STUDY OF DIALYZER MEMBRANE (POLYFLUX 210H) AND EFFECTS OF DIFFERENT PARAMETERS ON HEMODIALYSIS PERFORMANCE

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By

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ABSTRACT

Renal failure or kidney failure is a medical condition when the kidneys fail to filter toxins and waste products from the blood. Most of the time, problems encountered in kidney malfunction include abnormal fluid levels in the body, increased acid levels and abnormal levels of Urea, Glucose, Endothelin, β2-Microglobulin, Complement Factor D. In medicine, dialysis is a method that is used to remove waste products from blood when the kidneys are in a state of renal failure.

Parameters characterizing the structure of dialyzers are very important because they decide overall clearance of toxin molecules and at the same time should allow retaining useful molecules in the blood. It is however not clear how the changes of dialyzer parameters will affect the clearance. This can be found out by doing simulation of a dialysis process.

In this thesis, a numerical model was developed to simulate the process that goes on inside a dialyzer to determine which parameters are important for getting better clearance of toxin molecules and how the changes of those parameters can improve the performance of dialysis. In order to do that, a model of dialyzer membrane with details of the porosity is necessary. The dialyzer membrane that was considered in this research was Polyflux 210H. Here the cross sectional images of Polyflux 210H dialyzer membrane were taken by FESEM (Field Emission Scanning Electron Microscope) to obtain the porosity values of different layers. Using these porosity values, a multilayered membrane model was developed in Finite Element Software-COMSOL Multiphysics 4.3. Then a blood flow containing - Urea, Glucose, Endothelin, β2-Microglobulin, Complement Factor D and Albumin was introduced. For a certain blood flow rate the toxins diffuse through the membrane and on the other side of the membrane a dialysate flow was introduced to remove the toxins.

Two different definitions of effective diffusivity were considered for the phenomenon of the diffusion of the molecules in the membrane. Between the two, the better definition was found out by comparing the results with experimental data of the manufacturer of Polyflux 210H. Then for the chosen definition, further analysis was done and the results were compared with another set of experimental data to validate the model. Then different parameters - magnitude and direction of both blood and dialysate flow, length and diameter of the fiber, pore sizes were changed to simulate how these changes affect toxin clearance and the removal of useful molecules.

The results suggest some very interesting points to achieve better dialysis performance. First of all, the clearance rate of both Urea and Glucose increase rapidly with the increasing blood flow rate. When a maximum allowable blood flow rate is attained, increasing the dialysate flow rate can ensure better clearance rate for Urea and Glucose. In both the cases of increasing radius or length of the dialyzer fiber, the clearance rate of Glucose increases more rapidly than the clearance rate of Urea. For Endothelin and β2-Microglobulin the clearance rate increases twice compared to the initial condition. Meanwhile, the clearance rate of Albumin does not change that much. Also increasing the pore diameter up to 20 nm (but not more than that) can ensure higher clearance rate of Urea and Glucose, moderate clearance rate of middle molecules and minimum loss of Albumin.

ACKNOWLEDGEMENTS

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LIST OF ABBREVIATIONS

W	width of the path for dialysate flow
R_{ext}	outer radius of the dialyzer fiber
Φ	fiber packing density
D	diffusion coefficient of a molecule
c	concentration of a molecule in the flow
MW	molecular weight
Re	Reynolds Number
v_B	velocity of blood flow
Q_B	volume flow rate of blood
R_1	inner radius of the hollow fiber
r	radial coordinate
n	number of fibers in a dialyzer
v_D	velocity of dialysate flow
Q_D	volume flow rate of dialysate
D_e	effective diffusion coefficient
ε	porosity
K	Clearance rate of molecule
S	Sieving coefficient

CHAPTER 1

INTRODUCTION & OBJECTIVES

1.1 Introduction

Hemodialysis is an important process used to help thousands of people in society who are suffering from kidney disease or some other causes of reduced kidney functions. The process itself serves to replicate the functioning of healthy kidneys by filtering the blood to eliminate certain toxins as well as proteins which can become toxic when present in the blood in excessive amounts. The prefix "hemo" means "blood", while the word "dialysis" refers to the filtering process. It is well known that without this process, or a kidney transplant, the individuals with compromised kidney function would die. As a matter of fact, it is indicated by the Canadian Cancer Society's Advisory Committee on their Cancer Statistics, 2013 that around 1.5% of the deaths occur because of kidney disease [1].

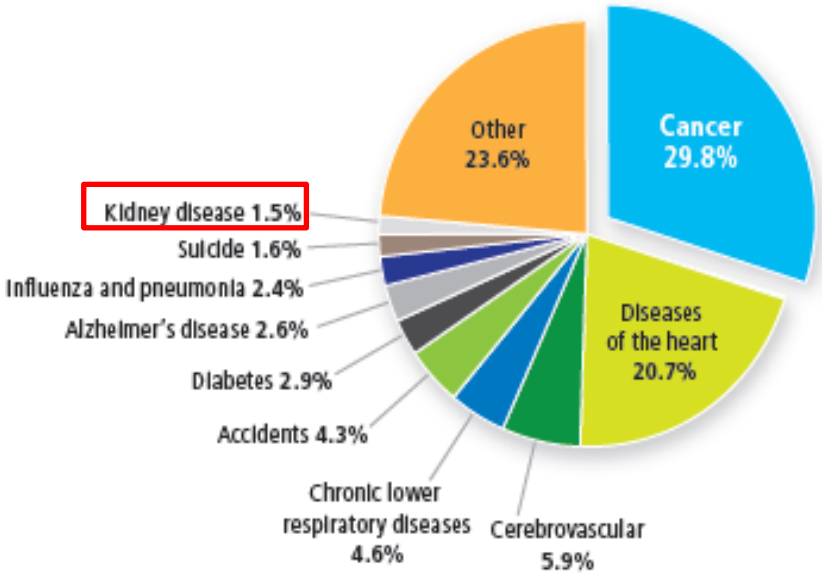

Figure 1.1 Proportion of deaths due to different causes, Canada, 2009 [1]

