UNIVERSITY OF STELLENBOSCH

Department of Applied Mathematics

Report to the

WATER RESEARCH COMMISSION

on

MATHEMATICAL MODELLING OF FLOW THROUGH POROUS MEMBRANES

by

J P du Plessis

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EXECUTIVE SUMMARY

MATHEMATICAL MODELLING OF FLOW THROUGH POROUS MEMBRANES

by

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Supplementary to the full report to the
WATER RESEARCH COMMISSION
on the project
MATHEMATICAL MODELLING OF FLOW THROUGH POROUS MEMBRANES

Profect Leader: Prof. J.P. du Plessis

BACKGROUND AND MOTIVATION

This project was initiated in 1991 to facilitate the application of recent international mathematical modelling advances in porous media research to water related phenomena in South Africa with particular emphasis on the enhancement of research on synthetic membrane systems and technology. Synthetic membrane technology presents powerful new concepts through which water treatment may be engineered. The successful prediction of resistance to flow through microporous and ultrafiltration membranes depends largely on a complete understanding of all flow phenomena in porous media. It therefore seems appropriate to contribute to our scientific understanding of membrane technological concepts by applying these newly developed mathematical tools in this area of research.

Since 1986 considerable success was achieved on an international basis towards the theoretical proof and understanding of fundamental flow phenomena within porous media. Since the accurate modelling of such phenomena on a pore-scale presents unique opportunities in studying and understanding the fundamental principles of the various transport processes, the time and effort devoted to this basic research has had almost immediate effect in the accuracy to within which such practical phenomena could be predicted. According to the new approach the theoretical development is driven as far as possible without introducing any arbitrary constants. The outcome is hopefully some mathematical equations from which practical situations in the laboratory or in field situations may be predicted quantitatively and without the necessity of adjustable parameters. If some level of arbitrariness has to be introduced for better correlation with experiment it is at a late stage of theoretical development when its harmful effects on the mathematics, describing the physics, is negligible. Scientifically this presents a very fortunate situation, since the resulting model cannot be adjusted to match experimental data. It either correctly describes the experiment satisfactorily or something is awry either with the modelling assumptions or with the experimental conditions. The performance of the model could thus be inferred directly.

Computational methods have become a necessity for thorough analysis towards system design in almost all fluid-related technologies. The capabilities of computational fluid dynamics have dramatically enlarged the horizon of quantitative understanding of flow phenomena and especially in cases where porous media are present. More often than not the equations which were developed decades ago to aid the correlation among different experimental and field results are no longer accurate and robust enough for use in numerical computations. In numerical work the flow phenomena are not treated on an average scale -local heterogeneities are computed directly and this causes the equations to be pushed beyond their limits of applicability and consistency. This warrants the development of new mathematical equations for use in computer programs by which water-related phenomena in synthetic membranes can be numerically simulated accurately.

The development of static tensiometer type soil moisture measurement meters depends to a large extent on the qualitative understanding and quantitative predictability of capillary force action in a partially saturated porous medium. Capillary action is directly related to the scale and structural geometry of the porous medium under consideration. The research efforts mentioned above are based on the pore-scale modelling of porous media with the description of the pore-scale morphology a very prominent aspect. It thus provides the ideal platform from which to do a quantitative analysis of capillary action to enhance understanding and predictability of this phenomenon.

OBJECTIVES

Three objectives of this research regarding flow in synthetic membranes were proposed namely

A The *analytical modelling* of flow through the different pore structures found in synthetic membranes.

B The establishment of a *computer code* providing the numerical means to study and predict flow phenomena in complex membrane systems.

C The study of quasi-stationary *capillary action* in foamlike porous media to provide theoretical support to the practical development of tensiometer type soil moisture meters.

MAJOR RESULTS AND CONCLUSIONS

Mathematical models were derived for flow in different kinds of porous structures as are found in the composite structure of a synthetic membrane. These models were incorporated in extensive computer codes by which flow and pressure drop data may be predicted for practical membrane systems. The most important result, however, is that a sound theoretical basis was secured from which future studies in membrane or other porous medium phenomena regarding water resources management may be conducted. To a large extent it eliminates the need for mathematical "models" by which porous flow phenomena are described by the introduction of haphazard and artificial correlation constants inferred from comparison between experimental data sets.

During the two years that this project was conducted, it was demonstrated beyond doubt that mathematical modelling can be conducted accurately so as to provide confidence in predicted results in the water engineering practice.

A computer code was developed for the prediction of flow through two-dimensional or axi-symmetrical membrane systems.

FULFILMENT OF CONTRACT OBJECTIVES

A Analytical modelling of flow through a membrane taking into account the morphology of the pore structure. This proposed modelling research was successfully advanced towards full fulfilment of contract objectives and results have been widely tested against available experimental results.

B Development of a computer program for prediction of flow in membrane systems. This activity was completed with successful test runs to validate the results qualitatively and quantitatively. Contract proposals in this regard were performed fully.

C Quantification of stationary capillary action in unsaturated porous media may be directly inferred from the explicit results obtained in the first part of this project. Although research on this front commenced on a high level of sophistication, it was stopped in favour of the enhancement of progress on the research carried out under section A. The termination was effected after it became known that the project on the development of tensiometer type moisture content meters by the Institute of Polymer Science was cancelled. As this activity was specifically aimed at supporting the latter project, this switch was considered in best interest of current needs of water research activities in South Africa.

CONTRIBUTIONS TO THE STATE OF ART

Pore-scale models were developed from which porous media with composite morphologies as is found in synthetic membranes, may be described. It opened the way for explicit calculation of pore lengths, tortuosity, surface areas and hydrodynamic permeability of membranes.

The Darcy-law for slow flow through porous media were proven quantitatively - given the type, the porosity and the length scale of the microstructure, the hydrodynamic permeability may be predicted directly.

Analytical proof of the Forchheimer effect, which refers to the nonlinear relationship between velocity and pressure gradient in porous media, were established. Since the real origin of this effect is now known, it may be studied in a much more scientific way.

A computational code was developed, incorporating the facility to ascribe different pore structures and permeabilities to different spatial regions. The code is based on a finite volume numerical procedure and contains no "black boxes" so that the actual progress through the numerical procedure may be traced completely.

The theoretical establishment of isotropic pore-scale models forms a sound basis from which studies on electrokinetic phenomena, contaminant transport and anisotropic conditions may be conducted.

SIGNIFICANCE OF THIS REPORT

This report presents a new set of equations for fluid movement through and adjacent to a synthetic membrane. These equations may be used in future mathematical and computational research on membrane processes and design of membrane systems. Although this report deals primarily with water seepage through synthetic membranes, the mathematical results are applicable generally for any Newtonian fluid or porous medium. This interdisciplinary applicability renders this study very cost-effective and may enhance research in various other fields of interest.

ACTIONS TO BE TAKEN

Due to the nature of this project no prescriptive action could be suggested, but the encouragement of the use of the results as basis or correlative measure in future membrane-related projects are recommended.

RECOMMENDATIONS

The fundamental theory developed under this project present a sound basis for enlargement of the applicability by research on the following aspects of membrane processes:

A Formalize introduction of the recirculatory model. This is intended to provide the full exposition of the modelling steps which leads to the improved results for granular media. This action will also align the foam and prismatic models with the improved version of the granular model, which compares favourably with experimental results over a very large range of parameter values.

B Macroscopic boundaries
Container walls have a marked influence on the macroscale characteristics of an enclosed porous medium since it alters the porosity in the near wall region. This problem is analogous to the proper inclusion of porosity variations on an intermediate scale.

C Tracer transport
Retention time of solutes and dispersion of contaminants may be studied in a logical manner, since a method now exists by which intrapore phenomena may be quantified.

D Electrokinetic phenomena

Ion movement due to externally applied electric fields may be modelled in a similar type of volumetric averaging.

E Anisotropic phenomena

Derivation of a suitable permeability tensor is of cardinal importance to make the theory available for use in non-isotropical membranes or other fields of application, such as groundwater transport or leaching.

F Velocity dispersion

This problem concerns the correction for smearing out of velocity gradients needed due to the neglect of the volumetric integral in the averaged equation. No such correction exists in world literature and is urgently needed for full application of the theory in cases where large velocity gradients exist.

G Pore size distribution

The present theory does not yet allow for variation in spatial variation in pore size and should be generalised to include calculation of the deviation due to given pore size distributions.

ACKNOWLEDGEMENTS

The research reported in this document emanated from a project funded by the Water Research Commission and entitled:

Modelling of flow through porous membranes.

The financing of the project by the Water Research Commission is gratefully acknowledged and so is the moral and scientific support by its members and especially Dr. T. Erasmus under whose supervision this project was conducted.

Cooperation by the University of Stellenbosch Institute for Polymer Science and the Pollution Research Institute at the University of Natal enhanced the scientific level of this work and they are both thanked heartily.

The University of Stellenbosch is also gratefully acknowledged for provision of computing and administrative facilities.

The following persons are also thanked for invaluable inputs:

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Margaret Collins, University of Stellenbosch
Jacob Masliyah, Department of Chemical Engineering, University of Alberta.
Ed Jacobs, Institute for Polymer Science, University of Stellenbosch.

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Contents

1 NOMENCLATURE

List of symbols

A_p	cross-sectional pore area,
d	microscopic characteristic length,
d_p	pore width,
d_s	cube side width,
F	microscopic shear factor,
g	gravitational body force per unit mass,
K	hydrodynamic permeability,
l	axial length in tubular arrangement,
p	fluid pressure,
q	specific discharge, $<v>$,
Re	pore flow Reynolds number, $2\rho v_p(d-d_s)/\mu$,
Re_{qd}	Reynolds number, $\rho\|q\|d/\mu$,
S	surface area,
T	tortuosity,
t	time,
V_f	fluid filled 'void' volume within RUC,
V_s	solid volume within RUC,
V_o	total volume of RUC,
v	fluid velocity field within V_f,
v_p	mean pore velocity within pore section,
ϵ	porosity (void fraction), V_f/V_o,
μ	fluid dynamic viscosity,
ν	normal surface vector pointing into solid,
ρ	fluid mass density,
ϕ	generic variable,
$<\phi>$	volumetric phase average of ϕ, $\frac{1}{V_f}\int\int_{V_f}\int \phi dV$,
$<\phi>_f$	volumetric intrinsic phase average of ϕ, $\frac{1}{V_f}\int\int_{V_f}\int \phi dV$,
$\mathring{\phi}$	deviation, $\phi-<\phi>_f$.

