s)</th>
<th>Predicted time (s)</th>
<th>Correlated time ‡ ‡ (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.036</td>
<td>2.5</td>
<td>1.353 ± 0.0032</td>
<td>150</td>
<td>0.002</td>
<td>250</td>
<td>0.0077 ± 3.6 x 10⁻⁵</td>
<td>3.38 ± 0.039</td>
<td>3.00 ± 0.039</td>
<td>2.85</td>
<td>2.91</td>
</tr>
<tr>
<td>2.725</td>
<td>3.5</td>
<td>1.700 ± 0.0041</td>
<td>200</td>
<td>0.002</td>
<td>250</td>
<td>0.0116 ± 6.4 x 10⁻⁵</td>
<td>2.62 ± 0.05</td>
<td>2.32 ± 0.049</td>
<td>2.20</td>
<td>2.31</td>
</tr>
<tr>
<td>3.380</td>
<td>4.5</td>
<td>2.008 ± 0.0082</td>
<td>200</td>
<td>0.002</td>
<td>250</td>
<td>0.0387 ± 9.2 x 10⁻⁵</td>
<td>2.22 ± 0.055</td>
<td>2.01 ± 0.055</td>
<td>1.81</td>
<td>1.95</td>
</tr>
<tr>
<td>3.380</td>
<td>5.5</td>
<td>1.685 ± 0.0047</td>
<td>200</td>
<td>0.002</td>
<td>250</td>
<td>0.0192 ± 5.2 x 10⁻⁵</td>
<td>2.38 ± 0.042</td>
<td>2.09 ± 0.042</td>
<td>1.99</td>
<td>2.12</td>
</tr>
<tr>
<td>3.380</td>
<td>6.5</td>
<td>1.356 ± 0.0047</td>
<td>150</td>
<td>0.002</td>
<td>250</td>
<td>0.0229 ± 5.2 x 10⁻⁵</td>
<td>2.66 ± 0.039</td>
<td>2.31 ± 0.040</td>
<td>2.24</td>
<td>2.35</td>
</tr>
<tr>
<td>3.380</td>
<td>7.5</td>
<td>0.961 ± 0.0014</td>
<td>150</td>
<td>0.002</td>
<td>250</td>
<td>0.0273 ± 1.5 x 10⁻⁵</td>
<td>3.11 ± 0.050</td>
<td>2.63 ± 0.050</td>
<td>2.71</td>
<td>2.78</td>
</tr>
<tr>
<td>4.055</td>
<td>6.0</td>
<td>2.177 ± 0.0065</td>
<td>200</td>
<td>0.002</td>
<td>250</td>
<td>0.0212 ± 7.3 x 10⁻⁵</td>
<td>1.97 ± 0.026</td>
<td>1.74 ± 0.026</td>
<td>1.60</td>
<td>1.75</td>
</tr>
<tr>
<td>4.055</td>
<td>7.0</td>
<td>1.767 ± 0.0081</td>
<td>200</td>
<td>0.002</td>
<td>250</td>
<td>0.0259 ± 9.1 x 10⁻⁵</td>
<td>2.16 ± 0.020</td>
<td>1.88 ± 0.020</td>
<td>1.79</td>
<td>1.93</td>
</tr>
<tr>
<td>4.055</td>
<td>8.0</td>
<td>1.424 ± 0.0073</td>
<td>150</td>
<td>0.002</td>
<td>250</td>
<td>0.0297 ± 8.2 x 10⁻⁵</td>
<td>2.36 ± 0.031</td>
<td>2.04 ± 0.030</td>
<td>2.00</td>
<td>2.13</td>
</tr>
<tr>
<td>4.055</td>
<td>9.0</td>
<td>1.082 ± 0.0064</td>
<td>150</td>
<td>0.002</td>
<td>250</td>
<td>0.0336 ± 7.1 x 10⁻⁵</td>
<td>2.73 ± 0.039</td>
<td>2.31 ± 0.038</td>
<td>2.31</td>
<td>2.41</td>
</tr>
</tbody>
</table>

† Mid channel pressure; § A&D balance full scale; £ Spectra-100 UV full scale; † † membrane area for permeation 84.48 cm²
‡ pulse half width added to the observed time; * plug flow assumed at the inlet and parabolic profile at the exit tubing.
* The mathematical prediction was scaled using the regression obtained from the tracer study: \( t_{corr} = t_{predict} \times 0.92714 + 0.27068 \)
Table 4.2.5 Results of pulse inputs of 1.6 μm radius particles in the porous channel using the Track-etch membrane.

<table>
<thead>
<tr>
<th>Flow in (ml/sec)</th>
<th>ΔP (psi)</th>
<th>Reject flow (ml/sec)</th>
<th>A&amp;DFS (grams)</th>
<th>AUFS</th>
<th>Pulse width (ms)</th>
<th>Permeation rate ( V_w ) (cm/sec)</th>
<th>Expt first response ( t^* ) (s)</th>
<th>Expt time spent in channel ( t ) (s)</th>
<th>Predicted time (s)</th>
<th>Correlated time ( t^* ) (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.725</td>
<td>3.50</td>
<td>1.688±0.017</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0126±2.0x10^-4</td>
<td>2.61±0.029</td>
<td>2.307±0.0254</td>
<td>2.20</td>
<td>2.31</td>
</tr>
<tr>
<td>2.725</td>
<td>4.75</td>
<td>1.25±9.1x10^-3</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0176±1.0x10^-4</td>
<td>3.09±0.026</td>
<td>2.722±0.0203</td>
<td>2.58</td>
<td>2.66</td>
</tr>
<tr>
<td>2.725</td>
<td>5.50</td>
<td>0.979±7.5x10^-3</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0206±8.4x10^-5</td>
<td>3.53±0.052</td>
<td>3.054±0.0395</td>
<td>2.95</td>
<td>3.01</td>
</tr>
<tr>
<td>3.380</td>
<td>4.75</td>
<td>1.896±0.0346</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0179±3.8x10^-4</td>
<td>2.25±0.065</td>
<td>1.995±0.0281</td>
<td>1.88</td>
<td>2.01</td>
</tr>
<tr>
<td>3.380</td>
<td>6.00</td>
<td>1.453±0.0146</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.023±1.6x10^-4</td>
<td>2.62±0.046</td>
<td>2.295±0.0454</td>
<td>2.16</td>
<td>2.27</td>
</tr>
<tr>
<td>3.380</td>
<td>6.75</td>
<td>1.175±0.0186</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0261±2.1x10^-4</td>
<td>2.95±0.024</td>
<td>2.543±0.0217</td>
<td>2.43</td>
<td>2.52</td>
</tr>
<tr>
<td>4.055</td>
<td>6.0</td>
<td>2.046±0.0293</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0237±3.3x10^-4</td>
<td>2.02±0.026</td>
<td>1.776±0.0131</td>
<td>1.65</td>
<td>1.80</td>
</tr>
<tr>
<td>4.055</td>
<td>7.0</td>
<td>1.656±0.0216</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0281±2.4x10^-4</td>
<td>2.26±0.027</td>
<td>1.978±0.0358</td>
<td>1.85</td>
<td>1.99</td>
</tr>
<tr>
<td>4.055</td>
<td>8.0</td>
<td>1.243±0.0128</td>
<td>10</td>
<td>0.005</td>
<td>400</td>
<td>0.0328±1.46x10^-4</td>
<td>2.67±0.036</td>
<td>2.382±0.04</td>
<td>2.17</td>
<td>2.28</td>
</tr>
</tbody>
</table>

\( ^\dagger \) Mid channel pressure; \( ^\S \) A&D balance full scale; \( ^\ddagger \) Spectra-100 UV full scale; \( ^{\dagger\ddagger} \) membrane area for permeation 84.48 cm²

\( ^\ddagger \) pulse half width added to the observed time; * plug flow assumed at the inlet and parabolic profile at the exit tubing.

\( ^\star \) The mathematical prediction was scaled using the regression obtained from the tracer study: \( t_{corr} = t_{predict} \times 0.92714 + 0.27068 \)
Table 4.2.6 Results of pulse inputs of 3.5 μm radius particles in the porous channel using the Track-etch membrane.

<table>
<thead>
<tr>
<th>Flow in (ml/sec)</th>
<th>ΔP †</th>
<th>Reject flow (ml/sec)</th>
<th>AUFS ‡</th>
<th>Pulse width (ms)</th>
<th>Permeation rate†† ( V_w ) (cm/sec)</th>
<th>Expt first response †‡ (s)</th>
<th>Expt time spent in channel * (s)</th>
<th>Predicted time (s)</th>
<th>Correlated time †* (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.725</td>
<td>3.5</td>
<td>1.765±2.9x10⁻³</td>
<td>0.002</td>
<td>300</td>
<td>0.0108±3.3x10⁻⁵</td>
<td>2.54±0.055</td>
<td>2.253±0.0559</td>
<td>2.15</td>
<td>2.26</td>
</tr>
<tr>
<td>3.380</td>
<td>4.25</td>
<td>2.071±0.017</td>
<td>0.002</td>
<td>300</td>
<td>0.0147±1.9x10⁻⁴</td>
<td>2.14±0.039</td>
<td>1.895±0.0391</td>
<td>1.78</td>
<td>1.92</td>
</tr>
<tr>
<td>4.055</td>
<td>5.0</td>
<td>2.359±0.029</td>
<td>0.002</td>
<td>300</td>
<td>0.0189±3.3x10⁻⁴</td>
<td>1.88±0.057</td>
<td>1.669±0.0576</td>
<td>1.52</td>
<td>1.68</td>
</tr>
<tr>
<td>4.681</td>
<td>6.0</td>
<td>2.602±5.5x10⁻³</td>
<td>0.002</td>
<td>300</td>
<td>0.0235±6.2x10⁻⁵</td>
<td>1.69±0.050</td>
<td>1.502±0.0501</td>
<td>1.36</td>
<td>1.53</td>
</tr>
<tr>
<td>5.378</td>
<td>7.0</td>
<td>2.825±8x10⁻³</td>
<td>0.005</td>
<td>300</td>
<td>0.0289±9.0x10⁻⁵</td>
<td>1.53±0.019</td>
<td>1.352±0.0197</td>
<td>1.22</td>
<td>1.40</td>
</tr>
</tbody>
</table>

† Mid channel pressure; ‡ Spectra-100 UV full scale; †† membrane area for permeation 84.48 cm²

‡ Pulse half width added to the observed time; * plug flow assumed at the inlet and parabolic profile at the exit tubing.

* The mathematical prediction was scaled using the regression obtained from the tracer study: \( t_{corr} = t_{predict} \times 0.92714 + 0.27068 \)
Figure 4.2.7 Residence time distribution of particles of radius 0.47 μm in the membrane filter (the response of the UV detector has been normalized to the area under the curve)
Figure 4.2.8 Residence time distribution of 1.6 μm radius particles in the membrane filter (the response of the UV detector is normalized by the area under the curve).
Figure 4.2.9 Residence time distributions of particles of radius 3.5 μm in the membrane filter (the response of the detector has been normalized by the area under the curve).
Figure 4.2.10 Computer simulation of the RTD of particles of radius 0.47 μm.

Qin = 4.055 ml/sec
Um = 39.91 cm/sec
Vw = 0.03 cm/sec
Length = 46 cms
input: Dirac pulse
β critical = 0.62
time(β = 0.99) = 35 sec
mid-channel shear rate: 667 1/sec
Figure 4.2.11 Computer simulation of the RTD of particles of radius 1.6 μm
Figure 4.2.12 Computer simulation of the RTD of particles of radius 3.5 \( \mu \)m.

Qin = 4.055 ml/sec
Um = 39.91 cm/sec
Vw = 0.019 cm/sec
Length = 46 cm
input: Dirac pulse
\( \beta \)critical = 0.45
\( \text{time}(\beta = 0.99) = 6.6 \text{sec} \)
mid-channel shear rate: 821 1/sec
Figures 4.2.7, 4.2.8 and 4.2.9 are similar to Figure 4.2.3 and they show the normalized experimental residence time distributions of particles of radius 0.47 μm, 1.6 μm and 3.5 μm respectively. In all cases a monomodal distribution is observed with a sharp leading edge and a long trailing edge. This indicates the importance of permeation drag in determining the transport of particles in this size range under the existing hydrodynamic conditions. Computer generated residence time distributions of these particles are given in Figures 4.2.10, 4.2.11 and 4.2.12. Observations similar to that of the smaller (a_p=0.24 μm) particle are also made in each of these cases. Finite pulse width of experimental inputs to the system result in wider responses at the channel exit than those calculated from theory. Also, particles are detected at times greater than the theoretically predicted last response. Leighton and Acrivos (1986) had demonstrated the phenomenon of resuspension of settled particles in viscous systems (at low values of the Reynolds number) arising from shear-induced interparticle interactions. Such processes are believed to transport particles deposited on the membrane (due to drag forces) in a direction towards the bulk flow. Eventually, these particles exit the channel at times far greater than values calculated from considerations of fluid inertia alone. This effect is seen clearly in the experimental response for the biggest particle investigated (a_p=3.5 μm). By including the effects of fluid inertia alone, the last response is expected to be around seven seconds after injection. The shear-induced transport is proportional to the shear-rate and to the square of the particle radius. The average value for the mid-channel shear rate for this particle is the highest (821 sec\(^{-1}\) compared to values around 660 sec\(^{-1}\) for
other particles). Thus, both shear and size effects are important in this case resulting in a long trailing edge for the experimentally determined RTD. Tables 4.2.7, 4.2.8 and 4.2.9 give estimates of the ratio of permeation drag and lift forces on these particles under the existing axial and transverse velocities. It should be noted that the particle Reynolds numbers, $Re_p$, in all the cases do not satisfy the necessary criterion for the theory described in section 3.3, i.e. $Re_p < 1$ and therefore higher order terms in the perturbation series expansion for the inertial effects should be considered. The relative importance of inertial effects can be observed to increase with particle size. For the small ($a_p = 0.47 \mu m$) particle, effects of permeation drag are three to four orders of magnitude greater than effects arising from fluid inertia while for the large ($a_p = 3.5 \mu m$) particle, permeation drag is only one order of magnitude larger than inertial effects.