Subscripts

c	critical point,
f	fluid phase,
fs	fluid-solid interface,
0	very low Reynolds number flow or total volume,
∞	very high laminar Reynolds number.

Notes on terminology

In this report a consistent manner is used to provide information on the pore-scale length dimensions, namely by the parameter d which gives the average length scale of the porous microstructure. In foamlike or tubular membranes it is defined as the average distance from pore centre to pore centre. The pore dimensions may then be inferred from d as is indicated in the respective sections of the report.

In granular or prismatic membranes d similarly gives the average distance from solid centre to solid centre. In these cases the solid diameters may be obtained by the explicit expressions given in the respective sections of the report.

In all references to numerical values a (.) will be used to indicate decimal fractions.

2 INTRODUCTION

This project was initiated in 1991 to facilitate the application of recent international research advances in mathematical modelling of flow phenomena in porous media to water related phenomena in South Africa, with particular emphasis on the enhancement of research on synthetic membrane systems and technology. Synthetic membrane technology presents powerful new concepts through which water treatment may be engineered. Optimal membrane process analysis and engineering design depend to a large extent on the quality of available or accessible quantitative knowledge about the basic flow phenomena present. The successful prediction of resistance to flow through microporous and ultrafiltration membranes depends largely on a good understanding of diverse flow phenomena in porous media. It, therefore, seems appropriate to contribute to our scientific understanding of membrane technological concepts by applying these newly developed mathematical tools in this area of research.

The object of the research project was three-fold: the first and most important objective was the development of a sound *mathematical model* from which flow phenomena in different porous environments may be predicted analytically or numerically. This may then enhance the design of membrane systems through the availability of *numerical simulation capabilities*, the creation of which was the second goal. A third objective was the analysis of *capillary force action* in porous media as aid to the investigation and design of tensiometer type soil moisture measurement meters. This last part of the project was scaled down considerably after it became known that the experimental programme regarding the tensiometer design investigations were halted. The time initially allocated to this activity was then used to enhance progress in the first goal by improving on the modelling of the so-called inertial effects in membrane flows.

At first it seems appropriate to discuss shortly the philosophy behind the approach followed in this project. A common practice in a complicated research field like transport phenomena in synthetic membranes is to conduct sets of controlled experiments from which correlation coefficients may be obtained for some phenomenon. Such correlations with adjustable coefficients are then regarded as models from which to infer the behaviour of similar or related phenomena. Although this is a justifiable practice when very little is known about the substance and its influence on a traversing fluid, the unknown interdependencies and reliability ranges of different parameters present difficulties during the assessment of numerical predictions.

In the present case the knowledge that is available about the substance under consideration is utilised to the full in developing a general theory, delaying the introduction of arbitrariness as long as possible. In this manner certain parameters can be determined to within a very narrow range and thus eliminate possible errors and or misconceptions. The real value of this type of modelling is that it carries over directly to an almost unlimited spectrum of applications and with it the confidence in its correctness.

Since 1986 considerable success was achieved on an international basis towards the *theoretical proof and understanding of fundamental flow phenomena within porous media.* Since the accurate modelling of such phenomena on a pore-scale presents unique opportunities in studying and understanding the fundamental principles of the various

transport processes, the time and effort devoted to this basic research have had almost immediate effect in the accuracy to within which such practical phenomena could be predicted. According to the new approach the theoretical development is driven as far as possible without introducing any arbitrary constants. The outcome is hopefully some mathematical equations from which practical situations in the laboratory or in field situations may be predicted quantitatively and without the necessity of adjustable parameters. If some level of arbitrariness has to be introduced for better correlation with experiment it is at a late stage of theoretical development when its harmful effects on the mathematics, describing the physics, is negligible. Scientifically this presents a very fortunate situation, since the resulting model cannot be adjusted to match experimental data. It either correctly describes the experiment satisfactorily or something is awry, either with the modelling assumptions or with the experimental conditions. The accuracy of the performance of the model could thus be inferred directly.

Computational methods have become a necessity for thorough analysis towards system design in almost all fluid-related technologies. The capabilities of computational fluid dynamics have dramatically enlarged the horizon of quantitative understanding of flow phenomena and especially in cases where porous media are present. More often than not the equations which were developed decades ago to aid the correlation among different experimental and field results are not any more accurate and robust enough for use in numerical computations. In numerical work the flow phenomena are not treated on an average scale -local heterogeneities are computed directly and this causes the equations to be pushed beyond their limits of applicability and consistency. This warrants the development of new mathematical equations for use in computer programs by which water-related phenomena in synthetic membranes can be accurately simulated numerically.

The development of static tensiometer type soil moisture measurement meters depends to a large extent on the qualitative understanding and quantitative predictability of *capillary force action* in a partially saturated porous medium. Capillary action is directly related to the scale and structural geometry of the porous medium under consideration. The research efforts mentioned above are based on the pore-scale modelling of porous media with the description of the pore-scale morphology a very prominent aspect. It thus provides the ideal platform from which to do a quantitative analysis of capillary action to enhance understanding and predictability of this phenomenon.

2.1 OBJECTIVES

Three objectives of this research regarding flow in synthetic membranes were proposed, namely

A The *analytical modelling* of flow through the different pore structures found in synthetic membranes.

B The establishment of a *computer code* providing the numerical means to study and predict flow phenomena in complex membrane systems and within the membranes themselves.

C The study of quasi-stationary *capillary action* in foamlike porous media to provide theoretical support to the practical development of tensiometer for soil moisture measurements.

The novel approach taken in this project, in addition to knowledge obtained from previous industrial projects, eliminated the need for an extensive literature survey. The theoretical basis of the work was developed only in 1986/87 as an international effort to eliminate some shortcomings in the theoretical basis of porous media flows. In a nutshell the overall purpose of the present project was to pave the way to differentiate mathematically between the hydrodynamic properties of different membrane structures such as those examples portrayed schematically as a composite in Figure 1 where the shaded areas denote membrane material.

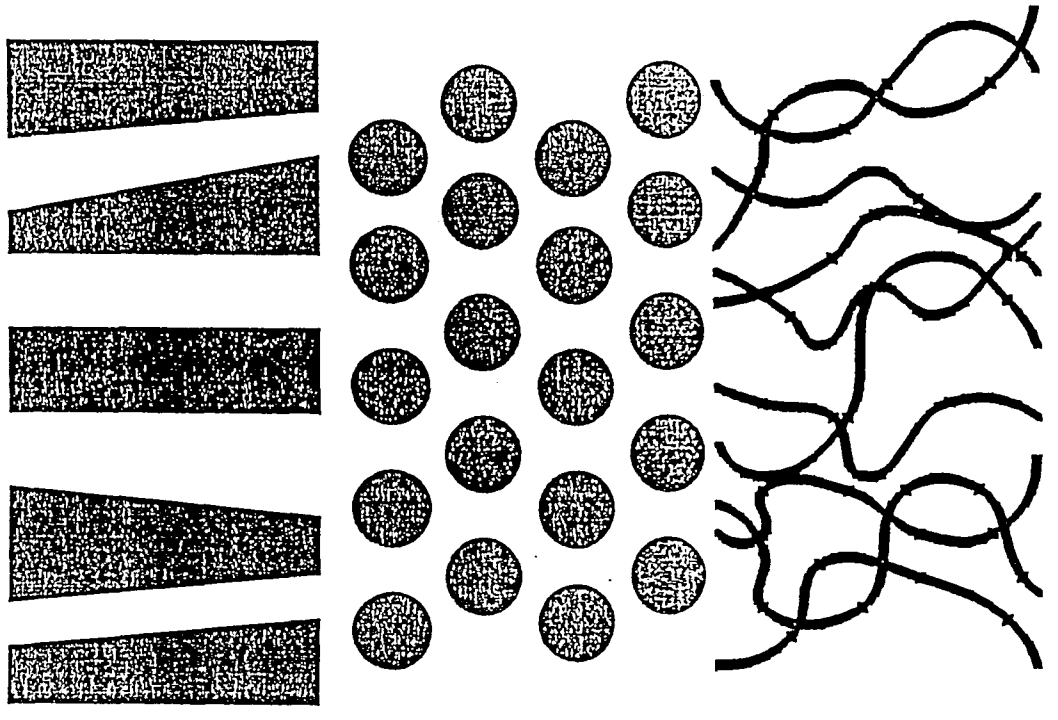

Figure 1. Basic Membrane Structures.

3 ANALYTICAL MODELLING

3.1 PHYSICAL PROBLEM STATEMENT

3.1.1 The Membrane

In general the membrane morphology is assumed to adhere to the following conditions:

- Stationary
  This condition implies that the motion of membrane material is negligible in comparison with the seepage velocity of the permeate.

- Isotropic
  The membrane is assumed to be a composite construction of different kinds of porous domains each of which can be described by one of the four basic geometric pore-structure models proposed, namely foamlike, granular, tubular, and prismatic.

3.1.2 The Fluid Phase

The traversing fluid is assumed to exhibit the following properties:

- Single phase.
- Constant density.
- Constant viscosity.

3.1.3 Micro-flow Properties

The following conditions apply as the fluid traverses the membrane pores:

- Laminar.
- A no-slip boundary condition applies to all fluid-solid interfaces.
- The entry velocity profile to each pore section is uniform.
- No local flow separation occurs within the pores.

3.1.4 Macro-flow properties

- Average velocity gradients small.