Table 4.2.7 Order of magnitude analysis of lateral forces on a $a_p = 0.47 \mu m$ particle in a channel of height 762 $\mu m$ under conditions listed below.$^8$

<table>
<thead>
<tr>
<th>$Q$ (ml/min)</th>
<th>$U_m$ (cm/sec)</th>
<th>$V_w$ (cm/sec)</th>
<th>$Re_p$ ($U_m a_p / \nu$)</th>
<th>permeation drag ($V_w / U_m$)</th>
<th>inertial lift ($Re_p \kappa^2$)</th>
<th>ratio of permeation drag to lift</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.306</td>
<td>22.70</td>
<td>0.0077</td>
<td>0.1067</td>
<td>3.39x10^{-4}</td>
<td>4.06x10^{-8}</td>
<td>8359.4</td>
</tr>
<tr>
<td>2.725</td>
<td>26.82</td>
<td>0.0116</td>
<td>0.1261</td>
<td>4.32x10^{-4}</td>
<td>4.80x10^{-8}</td>
<td>9018.4</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0155</td>
<td>0.1564</td>
<td>4.66x10^{-4}</td>
<td>5.95x10^{-8}</td>
<td>7832.5</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0192</td>
<td>0.1564</td>
<td>5.77x10^{-4}</td>
<td>5.95x10^{-8}</td>
<td>9702.2</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0229</td>
<td>0.1564</td>
<td>6.88x10^{-4}</td>
<td>5.95x10^{-8}</td>
<td>11571.9</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0273</td>
<td>0.1564</td>
<td>8.21x10^{-4}</td>
<td>5.95x10^{-8}</td>
<td>13795.4</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0212</td>
<td>0.1876</td>
<td>5.31x10^{-4}</td>
<td>7.14x10^{-8}</td>
<td>7443.2</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0259</td>
<td>0.1876</td>
<td>6.49x10^{-4}</td>
<td>7.14x10^{-8}</td>
<td>9093.3</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0297</td>
<td>0.1876</td>
<td>7.44x10^{-4}</td>
<td>7.14x10^{-8}</td>
<td>10427.5</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0336</td>
<td>0.1876</td>
<td>8.42x10^{-4}</td>
<td>7.14x10^{-8}</td>
<td>11796.7</td>
</tr>
</tbody>
</table>

$^8 \kappa = 0.0006$
Table 4.2.8 Order of magnitude analysis of lateral forces on a $a_p=1.6 \ \mu m$ particle in a channel of height 762 $\mu m$ under conditions listed below$^\S$.

<table>
<thead>
<tr>
<th>Q (ml/min)</th>
<th>$U_m$ (cm/sec)</th>
<th>$V_w$ (cm/sec)</th>
<th>$Re_p$ ($U_m a_p / \nu$)</th>
<th>permeation drag ($V_w / U_m$)</th>
<th>inertial lift ($Re_p \kappa^2$)</th>
<th>ratio of permeation drag to lift</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.725</td>
<td>26.82</td>
<td>0.0126</td>
<td>0.4291</td>
<td>4.70x10^{-4}</td>
<td>1.89x10^{-6}</td>
<td>248.3</td>
</tr>
<tr>
<td>2.725</td>
<td>26.82</td>
<td>0.0176</td>
<td>0.4291</td>
<td>6.56x10^{-4}</td>
<td>1.89x10^{-6}</td>
<td>346.8</td>
</tr>
<tr>
<td>2.725</td>
<td>26.82</td>
<td>0.0206</td>
<td>0.4291</td>
<td>7.68x10^{-4}</td>
<td>1.89x10^{-6}</td>
<td>405.9</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0179</td>
<td>0.5323</td>
<td>5.38x10^{-4}</td>
<td>2.35x10^{-6}</td>
<td>229.3</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0230</td>
<td>0.5323</td>
<td>6.91x10^{-4}</td>
<td>2.35x10^{-6}</td>
<td>294.6</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0261</td>
<td>0.5323</td>
<td>7.85x10^{-4}</td>
<td>2.35x10^{-6}</td>
<td>334.3</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0237</td>
<td>0.6386</td>
<td>5.94x10^{-4}</td>
<td>2.82x10^{-6}</td>
<td>210.9</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0281</td>
<td>0.6386</td>
<td>7.04x10^{-4}</td>
<td>2.82x10^{-6}</td>
<td>250.1</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0328</td>
<td>0.6386</td>
<td>8.22x10^{-4}</td>
<td>2.82x10^{-6}</td>
<td>291.9</td>
</tr>
</tbody>
</table>

$^\S \kappa=0.0021$

Table 4.2.9 Order of magnitude analysis of lateral forces on a $a_p=3.5 \ \mu m$ particle in a channel of height 762 $\mu m$ under conditions listed below$^\S$.

<table>
<thead>
<tr>
<th>Q (ml/min)</th>
<th>$U_m$ (cm/sec)</th>
<th>$V_w$ (cm/sec)</th>
<th>$Re_p$ ($U_m a_p / \nu$)</th>
<th>permeation drag ($V_w / U_m$)</th>
<th>inertial lift ($Re_p \kappa^2$)</th>
<th>ratio of permeation drag to lift</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.725</td>
<td>26.82</td>
<td>0.0108</td>
<td>0.9387</td>
<td>4.03x10^{-4}</td>
<td>1.98x10^{-5}</td>
<td>20.3</td>
</tr>
<tr>
<td>3.380</td>
<td>33.27</td>
<td>0.0147</td>
<td>1.1644</td>
<td>4.42x10^{-4}</td>
<td>2.46x10^{-5}</td>
<td>18.0</td>
</tr>
<tr>
<td>4.055</td>
<td>39.91</td>
<td>0.0189</td>
<td>1.3969</td>
<td>4.74x10^{-4}</td>
<td>2.95x10^{-5}</td>
<td>16.1</td>
</tr>
<tr>
<td>4.681</td>
<td>46.07</td>
<td>0.0235</td>
<td>1.6125</td>
<td>5.10x10^{-4}</td>
<td>3.40x10^{-5}</td>
<td>15.0</td>
</tr>
<tr>
<td>5.378</td>
<td>52.93</td>
<td>0.0289</td>
<td>1.8527</td>
<td>5.46x10^{-4}</td>
<td>3.91x10^{-5}</td>
<td>14.0</td>
</tr>
</tbody>
</table>

$^\S \kappa=0.0046$

Particle transport along the membrane surface because of fluid shear may also contribute to the long tails. The leading edge of the simulated and
experimental RTDs also show interesting differences. The computer generated RTD is the response of a hypothetical detector at the channel exit to an ideal Dirac pulse at the channel inlet at time zero. The "real" experimental apparatus is connected to the injection and detection systems using inert, non-porous tubing. This leads to dispersion at both the entry and exit regions. Therefore the output of the UV detector has a lower slope at the leading edge.

Experimental observations of the first responses in the RTD are plotted along with theoretical predictions as a function of the influent flow rate to the channel in Figures 4.2.13, 4.2.14 and 4.2.15 for particles of radius 0.47 μm, 1.6 μm and 3.5 μm respectively. The wall permeation rate was different for each pair of data points shown. As expected, particles take less time to cross the channel as the influent flow rate (and therefore the crossflow velocity) increases. Also, at any fixed inlet crossflow velocity, increasing the permeation rate (by increasing the transmembrane pressure drop) increases the first passage time both by increasing permeation drag as well as by decreasing the crossflow velocity along the channel length. From these figures it can be seen that there exists very good correlation between the values predicted by considerations of fluid mechanics and those observed from experiments.
Figure 4.2.13 Experimental observations and predicted values of the first response in a porous channel as a function of influent flow rate for a suspension of particles of radius $a_p = 0.47 \, \mu m$.

Figure 4.2.14 Experimental observations and predicted values of the first response in a porous channel as a function of influent flow rate for a suspension of particles of radius $a_p = 1.6 \, \mu m$. 
Figure 4.2.15 Experimental observations and predicted values of the first response in a porous channel as a function of the influent flow rate for a suspension of particles of radius $a_p = 3.5 \, \mu m$.

Comparisons of predicted first passage times and experimental observations are presented in Figures 4.2.16, 4.2.17 and 4.2.18, for different sized particles. For these particle sizes, experimental data and theoretical predictions are very well correlated. Statistically, the straight line fits for these plots pass through the origin with a slope of 1. It is recalled that a similar plot for the 0.24 $\mu m$ particle resulted in a straight line fit that had a positive intercept and a slope less than one. Also, the 95% confidence limits on the intercept and the slope are wider for these particles than the 0.24 $\mu m$ particle. Experiments with the 0.24 $\mu m$ particle were conducted using the Durapore membrane while all other particle experiments were performed with the track-etch membrane. It is speculated that the well defined pores in the track-etch membrane might lead to better
correlation with theory as compared to the Durapore membrane which is composed of a polymeric mesh and is characterized by a nominal pore size. The first response of the detector is associated with particles at lateral positions near the longitudinal axis of the channel, i.e., these particles are in the "far-field" region. Therefore, the surface character of the Durapore membrane is unlikely to influence the transport of these fast moving particles. However, there exists a statistical difference between the theoretical predictions of the first response and experimental observations with membrane characteristics. How exactly this influences transport in the "far-field" region and why should it play a role in the transport is not clear to the author at this stage.

Figure 4.2.16 Comparison of theoretical predictions of first passage time and experimental observations for particles of radius 0.47 μm. The 95% confidence intervals of the true slope and intercept are given.
Figure 4.2.17 Comparison of theoretical predictions of first passage time and experimental observations for particles of radius 1.6 μm. The 95% confidence intervals of the true slope and intercept are given.

Figure 4.2.18 Comparison of theoretical predictions of first passage time and experimental observations for particles of radius 3.5 μm. The 95% confidence intervals of the true slope and intercept are given.
The experimental observations of the first response in the RTD of all four particle are plotted as a function of the theoretical predictions in Figure 4.2.19. This nicely summarizes the results of Figures 4.2.6, 4.2.16, 4.2.17 and 4.2.18. Very good correspondence between theoretical considerations and experimental observations is observed. Thus, we may conclude that, overall, theory predicts transport in porous channels over a range of particle sizes for which permeation drag is much greater than inertial lift.

![Graph showing experimental vs predicted first response](image)

**Figure 4.2.19** Summary of all first response data. Comparison of experimental observations of the first response in the RTD and the predicted values of the first passage time for all four particle sizes investigated ($a_p = 0.24 \, \mu m$, $0.47 \, \mu m$, $1.6 \, \mu m$ and $3.5 \, \mu m$).

Several workers in the past have invoked inertial effects to explain the "flux-paradox" in the membrane filtration of colloidal suspensions (Porter, 1972; Green and Belfort, 1980; Wiesner et al., 1989) but according to the author's knowledge this is the first work to explicitly
investigate the importance of these effects under conditions typical of high permeate flux membrane filtration processes. Also, it is the author's belief that there exists some confusion in the literature about the nature of this phenomenon and the use of such a theory to obtain enhanced back-transport values for particle suspensions. It is suggested that initial particle deposition will be governed by a superposition of inertial and permeation drag forces and that for back-transport to occur, a concentration gradient must exist (either for Brownian or Shear-induced transport).
Chapter 5

Conclusions

The mechanics of neutrally buoyant particles in dilute suspensions undergoing laminar flow in a porous channel is the result of both drag forces and inertial lift. The fouling potential of different sizes of particles in a feed water can be estimated by computer simulations of particle trajectories. Large particles, like powdered activated carbon, experience greater inertial forces and hence are expected to cause less fouling in UF and MF applications. In contrast, the transport of smaller particles, like bacteria, is determined almost solely by fluid drag and are therefore predicted to contribute to the fouling of UF and MF membranes. Not only are smaller particles more likely to be deposited on the membrane but they are also expected to cause greater head loss and hence further decrease the flux of water through the membrane. Particles in the colloidal size range under hydrodynamic conditions typical of ultra and microfiltration applications, undergo transport almost purely due to fluid convection; inertial effects play a negligible role in their mechanics. Single peaks are predicted in the residence time distributions of these particles. In contrast, multiple peaks are expected in the residence time distributions of particles when inertial effects are important.

Experimental observations of first passage times of particles in the size range $0.24 \mu m \leq a_p \leq 3.5 \mu m$ undergoing permeation drag dominated transport in a microporous channel seem to be well described by theories of fluid mechanics. The first passage time approach followed here
potentially can be used to describe initial particle deposition on membranes. Experimental observations of particle residence time distributions show much longer tails than would be predicted by theory. This seems to indicate that there may be particle transport from the membrane surface to the bulk flow arising because of fluid shear and/or concentration gradients.

Numerical calculations of mass transfer in RO and NF systems show large differences in ionic environments along the direction of fluid permeation. At the membrane surface, where materials are rejected, the ionic strength is predicted to be high. Interactions between organic materials in the feed water and the rejected solutes might have implications on increased, irreversible adsorptive fouling of these membranes. Investigations of fluid slip show negligible effects at the free membrane surface whereas it is speculated to play a role on further mass deposition on to a fluidized cake. These effects should be incorporated into the mathematical description of polarization and fouling in pressure driven membrane filters used for potable water production.
Appendix A

Momentum Boundary Layer Calculations

In this section, we shall use some gross approximations and simplifications to develop momentum boundary layer profiles in different membrane systems. Potential flow theory is valid in infinite domains, here we shall apply it to the finite domain of the membrane filter.

A.1 The Potential Flow Problem

Consider first the flow far away from the membrane surface. The rotation of a fluid element is given by half the curl of the velocity vector \( \mathbf{V} \). We define the vorticity vector \( \mathbf{\omega} \) as

\[
\mathbf{\omega} = \frac{1}{2} \text{curl } \mathbf{V} = \frac{1}{2} \nabla \times \mathbf{V} \tag{A1.1.1}
\]

Flows with zero vorticity (\( \mathbf{\omega} = 0 \)) are called irrotational. i.e.

\[
\nabla \times \mathbf{V} = 0 \tag{A1.1.2}
\]

It follows from equation (A1.1.2) that \( \mathbf{V} \) can be expressed as the gradient of a scalar potential \( \Phi \). i.e.

\[
\mathbf{V} = -\nabla \Phi \tag{A1.1.3}
\]

When the velocity components satisfy

\[
\nabla \times \mathbf{V} = 0 \quad \text{(irrotational flow)}
\]

\[
\nabla \cdot \mathbf{V} = 0 \quad \text{(incompressible flow) and}
\]

\[
\mu = 0 \quad \text{(inviscid flow)}
\]

the flow is said to be potential.

Substituting equation (3) in equation (4) we get
\[ \nabla \cdot ( - \nabla \Phi ) = 0 = \nabla^2 \Phi \quad \text{(A1.1.5)} \]

Define the boundary layer (and potential flow) coordinate system as given below. We shall use capital letters for the potential flow parameters and small letters for the boundary layer parameters. Let \( h \) be the height of the membrane module, \( U_o \) be the uniform velocity at the leading edge of the membrane surface and \( V_w \) be the constant permeation (normal) velocity at the membrane surface.