3.2 MATHEMATICAL PROBLEM STATEMENT

Subject to the conditions stated above the flow of permeate within the membrane pores is governed by the continuity equation for conservation of mass

$$\nabla \cdot v = 0 \tag{1}$$

The Navier-Stokes equation, governing the transport of momentum according to the assumptions above, can be written as follows:

$$\rho \frac{\partial v}{\partial t} + \rho \nabla \cdot vv + \nabla p - \rho g - \mu \nabla^2 v = 0 \quad . \tag{2}$$

Since it is impossible to explicitly describe the flow in each pore section an averaging procedure is introduced whereby all parameters are volumetrically averaged over some control volume V_o [Bachmat and Bear, 1986]. Each fluid-related quantity or term is volumetrically averaged over the fluid part V_f of V_o and multiplied by the porosity to yield an average over the entire volume V_o, the porosity being defined by

$$\epsilon \equiv \frac{V_f}{V_o} \quad . \tag{3}$$

The specific discharge q denotes the volume average of the fluid velocity within the pores and it will be used here as dependent variable in the averaged equations. This vectorial quantity also determines the local streamwise direction. It follows directly from the volumetric averaging of the actual interstitial velocity v, namely

$$q \equiv \langle v \rangle = \frac{1}{V_o} \int\int\int_{V_f} v \, dV = \frac{\epsilon}{V_f} \int\int\int_{V_f} v \, dV \tag{4}$$

Volumetric phase averaging [Bachmat and Bear, 1986] of the continuity equation (1) yields the following generalized equation for fluid mass conservation during its traverse of a porous medium:

$$\nabla \cdot q = 0 \quad . \tag{5}$$

Similarly the volumetrically averaged form of the Navier-Stokes equation (2) can be written as [Du Plessis and Masliyah, 1988]:

$$\rho\frac{\partial q}{\partial t} + \rho\nabla\cdot(qq/\epsilon) + \epsilon\nabla p_f - \epsilon\rho g - \mu\nabla^2 q + \frac{\rho}{V_o}\int\int_{V_f}\int \nabla\cdot(\mathring{v}\mathring{v})dV - \frac{1}{V_o}\int\int_{S_p}\left(-\mathring{p}\nu+\mu\nu\cdot\nabla v\right) dS = 0 \quad . \tag{6}$$

The evaluation of the surface integral in equation (6) is subject to a description of the real velocity gradients at the pore surfaces. This in turn warrants a fairly accurate description of the porous microstructure, which was modelled by Du Plessis and Masliyah, 1988 for foams.

Due to the assumption that no large velocity gradients are present the volume integral of the velocity dispersion should be very small and may thus be discarded in comparison with the other terms present.

The flow through the porous matrix was modelled by Du Plessis and Masliyah, 1988 according to the assumption of laminar developing flow in the pore sections. If the surface integral in equation (6) is approximated according to these conditions, the final momentum transport equation, which is applicable for any 'local' porosity ϵ and 'local' characteristic length d, is as follows [Du Plessis and Masliyah, 1991]:

$$\rho\frac{\partial q}{\partial t} + \rho\nabla\cdot(qq/\epsilon) + \epsilon\nabla p_f - \epsilon\rho g - \mu\nabla^2 q + \mu F q = 0 \quad . \tag{7}$$

This equation, together with the continuity equation (5), now presents the means to calculate the flow field analytically or numerically, provided the factor F can be explicitly expressed in terms of known parameters. The factor F represents quantification of the frictional effects of the membrane on the permeate. In the next section results for F are given for six different basic membrane structures.

4 ANALYTICAL RESULTS

Evaluation of the drag factor F was done in accordance with the proposal by Du Plessis and Masliyah, 1988 to introduce a Representative Unit Cell (RUC). This allows the quantitative and qualitative evaluation of all the different contributions to the drag on the fluid explicitly in terms of the porosity ϵ, the scale length d of the microstructure, the type of microstructure through the tortuosity T and the seepage velocity q. The effective cross-sectional area of a single pore is given by the relation

$$A_p = \epsilon T d^2 \quad . \tag{8}$$

Consistent herewith the relation between the seepage velocity q and the mean pore velocity v_p is given for all subsequent models by

$$q = \epsilon T v_p \quad . \tag{9}$$

This relation determines the pore velocity uniquely, from which intrapore fluid dynamical phenomena may be deduced more accurately.

4.1 FOAM STRUCTURE

Consolidated porous media in spongelike form may be represented by a RUC containing three mutually orthogonal duct sections of square cross-section. In Figure 2 the pore section arrangement within the foam RUC is shown. This arrangement of pore sections is conceptually similar to the somewhat different geometry first proposed by Du Plessis and Masliyah, 1988.

The relationship between the pore diameter d_p and the characteristic length d of the microstructure is given by:

$$d_p = \frac{(3T-1)d}{2T} \quad . \tag{10}$$

The tortuosity for such a pore representation is given by [Du Plessis, 1992a]:

$$T = \frac{3}{4\epsilon} + \frac{\sqrt{9-8\epsilon}}{2\epsilon} \cos\left[\frac{4\pi}{3} + \frac{1}{3}\cos^{-1}\left\{\frac{8\epsilon^2-36\epsilon+27}{(9-8\epsilon)^{3/2}}\right\}\right] \quad . \tag{11}$$

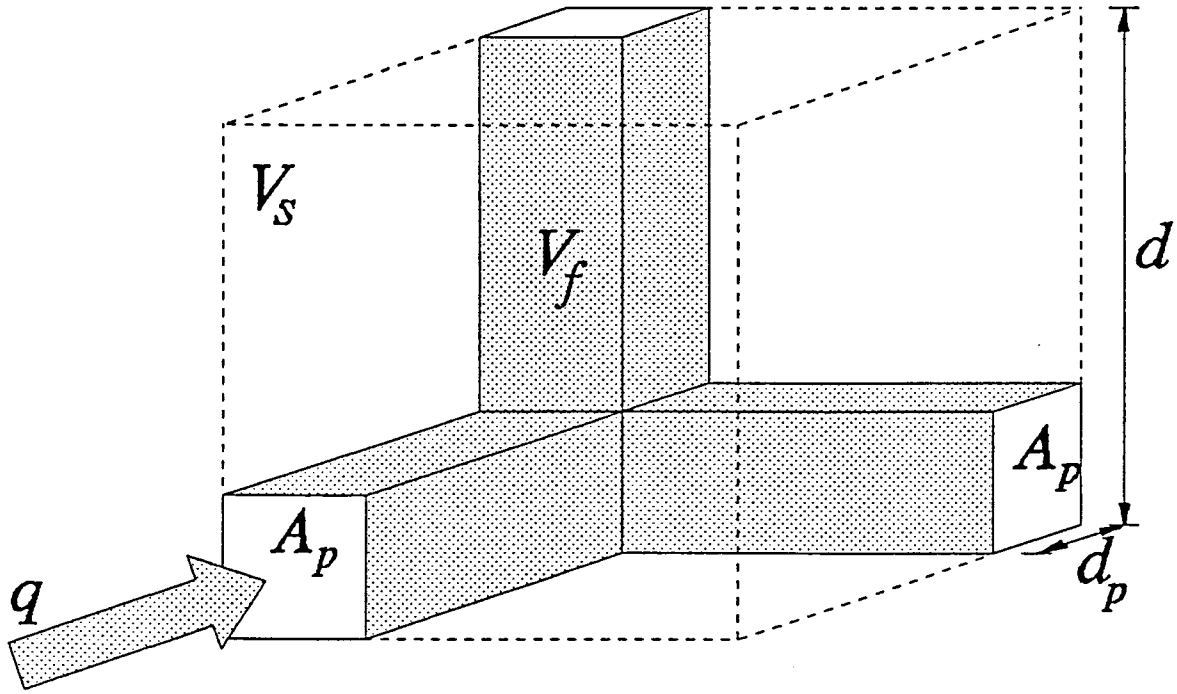

Figure 2. RUC for Foam Structure.

The shear stress factor F is given by [Du Plessis & Masliyah, 1988]:

$$F = \frac{42.69}{d^2}\,\frac{1-T}{\epsilon T^2}\sqrt{1 + \frac{0.117T}{1-T}\,Re_{qd}} \quad . \tag{12}$$

The critical Reynolds number which indicates the transition between Darcy and Forchheimer flow behaviour is given by

$$\left(Re_{qd}\right)_c = \frac{1-T}{0.117T} \quad . \tag{13}$$

In case of low Reynolds number flow the hydrodynamic permeability is given by

$$K = \frac{\epsilon^2 T^2 d^2}{42.7(1-T)} \quad . \tag{14}$$

4.2 GRANULAR STRUCTURE

The RUC introduced for granular structures consists of a cubic volume with a cubic solid placed centrally within and with faces aligned, Du Plessis & Masliyah, 1991. In Figure 3 the solid distribution within the granular RUC is shown.

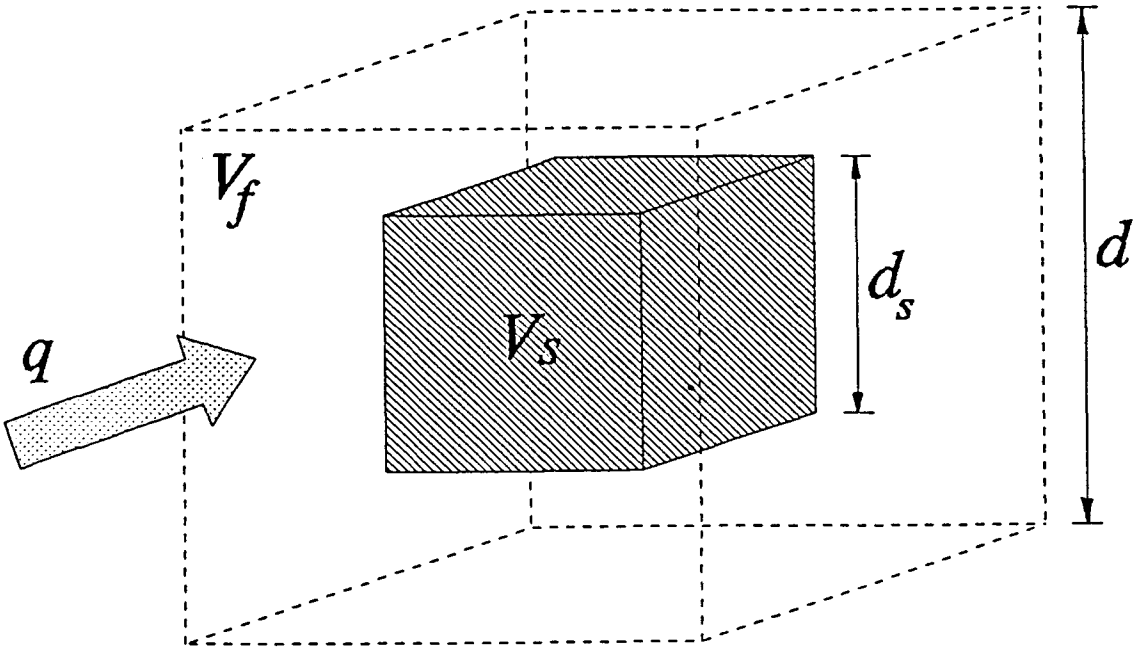

Figure 3. RUC for Granular Structure.