![Cartesian coordinate system for boundary and potential flow problems.](image)

Figure A1.1 The cartesian coordinate system for both the boundary layer and potential flow problems.

From a mass balance we can write the form of the axial velocity component, \( U \), as

\[ U = U_o - \frac{V_w x}{h} \quad \text{(A1.1.6)} \]

To satisfy the continuity equation and the boundary condition

\[ V = - V_w \text{ at } y = 0 \quad \text{(A1.1.7)} \]

the transverse velocity component, \( V \), can be derived as

\[ V = \frac{V_w (y-h)}{h} \quad \text{(A1.1.8)} \]
Thus, the velocity vector

\[ \mathbf{V} = (U_0 - \frac{V_w x}{h}) \mathbf{i} + \frac{V_w (y-h)}{h} \mathbf{j} \]  

(A1.1.9)

can be used to describe the potential flow in the porous channel where \( \mathbf{i} \) and \( \mathbf{j} \) are the unit vectors in the axial and normal directions respectively. The velocity potential that describes flow in the system can be derived from equations (2), (4) and (6) and is given below.

\[ \Phi(x,y) = -U_0 x + \frac{V_w}{2h} x^2 + V_w y - \frac{V_w y^2}{2h} + \text{Constant} \]  

(A1.1.10)

From Bernoulli's theorem:

\[ \frac{1}{2} U^2 + \frac{1}{2} V^2 + \frac{P}{\rho} = \text{Constant} \]  

(A1.1.11)

Differentiating w.r.t \( x \)

\[ U \frac{\partial U}{\partial x} + V \frac{\partial V}{\partial x} + \frac{1}{\rho} \frac{\partial P}{\partial x} = 0 \]

From Equation (A1.1.8)

\[ V = \frac{V_w (y-h)}{h} \Rightarrow \frac{\partial V}{\partial x} = 0 \]

\[ \therefore \frac{\partial U}{\partial x} = -\frac{1}{\rho} \frac{\partial P}{\partial x} \]  

(A1.1.12)

A.1.2 The Boundary Layer Problem

To formulate the boundary layer equations (Schlichting, 1968) we

a. Drop the momentum balance in the \( y \) direction.

b. Neglect the second order derivative w.r.t. \( x \).

c. Get the pressure drop in the axial direction from Potential theory.
Therefore for the steady flow of an incompressible Newtonian constant property fluid in 2-D the boundary layer problem is to solve:

\[ u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = - \frac{1}{\rho} \frac{\partial P}{\partial x} + v \frac{\partial^2 u}{\partial y^2} \quad (A1.2.1) \]

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (A1.2.2) \]

with the boundary conditions

\[ u(y=0) = 0 \quad (A1.2.3) \]

\[ v(y=0) = -V_w \quad (A1.2.4) \]

\[ u(y=\infty) = U(x) \quad (A1.2.5) \]

and the initial condition

\[ u(x=0) = U_0 \text{ where } \quad (A1.2.6) \]

\( u \) and \( v \) are the axial and transverse velocity components in the boundary layer. Note that we can apply only one boundary condition on \( v \) (\( v \) at the surface is specified) because the boundary layer equations are only first order in \( v \).

Substitute Equation (A1.1.12) in (A1.2.1) to get

\[ u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = U \frac{\partial U}{\partial x} + v \frac{\partial^2 u}{\partial y^2} \quad (A1.2.7) \]

We now try to get an estimate for the boundary layer thickness \( \delta \) using the approximate momentum-integral or the von Kármán integral method. In this method, the differential equations governing the flow are not satisfied for every fluid particle but are only satisfied in the regions near the inner (the membrane surface) and outer (near the potential flow) boundaries by enforcing the boundary conditions. In the rest of the
boundary layer, only an average of the equation of motion (by integrating over the entire boundary layer thickness) is satisfied. It is also necessary to assume a velocity profile within the boundary layer that satisfies both the inner and outer boundary conditions. For the two dimensional flow of incompressible fluid, the momentum-integral equation describing the boundary layer is:

\[
\frac{\partial}{\partial x} (\delta_2 U^2) + U \frac{\partial U}{\partial x} \delta_1 = -\frac{\tau_0}{\rho}, \quad \text{where} \tag{A1.2.8}
\]

\[\delta_1 \text{ is the displacement thickness } = \frac{1}{U} \int_0^\infty (U - u)\,dy \tag{A1.2.9}\]

\[\delta_2 \text{ is the momentum thickness } = \frac{1}{U^2} \int_0^\infty u(U - u)\,dy \quad \text{and} \tag{A1.2.10}\]

\[\tau_0 \text{ is the shear stress at the surface.}\]

Introduce the variable \( \eta = \frac{y}{\delta} \) and assume a parabolic profile for the velocity in the laminar boundary layer as given by:

\[
\frac{u}{U} = \begin{cases} 
a + b\eta + c\eta^2 & \text{if } y \leq \delta \\
1 & \text{if } y \geq \delta \end{cases} \tag{A1.2.11}
\]

subject to the boundary conditions

\[u = 0 \quad \text{at } y = 0 \tag{A1.2.12}\]

\[u = U \quad \text{at } y = \delta \text{ and} \tag{A1.2.13}\]

\[\frac{\partial u}{\partial y} = 0 \quad \text{at } y = \delta \tag{A1.2.14}\]

We solve for the coefficients \( a, b \) and \( c \) using the boundary conditions.

\[u(y = 0) = 0 \Rightarrow a = 0\]

\[u(y = \delta) = U \Rightarrow b + c = 1\]
\[ \frac{\partial u}{\partial y} = 0 \text{ at } y = \delta \Rightarrow b + 2c = 0 \]

or \( c = -1 \) and \( b = 2 \). Hence the axial velocity profile within the boundary layer is approximated by:

\[
\frac{u}{U} = \begin{cases} 2\eta - \eta^2 & y \leq \delta \\ 1 & y \geq \delta \end{cases}
\]  

(A1.2.14)

We now evaluate each of the terms in Equation (A1.2.7) as shown below:

\[
\tau_v = -\mu \frac{\partial u}{\partial y} \bigg|_{y=0} = -\mu \frac{\partial}{\partial y} \left[ U \left( \frac{2y}{\delta} - \frac{y^2}{\delta^2} \right) \right] \bigg|_{y=0} = -\frac{2\mu U}{\delta} \tag{A1.2.15}
\]

\[
\delta_1 = \frac{1}{U} \int_0^\infty (U - u)dy = \delta \int_0^1 (1 - 2\eta + \eta^2)d\eta = \frac{\delta}{3} \tag{A1.2.16}
\]

\[
\delta_2 = \int_0^\infty \frac{U}{U} (1 - \frac{U}{U})dy = \delta \int_0^1 (2\eta - \eta^2)(1 - 2\eta + \eta^2)d\eta = \frac{2}{15}\delta \tag{A1.2.17}
\]

Therefore, substituting Equations (A1.2.15), (A1.2.16) and (A1.2.17) in Equation (A1.2.17) we get:

\[
\frac{d}{dx} \left( \frac{2}{15} \delta U^2 \right) + U \frac{\delta}{3} \frac{dU}{dx} = \frac{2\mu U}{\rho \delta} \quad \text{or} \quad \frac{2U^2}{15} \frac{d\delta}{dx} + \frac{2\delta}{15} \frac{dU^2}{dx} + U \frac{\delta}{3} \frac{dU}{dx} = \frac{2\mu U}{\rho \delta} \tag{A1.2.18}
\]

Multiply Equation (A1.2.19) by \( \delta \) to get:

\[
\frac{U^2}{15} \frac{d\delta^2}{dx} + \frac{2\delta^2}{15} \frac{dU^2}{dx} + U \frac{\delta^2}{6} \frac{dU^2}{dx} = \frac{2\mu U}{\rho} \tag{A1.2.20}
\]

rearranging Equation (A1.2.20)
\[
\begin{align*}
\frac{d(\delta^2)}{dx} + \left(\frac{2\delta^2}{U^2} + \frac{15\delta^2}{6U^2}\right) \frac{d(U^2)}{dx} &= \frac{30\mu}{\rho U} \\
i.e. \quad \frac{d(\delta^2)}{dx} + \frac{27\delta^2}{6U^2} \frac{d(U^2)}{dx} &= \frac{30\mu}{\rho U}
\end{align*}
\] (A1.2.21)

Equation (A1.2.22) is an ordinary differential equation in \(\delta^2\) with the initial condition:
\[
\delta(x=0) = 0
\] (A1.2.23)

A fourth order Runge-Kutta method was used for the solution of Equation (A1.2.22) with Equation (A1.2.23) on the Macintosh SE/30 computer. The computer program BLAYER is shown in Appendix B. Boundary layer thickness profiles in Figures A1.2 - A1.5 using some operating parameters typical of reverse osmosis, ultrafiltration and microfiltration (using the same parameters used for generating Figures 3.2.2 - 3.2.8). Except in Figure A1.2, we see that the boundary layer fills the whole channel within approximately 40% of the channel length. This can be compared to Figures (3.2.2) - (3.2.8) showing the concentration profiles where even at mid-channel the concentration boundary layer occupied only about 3% of the channel height.

From these plots we can infer that viscous effects become important very early in the channel. Also, as is well known in the mass transfer of components with high Schmidt numbers, \((Sc=v/D)\), the concentration boundary layer is much smaller than the momentum boundary layer. Hence, the approach of separating the treatment of momentum and mass transfer seems to be valid.
Figure A1.2 Momentum boundary layer during a typical reverse osmosis application. Same parameters as used in Figure 3.2.3.

Figure A1.3 Momentum boundary layer during an ultrafiltration application: Filtration of humic acid from water. Same parameters as used in Figures 3.2.4 and 3.2.5.
Figure A1.4 Momentum boundary layer during an ultrafiltration application: Filtration of Bovine Serum Albumin. Same parameters as used in Figure 3.2.7.

Figure A1.5 Development of the momentum boundary layer during a typical experiment. Note that the boundary layer fills the channel very early.
Appendix B

Computer Programs

program blayer

! This is the program used for calculating the momentum
! boundary layers given in Appendix B.

implicit real (a - z)
integer nstep
common Uo, Vw
external f
x=0.0
o=0.0
nstep=1600
length=46
h=length/real(nstep)
write(9,*)'Enter Uo (cm/sec)'
read(9,*)Uo
write(9,*)'Enter Vw (cm/sec)'
read(9,*)Vw
call rk(f,x,o,h,nstep)
stop
end

subroutine rk(f,x,o,h,nstep)

! This is a fourth order Runge-Kutta algorithm for solving
! Equation A1.2.22 with the initial condition A1.2.23.

implicit real (a - z)
integer k, nstep
character*8 name
length = 46
Height = 0.0762
write(9,*)'Enter file name to store output file'
read(9,*'(a')'name
open(19, file = name)
open(20, file = 'xaxis')
write(19,3) sqrt(o)/Height
write(20,3)x/length
h2 = 0.5*h
p = x + h2
s = x + h
start = x

do 2 k = 1, nstep
   f1 = h*f(x,o)
   q = o + 0.5*f1
   f2 = h*f(p,q)
   r = o + 0.5*f2
   f3 = h*f(p,r)
   t = o + f3
   f4 = h*f(s,t)
   o = o + (f1+f2+f2+f3+f3+f4)/6.0
   x = start + h*real(k)
write(19,3)sqrt(o)/Height
write(20,3)x/length
2 continue
3 format(e15.3)
return
end

c

function f(x,o)
implicit real (a - z)
common Uo, Vw
ht=0.0762
nu=0.01
U = (Uo - Vw*x/ht)
f = 30.0*nu/U-27.0/6.0*o*(2*x*Vw*Vw/(ht*ht)-2*Uo*Vw/ht)/(U*U)
return
end
program Diffusion

this program solves the steady state convection diffusion

equation with the approximations for the first order derivatives:

x derivative - backward difference

y derivative - backward difference

for a channel with one porous wall (at y = h)

parameter (nj = 5001, nm = 5001)
double precision Le, h, Uo, Vw, Rew, D, lastx
double precision dl, dz, l, x, z, f0, f1
double precision nu, slip, mult
double precision vvel(nj), uvel(nj), C1, C2, f0prime, f1prime,
double precision a(nj), b(nj), e(nj), f(nj), x1(nj), c(nj)
integer i, j, m, iterations
implicit none

define the fluid parameters and channel geometry
data h/0.3820/
data Le/48.00/
data Uo/34.5600/
data nu/0.0100/
lastx = Le / 2.000

write(*,*)'Enter the slip coefficient'
read(*,*)slip

calculate the first order coefficients for the velocity profiles

C1 = ((24.000/35.000)*(1.+slip)**3) - 
   2.400*(1.+slip)**2*(1.+2.*slip) 
   + 3.600*(1.+slip)**2*(1.+2.*slip)**2) - 
   2.400*(1.+slip)**2*(1.+6.*slip) + 
   7.200*(1.+slip)**2*(1.+2.*slip)*((1.+5.*slip) - 9.*(1.+4.* 
   slip)**2)) / ((1.+2.*slip)**2) / (-1.000)

c
C2 = ( (12./35.)*(1.+2.*slip)**2*(1.+slip)**2) - 
   0.800*(1.+slip)**2*(1.+ 
   2.000*(1.+slip)**2*(1.+2.*slip)**2) + 
   2.400*(1.+slip)**2*(1.+2.*slip)**2*(1.+5.*slip) 
   + 1.800*(1.+2.*slip)**3 - 3.*(1.+4.*slip) 
   *((1.+2.*slip)**2) / ((1.+4.*slip)**3)

write(*,*)'Enter the diffusion coefficient in cm2 / sec'
read(*,*)D
write(*,*)'Enter the wall permeation rate'
read(*,*)Vw

determine the dimensionless wall Reynolds number
Rew = Vw * h / nu

fix the dimensionless grid size in the y and x directions respy

dl = 1.000 / dble(nj - 1)
dz = 1.000 / dble(nm - 1)
write(*,*)'dl = ',',dl
write(*,*)'dz = ',',dz

C********************************************************************
C set the initial conditions for the concentration profile
do 15 i = 1, nj
   c(i) = 1.0D0
15 continue

C********************************************************************
C develop the dimensionless transverse velocity profile.
do 10 i = 1, nj
   l = dble(i - 1) * dl
   f0 = ((l**1)/(1.0D0+4.0D0*slip))*(-2.0D0*(1.0D0+slip)*l + 3.0D0*
       (1.0D0 + 2.0D0*slip))
   fl = C1*l**1*l/6.0D0+C2*l**1/2.0D0+((l**5)
       (1.0D0+4.0D0*slip)**2)*
       (-12.0D0*l**1*((1.0D0+slip)**2)/210.0D0 +
       0.2D0*l*(1.0D0 + slip)*(1.0D0+2.0D0*slip)
       - 0.3D0*((1.0D0+2.0D0*slip)**2))
   vvel(i) = (f0 + Rew*fl)
10 write(52,901) vvel(i)