The tortuosity of the porous microstructure is given by

$$T = \frac{1-(1-\epsilon)^{2/3}}{\epsilon} \tag{15}$$

and the scale length of the granules by

$$d_s = (1-\epsilon)^{1/3}\, d \quad . \tag{16}$$

Evaluation of the non-linear dependence of F on the specific discharge q was done by the modelling of two intrapore effects which may give rise to such nonlinear behaviour, namely intrapore flow development and intrapore flow recirculation.

4.2.1 Flow Development Model

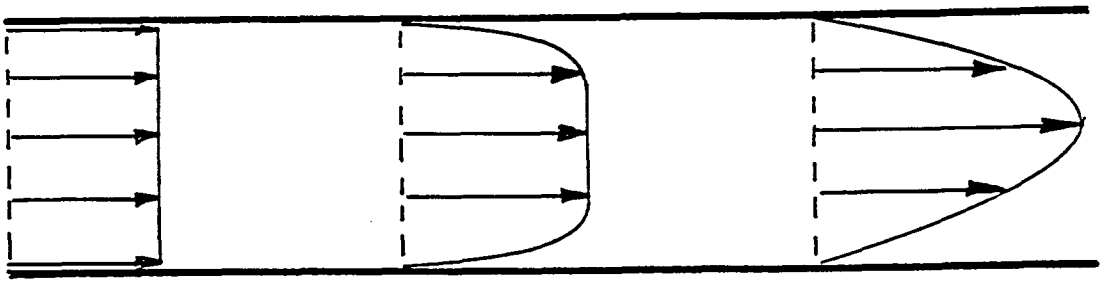

Figure 4. Flow Development in a RUC Pore Section.

The frictional effects introduced by the presence of the granules is governed by the term $\mu F q$, the factor F being given by the following expression [Du Plessis and Masliyah, 1991] for the case of granular porous media:

$$F = \frac{36}{d^2} \frac{(1-\epsilon)^{2/3}}{\left[1-(1-\epsilon)^{1/3}\right]\left[1-(1-\epsilon)^{2/3}\right]} \sqrt{1 + \frac{0.0822\ Re_{qd}\left[(1-\epsilon)^{-1/3}-1\right]}{\left[1+(1-\epsilon)^{1/3}\right]}} \quad . \tag{17}$$

The Reynolds number dependent term originates from inclusion of flow development within each pore section, according to which the velocity profile changes from a uniform inlet profile towards a fully developed parabolic profile as illustrated schematically in Figure 4.

The critical Reynolds number $(Re_{qd})_c$ gives the Reynolds number at the centre of the transition region between the Darcy region of velocity-independent F and the Forchheimer region, where non-linearity is introduced by the inertial effects. From equation (17) it can be expressed explicitly in terms of porosity as follows:

$$\left(Re_{qd}\right)_c = \frac{1+(1-\epsilon)^{1/3}}{0.0822\left[(1-\epsilon)^{-1/3}-1\right]} \quad . \tag{18}$$

In the case of small Reynolds number flow, the square-rooted factor on the RHS of equation (17) approaches unity, rendering the term $\mu F q$ linear in velocity. The hydrodynamic permeability, inclusive of the non-linear microscopic inertial effects, is given by ϵ / F and this leads to a velocity-independent Darcy-permeability for very low Reynolds number flow ($Re_{qd} \ll \left(Re_{qd}\right)_c$) of

$$K = \frac{d^2}{36} \frac{\epsilon}{(1-\epsilon)^{2/3}} \left[1-(1-\epsilon)^{1/3}\right] \left[1-(1-\epsilon)^{2/3}\right] \quad . \tag{19}$$

The intrapore flow Reynolds number Re, based upon a flat plate configuration of the pore microstructure, is given by

$$Re = \frac{2}{1+(1-\epsilon)^{1/3}} Re_{qd} \quad . \tag{20}$$

The results for this type of medium may be simplified considerably by restriction to a small range of porosities. As a typical example, results are presented here for low and very low porosities. Similar simplifications are possible for other bounds on porosity values.

Low Porosities

In case of low porosity values the above expression for F may be subjected to a series expansion and truncation [R8], yielding

$$F = \frac{27}{d^2} \frac{(6-7\epsilon)}{\epsilon^2} \sqrt{1 + 0.00228\epsilon(6+5\epsilon)\, Re_{qd}} \tag{21}$$

with the critical Reynolds number

$$\left(Re_{qd}\right)_c = \frac{6-5\epsilon}{0.0822\epsilon} \quad . \tag{22}$$

The corresponding hydrodynamic Darcy permeability is given by

$$K = \frac{\epsilon^3 d^2}{972} (6+7\epsilon) \quad . \tag{23}$$

These simplified results may also be used for intermediate porosity values, provided the truncation is accompanied by throwback at the appropriate porosity level [Roos, 1992].

Very Low Porosities

Further truncation of the results above leads to the following results, accurate only at very low porosities

$$F = \frac{162}{d^2} \frac{1}{\epsilon^2} \sqrt{1 + 0.0137\epsilon \, Re_{qd}} \tag{24}$$

with

$$\left(Re_{qd}\right)_c = \frac{73}{\epsilon} \tag{25}$$

and

$$K = \frac{\epsilon^3 d^2}{162} \quad . \tag{26}$$

4.2.2 Flow Recirculation Model

At the closing stages of the project a breakthrough was made in the theoretical modelling through the successful inclusion of flow separation within the pores on the local lee side of each granule [Du Plessis, 1992c] as indicated in Figure 5. Due to this improvement the Ergun equation, which encompasses experimental results over a wide range of parameters, can be proven quantitatively. Although, due to the low Reynolds numbers encountered in membrane flows, recirculation will not be a prominent feature, its gradual increase is affecting the velocity-pressure drop relationship already at very low Reynolds numbers.

According to this analysis the F-factor is given by

$$F = \frac{36}{d^2} \frac{(1-\epsilon)^{2/3}}{\left[1-(1-\epsilon)^{1/3}\right]\left[1-(1-\epsilon)^{2/3}\right]} + \frac{(1-\epsilon)^{2/3}}{\left[1-(1-\epsilon)^{2/3}\right]^2} \frac{Re_{qd}}{d^2} \tag{27}$$

with a critical Reynolds number of

$$\left(Re_{qd}\right)_c = \frac{36\left[1-(1-\epsilon)^{2/3}\right]}{\left[1-(1-\epsilon)^{1/3}\right]} \quad . \tag{28}$$

The hydrodynamic permeability is given by

$$K = \frac{\epsilon d^2}{36(1-\epsilon)^{2/3}} \left[1-(1-\epsilon)^{1/3}\right]\left[1-(1-\epsilon)^{2/3}\right] \quad . \tag{29}$$

These equations predict the Ergun equation almost exactly in the range for which the latter is reported to be applicable.

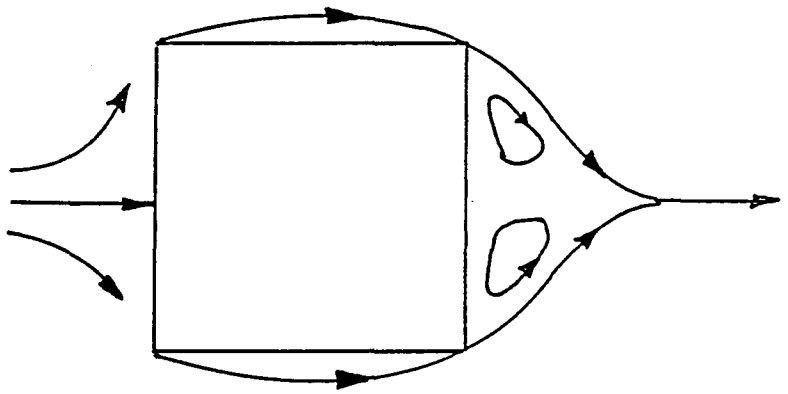

Figure 5. Flow Recirculation in Pore Section.

4.3 2D TUBULAR STRUCTURE

4.3.1 Square Cross-section

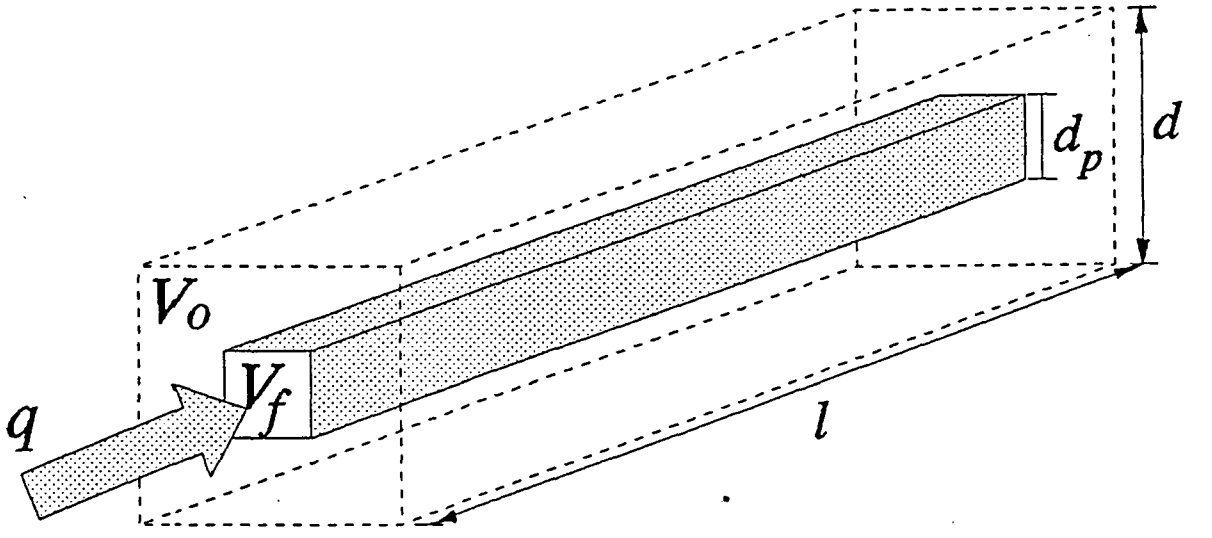

Figure 6. RUC for Tubular Structure of Square Cross-Section.