C********************************************************************
iterations = nint(lastx/Le/dz + 1)
write(*,*)'The total # of iterations = ',', iterations
write(*,*)'last x = ',',Le*dble(iterations - 1.0)*dz
do 50 m = 2, iterations
   z = dble(m - 1) * dz
   x = Le * z
   if ( (mod(m,50.0D0)) .eq. 0) then
      write(*,*)'x = ',',x, ' iteration # = ',',m
   endif

C********************************************************************
C develop the dimensionless axial velocity profile
do 35 j = 1, nj
   l = dble(j - 1) * dl
   f0prime = 6.0D0*l/(1.0D0+4.0D0*slip) *
       (1.0D0+2.0D0*slip)
   flprime = C1*l**1/2.0D0 + C2*1 +
       (l**4)/((1.0D0+4.0D0*slip)**2)
   * ( -0.4D0*((1.0D0+slip)**2)*l**1 + 1.2D0*
       (1.0D0+slip)*(1.0D0+2.0D0*slip)*l**1 - 1.5D0*
       ((1.0D0+2.0D0*slip)**2) )
   uvel(j) = (Uo - Vw*x/h) * (f0prime + Rew*flprime)
   uvel(j) = uvel(j) / Uo
35 continue
b(l) = (2.0D0 * D * Le )/ (h * h * dl * dl * Uo) +
      (vvel(i) * Vw * Le) / (dl * Uo * h)

e(l) = -(2.0D0 * D * Le )/ (h * h * dl * dl * Uo) -
      (vvel(i) * Vw * Le) / (dl * Uo * h)
f(l) = 0.0D0

do 45 i = 2, nj-1
    1 = dble(i - 1) * dl

c
    a(i-1) = (-Le * Vw * vvel(i) ) / ( h * Uo * dl ) -
             ( (D * Le) / (h * h * Uo * dl * dl) )

c
    b(i)=(vvel(i)/dz) + (2.0D0 * D * Le/(dl * dl * Uo * h * h))
    + (Vw * Le * vvel(i)) / (Uo * h * dl)

c
    e(i) = -(D * le) / (h * h * Uo * dl * dl)

c
    f(i) = ( uvel(i) / dz ) * c(i)

c
        continue

c
    a(nj-1)= -(Vw * Le)/(Uo * h* dl * vvel(nj)) -
             (2.0D0 * D* Le/(h * h * Uo * dl * dl))
    b(nj) = (vvel(nj) * Vw * Le/(Uo*h* dl)) +
             2.0D0 * D * Le/(h * h* Uo *dl * dl)
    2 - 2.0D0 * vvel(nj)*Vw * Le/(h * Uo * dl) + uvel(nj)/dz
    e(nj) = 0.0D0
    f(nj) = uvel(nj) * c(nj) /dz
    a(nj) = 0.0D0

c
call tridiag(nj, a, b, e, f, x1)
do 47 j = 1, nj
    c(j) = x1(j)
x1(j) = 0.0D0

47 continue

50 continue
    i = m - 1
    x = Le * dble(i - 1) * dz
    write(*,*)'x = ',x

do 65 j = 1, nj
    mult = (j - 1.0D0) * dl
    write(23,902)c(j)
    write(24,901)(1.0D0 - mult)

65 continue
901 format(2f15.10)
902 format(f15.3)
end
doubleprecision function f(b) 

implicit doubleprecision (a - z) 

f = 1.532139d0 - 12.182786d0*b + 21.652283d0*b*b + 
   1 4.495068*(b**3) - 28.176666d0*(b**4) + 10.950694*(b**5) 
   2 + 0.198042*(b**6) 

c end
doubleprecision function g(s)

implicit doubleprecision (a - z)
doubleprecision s, g

g = -(2.0DO*s + 1.0DO) * ( (1.0D0 - s)**2 )

end
doubleprecision function integrand(z)

implicit doubleprecision (a - z)
common gamma
external f, g

integrand = f(z) + gamma*g(z)

return
end
doubleprecision function lateral(z,b)

C***************************************************************************
C Here I solve for dbeta/dz to get beta = beta(z)
C I use this directly in the beta vs z plot.
C i.e. in the lateral position vs axial position trajectory plot
C***************************************************************************

implicit doubleprecision (a - z)

common Um,Vw,h,rad,length,nu
external f, g

Umlocal = ( Um - 1.5D0*Vw*z/h )
Replocal = Umlocal * rad / nu
kappa = rad / h
denom = 4.D0 * h * Umlocal * b * (1.0D0 - b)
umer = Replocal * kappa * kappa * Umlocal * f(b) + Vw * g(b)
lateral = numer / denom
return
end
program pulse

This program calculates the time needed for a particle to cross
the membrane module. The module here is of one with one porous
wall. The initial position of release is beta0.

parameter (n = 128)
doubleprecision Um, Vw, h, rad, nu, f, g, lateral, length
doubleprecision beta, beta0, z, z0, step, t0, t, tcross
integer i
logical capture
implicit none
common Um, Vw, h, rad, length, nu

external f, g, lateral, tcross

data length/46.0D0/
data Um/100.00D0/
data Vw/0.00D0/
data h/2.6D-1/
data nu/0.01D0/
write(*,*)'Enter the particle radius in microns'
read(*,*)rad
rad = rad * 1.0D-4

do 10, file='time.m'
do 11, file='beta.m'

capture = .false.
step = 1.0D0 / dble(n)
do 90 beta0 = 0.98D0, 0.01D0, -0.01D0
  write(11,901) beta0
  z0 = 0.0D0
t0 = 0.0D0
  beta = beta0
  z = z0
t = t0
do 30 i = 1, int(n*length)
  beta = beta + step * lateral(z, beta)
  if (beta .le. 0.0D0) then
    beta = 0.0D0
    write(*,*)'***Particle at membrane surface***'
    write(*,*)'Point of release = ', beta0
    capture = .true.
goto 100
endif
z = z + step
t = t + step * tcross(z,beta)

C*****************************************************************************
C   We now have the relationship between z and beta as beta=beta(z)
C*****************************************************************************
30    continue
       write(10,901)t
       if (beta0 .eq. 0.99) write(*,*)'Time = ',t
90    continue
100   if (capture) write(10,901)t
901   format(f10.4)
    end
program rtd

This program calculates the RTD for a pulse input in the channel
This uses the output of the program 'pulse' and then calculates
the number of trajectories that emerge at fixed time intervals.

parameter (n = 128)
doubleprecision Um, Vw, h, rad, nu, f, g, lateral, length
doubleprecision beta, beta0, z, z0, step, t0, t, tcross
integer i, j, k
logical capture
doubleprecision low, high, inter, artime(500), arbeta(500), sum,
doubleprecision crap, count
implicit none
common Um, Vw, h, rad, length, nu
external f, g, lateral, tcross

data length/46.0D0/
write(*,*)'Enter Um'
read(*,*)Um
write(*,*)'Enter Vw'
read(*,*)Vw
data h/0.0762/
data nu/0.01D0/
write(*,*)'Enter the particle radius in microns'
read(*,*)rad
rad = rad * 1.0D-4

open(10,file='time.m')
open(11,file='beta.m')
open(12,file='rtptime.m')
open(13,file='rtdbeta.m')
j = 1
capture = .false.
step = 1.0D0 / dble(n)
do 90 beta0 = 0.98D0, 0.01D0, -0.002D0
   write(11,901)beta0
   arbeta(j)=beta0
   z0 = 0.0D0
t0 = 0.0D0
   beta = beta0
   z = z0
   t = t0
   do 30 i = 1, int(n*length)
      do 20 j = 1, n
         ...
beta = beta + step * lateral(z,beta)
if (beta .le. 0.0D0) then
    beta = 0.0D0
    write(*,*)'*** Particle at membrane surface'
    write(*,*)'Point of release = ', beta0
    capture = .true.
    goto 100
endif
z = z + step
 t = t + step * tcross(z,beta)