Straight parallel tubular ducts are assumed [Roos, 1992] through the medium as is shown in Figure 6, yielding a tortuosity

$$T = 1 \quad . \tag{30}$$

The relationship between the pore width d_p and the characteristic length d of the pore structure is

$$d_p = \sqrt{\epsilon}\, d \quad . \tag{31}$$

Internal friction is governed by the factor F, following from

$$Fd^2 = \frac{28.5}{\epsilon}\sqrt{1 + 0.0584\ Re_{qd}\ \frac{d}{l}} \quad . \tag{32}$$

This gives a critical Reynolds number of

$$\left(Re_{qd}\right)_c = 17.1\ \frac{l}{d} \tag{33}$$

and a hydrodynamic permeability of

$$K = \frac{\epsilon^2 d^2}{28.46}\ \frac{1}{\sqrt{1 + 0.0584\ Re_{qd}\ \frac{d}{l}}} \quad . \tag{34}$$

4.3.2 Circular Cross-section

The tubular structure given above may be relaxed to that of a tubular structure comprising tubes of circular cross section [Roos, 1992] as is shown in Figure 7.

The tortuosity for this RUC structure is

$$T = 1 \tag{35}$$

due to the assumption of coherent straight channels.

$$d_p = 2\sqrt{\frac{\epsilon}{\pi}}\ d \quad . \tag{36}$$

Internal friction is governed by the factor

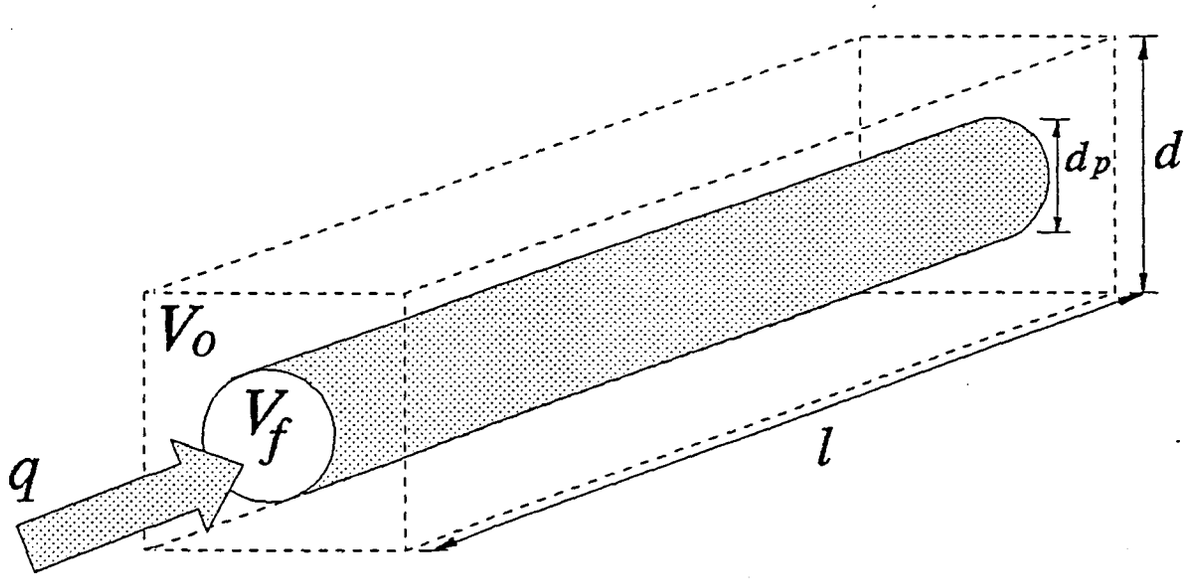

Figure 7. RUC for Tubular Structure of Circular Cross-Section.

$$Fd^2 = \frac{25.13}{\epsilon}\sqrt{1 + 0.0586\, Re_{qd}\,\frac{d}{l}} \tag{37}$$

and this leads to a critical Reynolds number of

$$\left(Re_{qd}\right)_c = 17\,\frac{l}{d} \tag{38}$$

and a Darcy permeability of

$$K = \frac{\epsilon^2 d^2}{25.13}\,\frac{1}{\sqrt{1 + 0.0586\, Re_{qd}\,\frac{d}{l}}} \tag{39}$$

Comparison of results for the two cases suggests that either of the two may be taken as representative of a tubular structure.

4.4 2D PRISMATIC STRUCTURE

The RUC may be defined as infinitely long prisms of square cross-section as is shown in Figure 8. The solid constituent of each RUC is a solid bar of infinite length and square cross-section placed concentric to the RUC itself and with its sides aligned with that of the RUC.

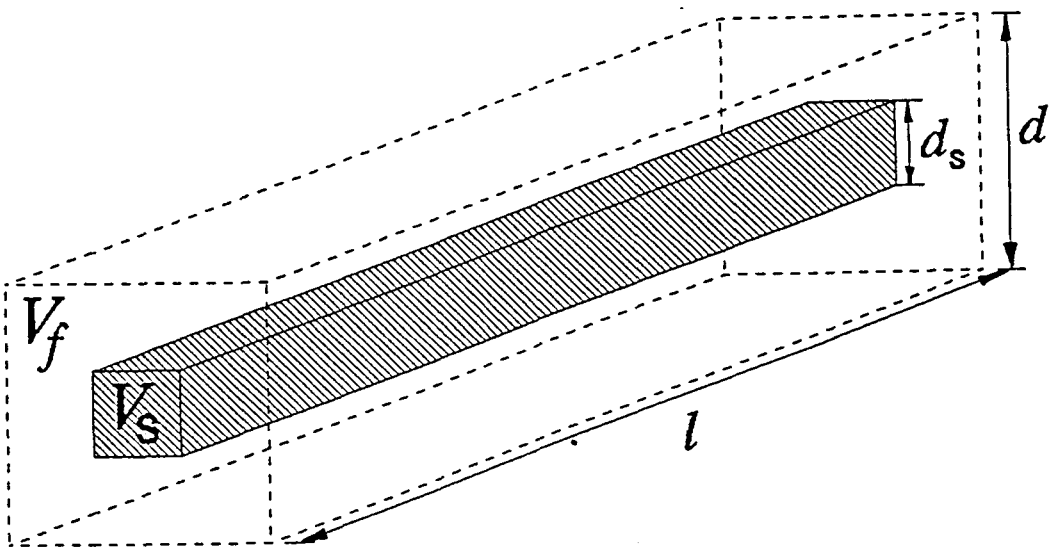

Figure 8. RUC for Prismatic Structure.

4.4.1 Crossflow

During crossflow the flow takes place perpendicular to the longitudinal axes of the prismatic arrangement. The tortuosity for crossflow through the particular arrangement is given by

$$T = \frac{1-\sqrt{1-\epsilon}}{\epsilon} \tag{40}$$

and the cross-sectional scale length of the solid structure by

$$d_s = \sqrt{1-\epsilon}\; d \quad . \tag{41}$$

Friction provided to the fluid by the solid bars can thereupon be approximated by the following expression [Du Plessis, 1991a,b]:

$$Fd^2 = \frac{24\sqrt{1-\epsilon}}{\left[1-\sqrt{1-\epsilon}\right]^2}\sqrt{1 + 0.0822\, Re_{qd}\,\frac{1-\sqrt{1-\epsilon}}{\sqrt{1-\epsilon}}} \quad . \tag{42}$$

The critical Reynolds number is accordingly given by

$$\left(Re_{qd}\right)_c = \frac{12.2\sqrt{1-\epsilon}}{1-\sqrt{1-\epsilon}} \tag{43}$$

and the Darcy permeability by

$$K = \frac{\epsilon d^2\left[1-\sqrt{1-\epsilon}\right]^2}{24\sqrt{1-\epsilon}} \quad . \tag{44}$$

4.4.2 Longitudinal Flow

In this case the results are given in terms of an axial length l along the prismatic bar [Roos, 1992] as is shown in Figure 8. The flow now takes place longitudinally along the prismatic bar. For the tortuosity it follows that

$$T = 1 \tag{45}$$

and for the cross-sectional scale length of the solid structure that

$$d_s = \sqrt{1-\epsilon}\; d \quad . \tag{46}$$

Internal friction is governed by

$$Fd^2 = \frac{24\sqrt{1-\epsilon}}{\epsilon\left[1-\sqrt{1-\epsilon}\right]}\sqrt{1 + 0.0822\, Re_{qd}\,\frac{d}{l}\,\frac{\left[1-\sqrt{1-\epsilon}\right]^2}{\epsilon}} \tag{47}$$

leading to a critical Reynolds number of

$$\left(Re_{qd}\right)_c = \frac{\epsilon}{0.0822\left[1-\sqrt{1-\epsilon}\right]^2}\,\frac{l}{d} \quad . \tag{48}$$

In the low Reynolds number regime the Darcy permeability is given by

$$K = \frac{\epsilon^2 d^2\left[1-\sqrt{1-\epsilon}\right]}{24\sqrt{1-\epsilon}} \quad . \tag{49}$$

4.5 DIFFERENCES BETWEEN STRUCTURES

In Figure 9 the hydrodynamic permeability as predicted by the different porous structures is presented graphically as a function of the porosity. It is clear that, for certain porosities and all other scale parameters being the same, the permeabilities predicted for the different models may differ by almost two orders of magnitude. This is especially important in the case of comparison between tubular and granular media, the latter conforming to actual structures present in some membranes and the former to the model on which most analyses available in literature have been based. This fact is, therefore, responsible for the need for experimental callibration of empirical constants, which may need to be eliminated after proper introduction of the present results.

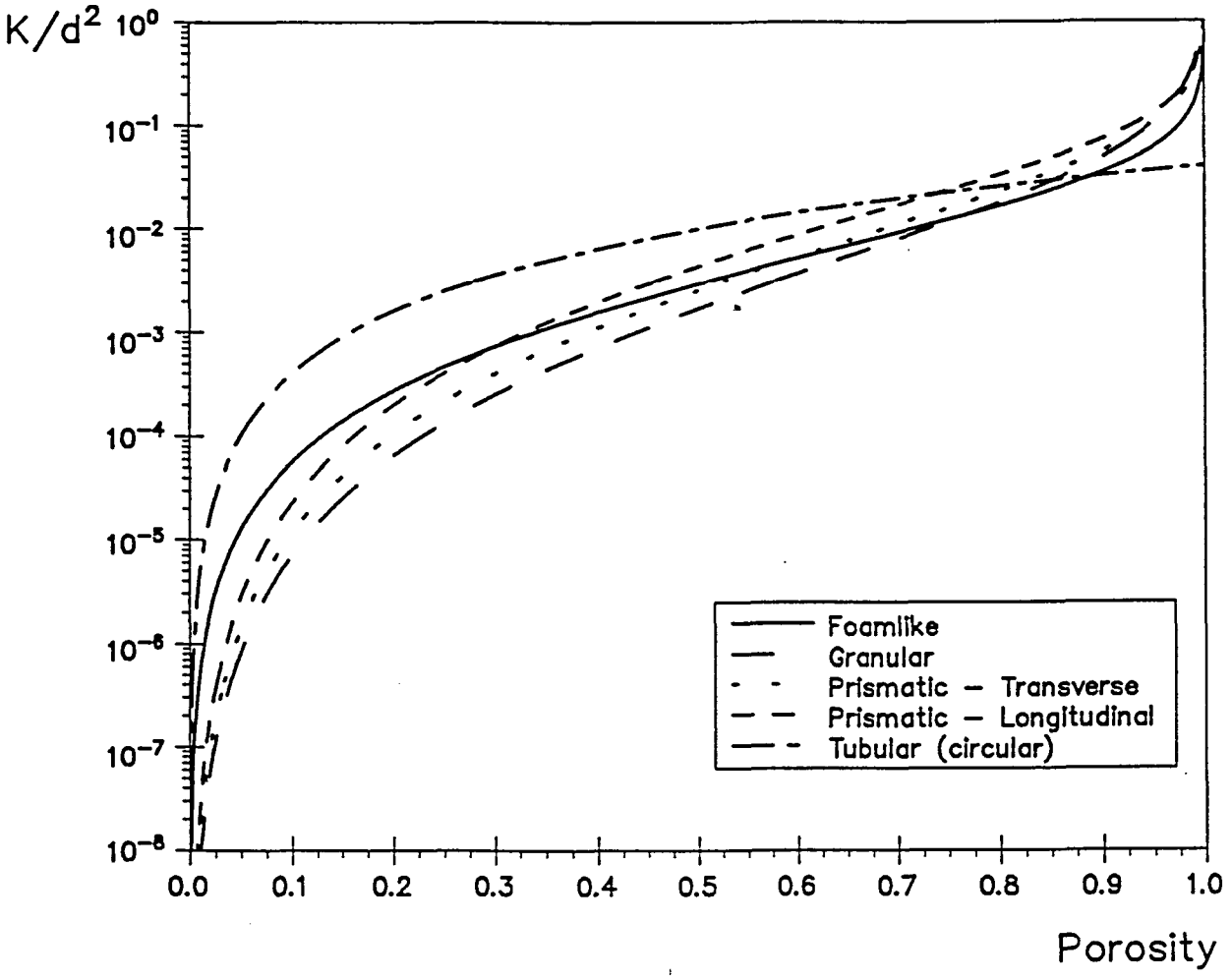

Figure 9. Permeabilities Predicted for Different Structures.

4.6 COMPARISON WITH STATISTICAL MODEL

The theoretical results derived for tubular structures were tested against numerical results obtained by Arnold et al, 1989. In Table 1 the results are compared directly, showing that the present theory predicts similar results for the discharge through a membrane of tubular structure. It should be noted that for this comparison the present method has a large computational advantage above the statistical method, the latter requiring 35 times more CPU time for execution.

Table 1: Specific Discharge Values $q/\left(-\frac{dp}{dz}\right)$.

ϵ	Tubular Model $d_p = 5.5\times10^{-10}$	Statistical Model $\bar{d}_p = 5.5\times10^{-6}$	
		$\sigma = 0.1\times10^{-6}$	$\sigma = 0.375\times10^{-6}$
0.1	0.9453×10^{-10}	0.9479×10^{-10}	0.9704×10^{-10}
0.2	1.8906×10^{-10}	1.8948×10^{-10}	1.9379×10^{-10}
0.3	2.8359×10^{-10}	2.8404×10^{-10}	2.9020×10^{-10}
0.4	3.7812×10^{-10}	3.7872×10^{-10}	3.8618×10^{-10}
0.5	4.7265×10^{-10}	4.7355×10^{-10}	4.8351×10^{-10}
0.6	5.6718×10^{-10}	5.6851×10^{-10}	5.8177×10^{-10}
0.7	6.6171×10^{-10}	6.6306×10^{-10}	6.7798×10^{-10}
0.8	7.5624×10^{-10}	7.5821×10^{-10}	7.7645×10^{-10}
0.9	8.5077×10^{-10}	8.5243×10^{-10}	8.7143×10^{-10}

4.7 COMPARISON WITH EXPERIMENT

The Institute for Polymer Science at the University of Stellenbosch supplied data regarding pure water flow through tubular membranes. These mambranes were constructed of polyethylene glycol with molecular weight of 12000, 20000 and 35000 , respectively, and are being used for ultra filtration processes. The average pore diameter of an ultra filtration membrane may range from approximately 2 nm to 250 nm. According to a process selection chart distributed by Membratek (Pty) Ltd, the average pore diameter of a membrane with a molecular weight of 20000 is in the order of 10 nm.

In order to demonstrate the comparison of results, the data regarding membranes with molecular weight of 20000 will be given here. The data supplied includes the following:

Table 2: Data Supplied for a 20000 Polyethylene Glycol Membrane.

Pressure drop over membrane (kPa)	200	300	400
Pure water flux ($l/m^2/h$)	190	304.2	418.9

According to information obtained from the Institute of Polymer Science, the thickness of the membrane lies in the range of $1\mu m$ to $250\mu m$. The objective now is to incorporate the given experimental data in the relevant volumetric averaging models derived here to predict an average pore diameter for a membrane of the specified thickness.

In order to compare the experimental values to results derived here for tubular membranes, the notation should be brought in correspondance. For low Reynolds number flow equation (37) yields:

$$Fd^2 = \frac{25.13}{\epsilon} \tag{50}$$

and, by substituting d^2 by $\frac{\pi}{4\epsilon} d_p^2$ we get

$$F = \frac{100.532}{\pi d_p^2} \quad . \tag{51}$$

In case of steady, incompressible flow in the z-direction, equation (7) becomes

$$\frac{q}{\left(-\frac{dp}{dz}\right)} = \frac{\epsilon \pi d_p^2}{100.532 \mu} \quad . \tag{52}$$

The following expression for the pore diameter d_p may thereupon be derived for the tubular model:

$$d_p = \sqrt{\frac{q}{\left(-\frac{dp}{dz}\right)} \cdot \frac{100.532 \mu}{\epsilon \pi}} \quad . \tag{53}$$

In the case of the volumetric averaging model for foamlike porous media, equation (12) for low Reynolds number flow is given by

$$Fd^2 = \frac{42.69(1-T)}{\epsilon T^2} \tag{54}$$

where T is given by equation (11).

Using equation (10) in (54) the following expression for F is derived:

$$F = \frac{10.6725(1-T)(3T-1)^2}{\epsilon d_p^2 T^4} \quad . \tag{55}$$

For steady, incompressible flow in the z-direction, equation (7) then becomes

$$\frac{10.6725(1-T)(3T-1)^2}{\epsilon d_p^2 T^4} \mu q = \epsilon \left[-\frac{dp}{dz}\right] \quad . \tag{56}$$

The pore diameter may then be determined through the following relation:

$$d_p = \sqrt{\frac{q}{\left(-\frac{dp}{dz}\right)} \cdot \frac{10.6725\mu(1-T)(3T-1)^2}{\epsilon^2 T^4}} \quad . \tag{57}$$

For the purpose of validating results, a value of 0.5 for the porosity seems reasonable and this value was confirmed by the Institute for Polymer Science. The dynamic viscosity μ for pure water is 0.001 Nsm^{-2}. Using the values given in Table 2, the values obtained for d_p are given in Table 3.

Table 3: Predicted Pore Diameter Values (in m).

	dp (kPa)	200	300	400
dz (μm)	*q* ($l/m^2/h$)	190	304.2	418.9
1	Foam	4.747×10^{-9}	4.904×10^{-9}	4.984×10^{-9}
	Tubular	4.110×10^{-9}	4.246×10^{-9}	4.315×10^{-9}
5	Foam	1.061×10^{-8}	1.097×10^{-8}	1.114×10^{-8}
	Tubular	9.189×10^{-9}	9.494×10^{-9}	9.648×10^{-9}
10	Foam	1.501×10^{-8}	1.551×10^{-8}	1.576×10^{-8}
	Tubular	1.300×10^{-8}	1.343×10^{-8}	1.364×10^{-8}
50	Foam	3.356×10^{-8}	3.468×10^{-8}	3.524×10^{-8}
	Tubular	2.906×10^{-8}	3.002×10^{-8}	3.051×10^{-8}
100	Foam	4.474×10^{-8}	4.904×10^{-8}	4.984×10^{-8}
	Tubular	4.110×10^{-8}	4.246×10^{-8}	4.315×10^{-8}
150	Foam	5.813×10^{-8}	6.006×10^{-8}	6.104×10^{-8}
	Tubular	5.033×10^{-8}	5.200×10^{-8}	5.285×10^{-8}
200	Foam	6.713×10^{-8}	6.935×10^{-8}	7.048×10^{-8}
	Tubular	5.812×10^{-8}	6.004×10^{-8}	6.102×10^{-8}
250	Foam	7.505×10^{-8}	7.754×10^{-8}	7.880×10^{-8}
	Tubular	6.498×10^{-8}	6.713×10^{-8}	6.822×10^{-8}

As the specified pressure difference - flux combinations are given for a specific membrane, it is expected that the calculated pore diameter values for these combinations should remain constant for a specified membrane thickness. This can indeed be seen in Table 3, the horizontal rows giving similar values for the three different pressure drops. Furthermore, the average pore diameter (over all membrane thicknesses considered) using the foam model is 4×10^{-8}m and using the tubular model 3.5×10^{-8}m. This is well in the range for ultra filtration membranes, and is in the order of 1×10^{-8}m as given in the process selection chart for membranes with molecular weight of 20000.

The comparison presented here clearly demonstrates that theoretical results are capable of accurately predicting pore characteristics from overall experimental data provided that the porosity and membrane thickness are known. Should a whole range of data on the same membrane be available it should also be posssible to determine either the porosity or the membrane thickness, should only one be known.