C**************************************************************************************************************************************************
C We now have the relationship between z and beta as beta=beta(z)
C**************************************************************************************************************************************************
30    continue
    write(10,901)t
    artime(j)=t
    if (beta0 .eq. 0.99) write(*,*)'Time = ',t
    j = j + 1
90   continue
100  if (capture) then
    write(10,901)t
    artime(j)=t
endif
    write(*,*)'The last j = ',j

C**************************************************************************************************************************************************
C Now start the rtd generation code
C**************************************************************************************************************************************************
inter = 0.1D0
do 130 i = 1, 50
    low = dble(i) * inter
    high = dble(i + 1) * inter
    sum = 0.0D0
    count = 0.0D0
    do 110 k = 1, j-1
        if ((artime(k) .lt. high) .and. (artime(k) .ge. low)) then
            count = abs(arbeta(k) - arbeta(k+1))
            sum = sum + count
        endif
110    continue
    write(12,901)(low+high)/2.0
    write(13,901)sum
130   continue
901  format(f10.4)
end
program sconc

parameter (nt = 100, nb = 200)
doubleprecision sum, a, b, h, sum, integral, integrand
doubleprecision sub, sumd, nu, trapezoid, Temp
integer i, j, k, n, m
doubleprecision x(0:2*nt), dintegrand(0:nb), beta(0:nb),
doubleprecision denominator, Um, height, radius, nu, boltz, Vw,
doubleprecision pi, D, Rep, kappa, gamma, K1
implicit none

common gamma

external integrand

data Um/41.0D0/
data height/0.0762D0/
data nu/0.01D0/
data boltz/1.380662D-23/
data Vw/0.01D0/
data Temp/298.0D0/
data mu/1.0D-3/
pi = 4.0D0 * atan(1.0D0)
write(*,*)'Enter particle radius (in microns) '
read(*,*)radius

calculate the Brownian diffusivity using Stokes-Einstein formula

D = boltz * Temp / (6.0D0 * pi * mu * (radius*1.D-6))
D = D * 1.D4
write(*,*)'D = ',D
Rep = Um * radius * 1.D-4 / nu
write(*,*)'Re particle = ',Rep
kappa = radius * 1.0D-4 / height
write(*,*)'kappa = ',kappa
K1 = Rep * kappa * kappa * Um * height / D
write(*,*)'K1 = ',K1
gamma = Vw / (Rep * kappa * kappa * Um)
write(*,*)'gamma = ',gamma

a = 0.0D0
sub = 1 / dble(nb)
do 20 j = 0, nb
if (mod(j,25) .eq. 0) write(*,*)'outer iter to go =',(nb - j)

20 continue
b = dble(j) * sub
do 15 i = 1, nt
    sum = 0.0D0
    n = 2 * i
    h = (b - a) / dble(n)
    do 14 k = 1, 2*i+1
       x(k-1) = a + dble(k-1)*h
       if ((k .eq. 1) .or. (k .eq. (2*i+1))) then
          m = 1
       else if (mod(k, 2) .eq. 0) then
          m = 4
       else if (mod(k, 2) .eq. 1) then
          m = 2
       endif
       sum = sum + dble(m)*integrand(x(k-1))
    14 continue
    integral = h * sum / 3.D0
15 continue
    beta(j) = b
    dintegrand(j) = exp(K1*integral)
    if ( ( j .gt. 0 ) .and. ( j .lt. nb ) ) then
       trapezoid = trapezoid + dintegrand(j)
    endif
20 continue
    sumd = 0.5D0 * ( dintegrand(0) + dintegrand(nb) )
    denominator = sub * (trapezoid + sumd)
    do 30 j = 0, nb
       write(10,902)beta(j)
       write(11,901)dintegrand(j)/denominator
30 continue
901 format(E15.8)
902 format(f6.3)
end
doubleprecision function tcross(z,beta)

implicit doubleprecision (a - z)

common Um,Vw,h,rad,length,nu

external lateral, f, g

Umlocal = Um - 1.5D0*Vw*z/h

tcross = 1.D0 / ( 4.D0 * Umlocal * beta * (1.D0 - beta) )

return

derend
program timetraj

C*******************************************************************************
C First we need the relationship
C
C first we determine z = z(beta). Then we can use the function
C
central to numerically integrate (Euler's method) to any time
C limit. This program calculates both the time and the z trajectory
C of a neutrally buoyant sphere in a channel with one porous wall.
C
C The length scale used for non-dimensionalizing the axial distance
C is the channel length while the time scale used is the residence
C time of the particle in the channel in the fluid phase.
C*******************************************************************************

parameter (n = 128)
double precision Um, Vw, h, rad, nu, f, g, lateral, length
double precision beta, beta0, z, z0, step, t0, t, tcross, tfinal
double precision array(10000)
integer i, j
implicit none

C

common Um, Vw, h, rad, length, nu

C

external f, g, lateral, tcross

C
data length/46.00D0/
data Um/50.00D0/
data Vw/1.5D-2/
data h/7.62D-2/
data nu/0.01D0/
write(*,*)'Enter the particle radius in microns'
read(*,*)rad
rad = rad * 1.0D-4

C

open(10,file='time.m')
open(11,file='beta.m')
open(12,file='z.m')

C

step = 1.0D0 / dble(n)
write(*,*)'Enter the initial particle position'
read(*,*)beta0
z0 = 0.00D0
t0 = 0.00D0
beta = beta0
z = z0
t = t0
do 30 i = 1, int(n*length)
    beta = beta + step * lateral(z,beta)
    if (beta .le. 0.0D0) then
        beta = 0.0D0
        write(*,*)'*** Particle at membrane surface ***'
        goto 100
    endif
    z = z + step
    t = t + step * tcross(z,beta)
    c**********************
    c We now have the relationship between z and beta as beta=beta(z)
    c**********************
    tarray(i) = t
    write(11,901)beta
    write(12,901)z
30 continue
100 tfinal = t
    do 40 j = 1, (i-1)
        write(10,901)tarray(j)
40 continue
    write(*,*)'Time to cross length of the channel ',tfinal,' sec'
901 format(f10.4)
end
subroutine tridiag(n,a,d,c,b,x)
imPLICIT doubleprecision (a - z)
ingteger n, i
dimension a(n),d(n),c(n),b(n),x(n)
   
do 10 i = 2, n
       xmult = a(i-1)/d(i-1)
       d(i) = d(i) - xmult*c(i-1)
       b(i) = b(i) - xmult*b(i-1)
 10 continue
   
x(n) = b(n)/d(n)
do 20 i = n-1, 1, -1
    x(i) = (b(i) - c(i)*x(i+1))/d(i)
 20 continue
return
end
List of References


Green, G. "unpublished work." (1979):