5 NUMERICAL SIMULATION

5.1 FINITE DIFFERENCE NUMERICAL PROCEDURE

Equations (5) and (7) may be solved by any suitable numerical procedure, which allows computation with predominant source terms in some areas of the flow regime. During this project a finite difference procedure, based on the SIMPLEC improvement [Van Doormaal and Raithby, 1984] on the SIMPLE procedure [Patankar, 1980] was used. To avoid all the pitfalls of programming and other teething errors a proven basic FORTRAN code for computational fluid dynamics was adapted to include the presence of porous material in any subsection of the computational domain. Suitable analytical expressions for fully developed average flow were also developed to serve as benchmark tests of the coding [Du Plessis and Van Der Merwe, 1992].

The adapted version of the FORTRAN computer code used to solve the momentum transport equations with a finite volume numerical procedure is being filed as Report PMG-92-01 of the Department of Applied Mathematics at the University of Stellenbosch. In accordance with the contractual agreement this program is available as it is without any user-friendly documentation or any other user aid or guidance.

5.2 NUMERICAL RESULTS

It proved very difficult to obtain data sets from controlled experiments with which to compare the results. Apart from some comparisons, therefore, a range of fictitious membrane conditions were subjected to the six different membrane models as well as some arbitrary composite structures. Some numerical results are graphically presented below to convey the capabilities of the present approach.

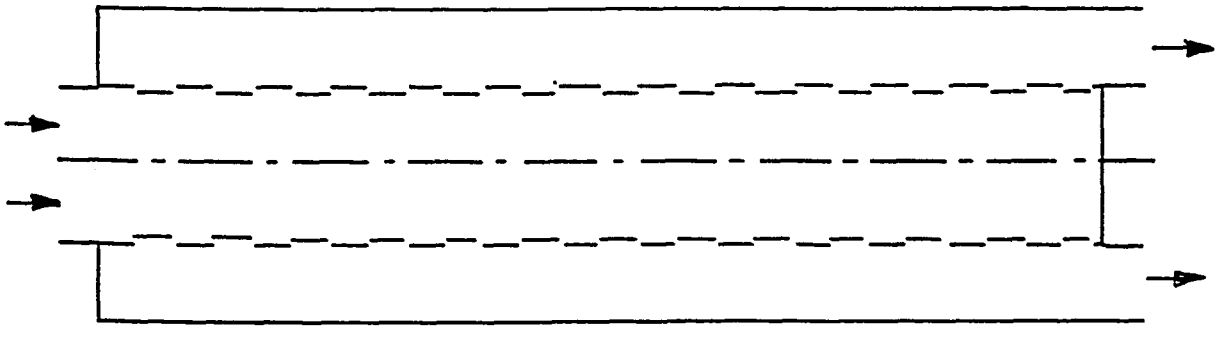

Figure 10. Hypothetical tubular arrangement of membrane process.

In Figure 10 a tubular membrane arrangement, according to which some demonstrative numerical simulations are done, is shown. The arrangement consists of a tubular membrane, housed co-axially within an outer shell. Fluid enters the inner membrane tube, filters through the membrane due to a dead end of the inner tube and flows out of the annular area.

In Figure 11 the numerical results are shown for the tubular arrangement when the membrane consists of a foamlike structure. Results (a), (b) and (c) for are given respectively for the three porosities 0.1, 0.5 and 0.9.

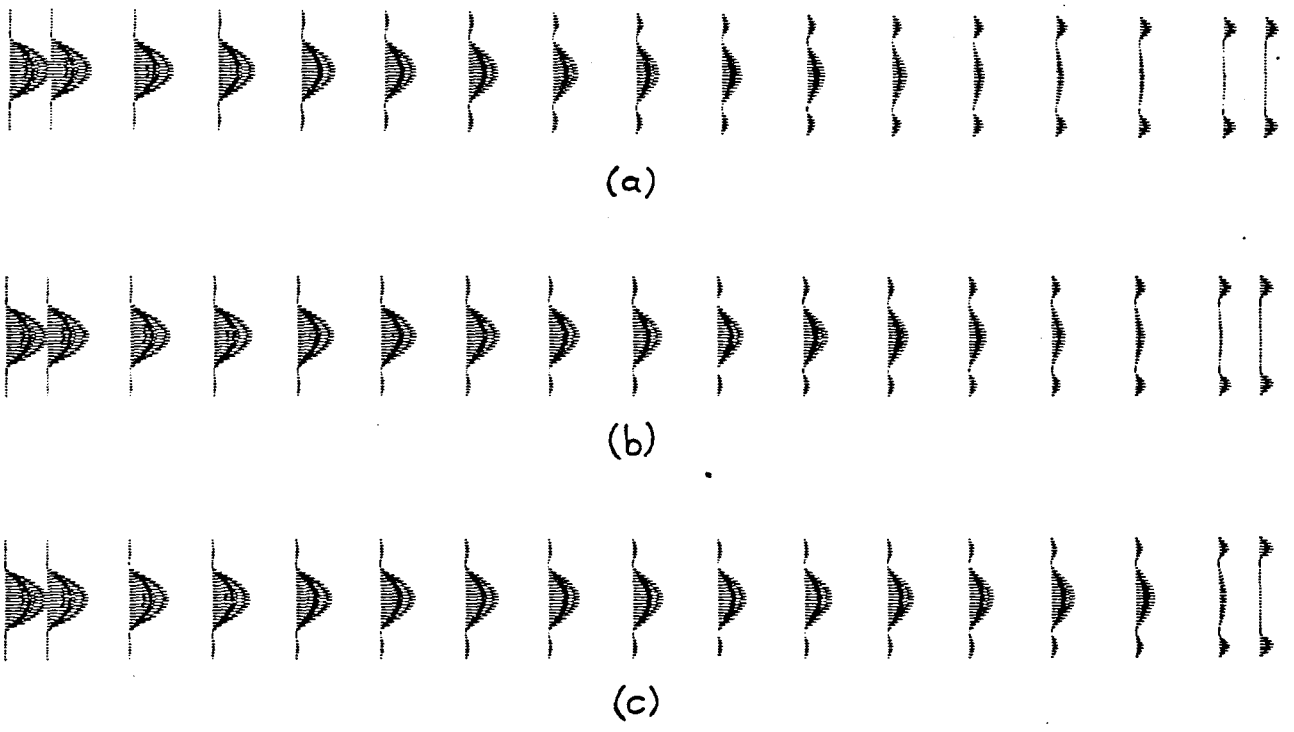

Figure 11. Flow for Foam Structure.

In Figure 12 the numerical prediction of normalised cumulative discharges are shown for a foamlike membrane structure in the tubular arrangement, but with different porosities. Normalised cumulative discharges for different membrane structures as predicted numerically are given in Figure 13. In all these cases the porosity and characteristic lengths were identical. For optimal membrane performance the curve should be a straight line and it should be clear from this hypothetical example that, even in cases of more complicated axi-symmetric geometries, the numerical capability may considerably enhance the engineering design.

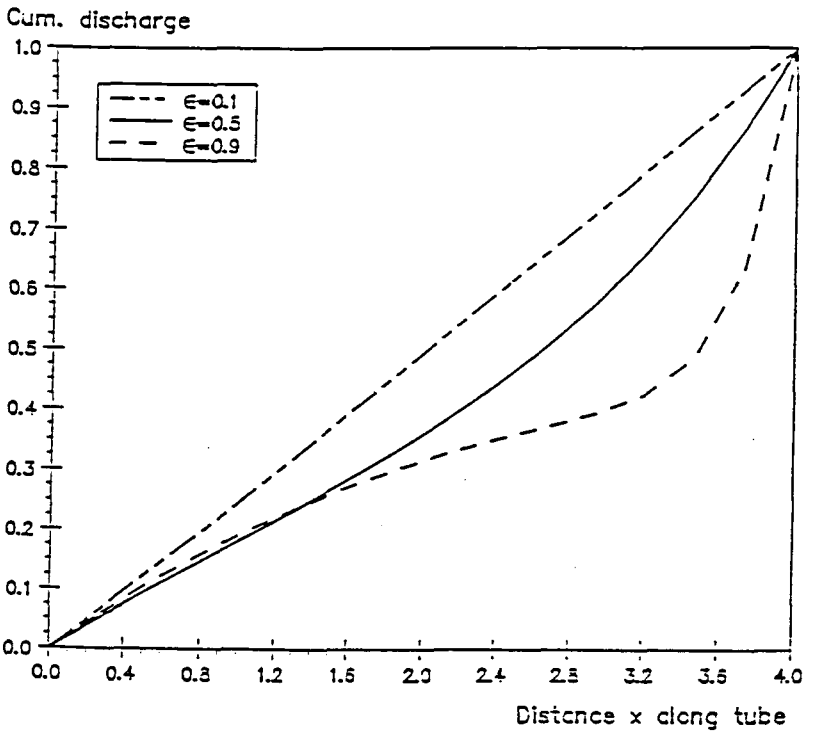

Figure 12. Normalised Cumulative Discharge for Different Membrane Porosities.

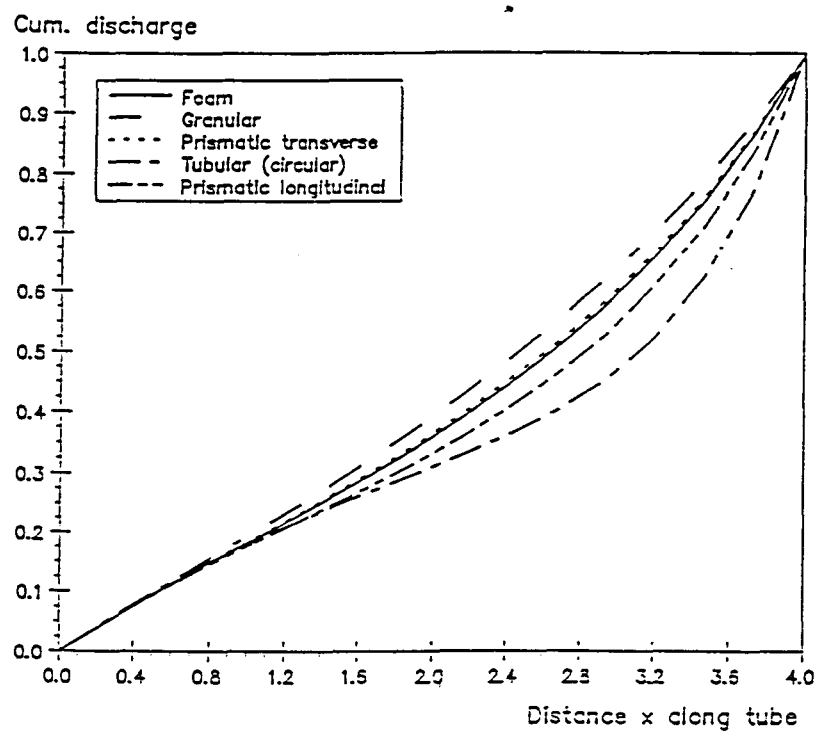

Figure 13. Normalised Cumulative Discharge for Different Membrane Structures.

6 CAPILLARY FORCE ACTION

6.1 INTRODUCTION

The geometrical models for the substructures of the membrane may all be applied to the study of the capillary force action. In particular, the foam model appears to be the closest to what was intended for the groundwater potensiometers. In its present form these results apply only to isotropic foams with uniform pore cross-sections. If smaller pore throats do play a predominant part in the capillary force action, the results will have to be generalised accordingly.

6.2 LITERATURE SURVEY

An extensive literature survey was conducted to obtain the most up to date mathematical methods used in the modelling of capillary action. Some of the most prominent mathematical analyses studied are listed in the reference list, namely Bear and Bachmat, 1991, Adamson, 1982, and Lowell and Shield, 1984.

As already mentioned above the research effort in this branch of the project was terminated when it became known that the experimental part was not being pursued any further. The most cost-efficient way to make available the preliminary work without pushing the overhead costs too high is to make the study material available as is in an informal document. This material is therefore available under the title Informal Research Notes on Capillary Force Action and filed as Report PMG-92-02 of the Porous Medium Research Group at the Department of Applied Mathematics, University of Stellenbosch [Collins and Du Plessis, 1992].

6.3 FINAL REMARKS

It should be noted that the complete analytical description given above for the mathematical modelling of the foamlike and other membrane structures apply directly to the investigation of capillary force action in porous media. Since the pore structure determines the cross-sectional pore area A_p and this in turn the surface tension, quantification of the latter may be substantially aided by the results derived above. The crucial equation derived is therefore the following expression for the cross-sectional pore area

$$A_p = \epsilon T d^2 \tag{58}$$

from which the magnitude of the particular surface tension may be obtained.

7 CLOSURE

Mathematical models were derived for flow in different kinds of porous structures as are found in the composite structure of a synthetic membrane. These models are deterministic and expressed in terms of basic parameters of the membrane structure. They allow pressure drop and flow rates to be determined directly and conversely knowledge about the membrane structure may be inferred from a study of overall pressure drop-flow rate data.

These models were also incorporated in extensive two-dimensional computer code by which flow and pressure drop data may be predicted for practical membrane systems. The code may also be used in axi-symmetric mode to allow for computation of flow phenomena in tubular configurations. These predicting possibilities may enhance better design of new or upgrading of existing membrane systems.

The most important result, however, is that a sound theoretical basis was secured from which future studies in membrane or other porous medium phenomena regarding water resources management may be conducted. To a large extent it eliminates the need for mathematical "models" by which porous flow phenomena are described by the introduction of haphazard and artificial correlation constants inferred from comparison between experimental data sets.

During the two years that this project was conducted, it was demonstrated beyond doubt that mathematical modelling can be conducted accurately so as to provide confidence in predicted results in the water engineering practice.

Overall the project was very successful and significant advances in the development of a unified theoretical approach to flow through synthetic membranes were made. Since the development was kept as general as possible, validation could be effected by comparisons outside of the particular membrane field - this was very useful since it proved extremely difficult to obtain basic data of controlled experiments for particular membranes.

7.1 RESEARCH OUTPUT

The research done during this stage of the project has already been published widely and tested on various local and international forums.

1. COLLINS, M.R., & DU PLESSIS, J.P. 1992
   Informal Research Notes on Capillary Force Action, Porous Medium Research Group Report PMG-92-02, Department of Applied Mathematics, University of Stellenbosch.

2. DU PLESSIS, J.P. 1991a
   Similarities between flow across tube bundles and through porous media, Proceedings of the 32nd Heat Transfer and Fluid Mechanics Institute, Sacramento, California, USA, June 6-7, 1991, pp. 267-270.

3. DU PLESSIS, J.P. 1991b
   Saturated flow through a two-dimensional porous domain, Advances in Water Resources Vol. 14(3), 131-137.

4. DU PLESSIS, J.P. 1992a
   Pore-scale modelling for flow through different types of porous environments, in Heat and Mass Transfer in Porous Media, editors M. Quintard and M. Todorovic, Elsevier, Amsterdam, edited Proceedings of the ICHMT International Seminar on Heat and Mass Transfer in Porous Media, Dubrovnik, Yugoslavia, May 20-24, 1991.

5. DU PLESSIS, J.P. 1992b
   Geometrical porous medium models for membrane morphologies, Proceedings of the IAWPRC Specialized Conference on Membrane Technology in Wastewater Management Cape Town, March 2-5.

6. DU PLESSIS, J.P. 1992c
   High Reynolds number flow through granular porous media, in Computational Methods in Water Resources IX, Vol. 2: Mathematical Modeling in Water Resources, editors T.F. Russel et al, Computational Mechanics Publications, Southampton, pp. 179-186, edited Proceedings of the IX International Conference on Computational Methods in Water Resources, Denver, Colorado, USA, June 9-12, 1992.

7. DU PLESSIS, J.P. & MASLIYAH, J.H. 1991
   Flow through isotropic granular porous media, *Transport in Porous Media*, vol. 6(3). pp. 207-221.

8. DU PLESSIS, J.P. & VAN DER MERWE, L.M. 1992
   On fully developed flow in porous media, Tenth Canadian Symposium on Fluid Dynamics, Saint John, NB, Canada, June 4-6, 1992.

9. ROOS, L.I. 1992
   Mathematical modelling of synthetic membrane morphology, MSc Thesis (cum laude), Department of Applied Mathematics, University of Stellenbosch, 1992.

10. ROOS, L.I. & DU PLESSIS, J.P. 1992
FORTRAN code for prediction of water seepage through a tubular membrane system, Porous Medium Research Group Report PMG 92-01, Department of Applied Mathematics, University of Stellenbosch, 1992.

7.2 FULFILMENT OF CONTRACT OBJECTIVES

A Analytical modelling of flow through a membrane taking into account the morphology of the pore structure. This proposed modelling research was successfully advanced towards full fulfilment of contract objectives and results have been widely tested against available experimental results.

B Development of a computer program for prediction of flow in membrane systems. This activity was completed with successful test runs to validate the results qualitatively and quantitatively. Contract proposals in this regard were performed in the full.

C Quantification of stationary capillary force action in unsaturated porous media may be directly inferred from the explicit results obtained in the first part of this project. Although research on this front commenced on a high level of sophistication, it was stopped in favour of the enhancement of progress on the research carried out under section A. The termination was effected after it became known that the project on the development of tensiometertype soil moisture content meters by the Institute of Polymer Science were cancelled. As this activity was specifically aimed at supporting the latter project, this switch was considered in best interest of current needs of water research activities in South Africa.

7.3 CONTRIBUTIONS TO THE STATE OF ART

Pore-scale models were developed from which porous media with composite morphologies as found in synthetic membranes, may be described. It opened the way for explicit calculation of pore lengths, tortuosity, surface areas and hydrodynamic permeability of membranes.

The Darcy-law for slow flow through porous media were proven quantitatively - given the type, the porosity and the length scale of the microstructure, the hydrodynamic permeability may be predicted directly.

Analytical proof of the Forchheimer effect, which refers to the nonlinear relationship between velocity and pressure gradient in porous media, was established. Since the real origin of this effect is now known, it may be studied, both qualitatively and quantitatively, in a much more rigorous manner.

A computational code was developed, incorporating the facility to ascribe different pore structures and permeabilities to different spatial regions. The code is based on a finite volume numerical procedure and contains no "black boxes" so that the actual progress through the numerical procedure may be traced completely.

The theoretical establishment of isotropic pore-scale models forms a sound basis from which studies on electrokinetic phenomena, contaminant transport and anisotropic conditions may be conducted.

7.4 SIGNIFICANCE OF THIS REPORT

This report presents a new set of equations for fluid movement through and adjacent to a synthetic membrane. These equations may be used in future mathematical and computational research on membrane processes and design of membrane systems. Although this report deals primarily with water seepage through synthetic membranes, the mathematical results are applicable generally for any Newtonian fluid or porous medium. This interdisciplinary applicability renders this study very cost-effective and may enhance research in various other fields of interest.

7.5 ACTIONS TO BE TAKEN

Due to the nature of this project no prescriptive action could be suggested other than the encouragement of the use of the results as basis or correlative measure in future membrane-related projects and the application in other water-related fields concerning filtration, leaching and groundwater phenomena. A prominent problem encountered during the project was the lack of suitable sets of controlled laboratory test data giving fluxes and pressure drops for any pure fluid with known physical properties, like water. Promotion of such basic benchmark tests with full specifications is recommendable.

7.6 RECOMMENDATIONS

The fundamental theory developed under this project presents a sound basis for enlargement of the applicability by research on the following aspects of membrane processes:

A Formalize introduction of the recirculatory model.
This is intended to provide the full exposition of the modelling steps which lead to the improved results for granular media. This action will also align the foam and prismatic models with the improved version of the granular model, which compares favourably with experimental results over a very large range of parameter values.

B Macroscopic boundaries
Container walls have a marked influence on the macroscale characteristics of an enclosed porous medium since it alters the porosity in the near wall region. This problem is analogous to the proper inclusion of porosity variations on an intermediate scale.

C Tracer transport
Retention time of solutes and dispersion of contaminants may be studied in a logical manner, since a method now exists by which intrapore phenomena may be quantified.

D Electrokinetic phenomena
Ion movement due to externally applied electric fields may be modelled in a similar type of volumetric averaging.

E Anisotropic phenomena
Derivation of a suitable permeability tensor is of cardinal importance to make the theory available for use in non-isotropical membranes or other fields of application, such as groundwater transport or leaching.

F Velocity dispersion
This problem concerns the correction for smearing out of velocity gradients needed due to the neglect of the volumetric integral in the averaged equation. No such correction exists in world literature and is urgently needed for full application of the theory in cases where large velocity gradients exist.

G Pore size distribution
The present theory does not yet allow for variation in spatial variation in pore size and should be generalised to inlude calculation of the deviation due to given pore size distributions.

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