In addition, the prevalence of this problem is large and on the rise. For example, the Kidney Foundation of Canada reported in 2013 that "1 in 10 Canadians has kidney disease and millions more are at risk. Each day, an average of 15 people are told that their kidneys have failed." [2]

Doctors often use the term - renal function to describe the efficiency levels of the kidneys. A human body with two healthy kidneys, has 100 percent capability of its kidney functions. Many people suffer from reduced kidney function without even knowing about it. Often this gets worse

unless the patient undergoes proper treatment. The problems really become noticeable when the renal function reduces to 25 percent or less. In case of kidney function dropping below 10 to 15 percent, a patient needs dialysis or a kidney transplant [3].

The prolonged problems related to kidney disease can eventually lead to cancer. An increasing trend of ASIR (Age-standardized incidence rate: The number of new cases of cancer per 100,000 people, standardized to the age structure of the 1991 Canadian population to account for changes in age distribution over time) is noticed in male population which suggests that kidney related cancer is ever-growing since 1984 (Figure 1.2).

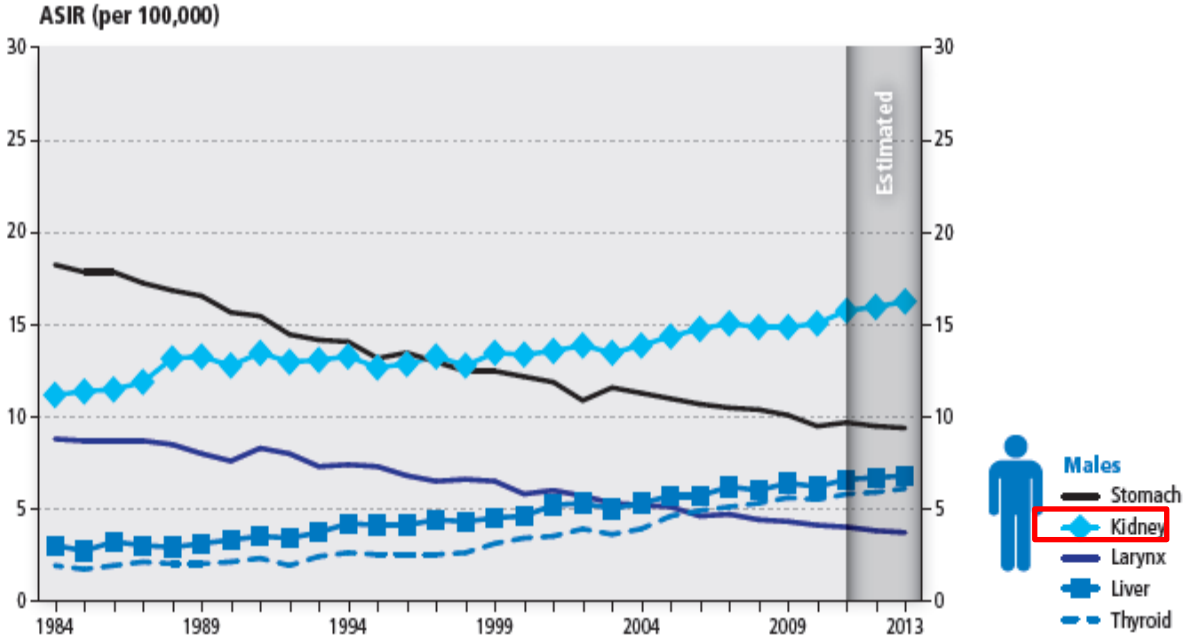

Figure 1.2 Five most frequent cancers with a statistically significant change in incidence rate of at least 2% per year. [1]

At present, a big concern with the presently used hemodialysis system is that often it takes several hours for a dialysis treatment session, and patients must repeat the whole procedure a couple of times in the same week [2]. So, researchers are always looking for new ways to reduce these long, stressful sessions for the patients and at the same time achieve the same or even better level of dialysis performance.

Although hemodialysis is of critical importance to the health and welfare of society, little quantitative engineering-based research has been performed to optimize the process. Numerous

medical case studies have been conducted to compare the performance of different dialyzers, but this approach has not provided a systematic quantitative method for determining the effects of various parameters involved in a dialysis process. If such a quantitative method were developed, it might be possible to improve or even optimize the dialysis process.

The broad objective of the research described in this thesis was to develop a model to simulate the hemodialysis process, and to use this model to perform a parametric study examining the effects of various parameters. In sections 1.2 and 1.3 to follow, kidney functions and hemodialysis operations are described in detail, and this is followed by a review of pertinent literature in Section 1.4. Together, sections 1.2 to 1.4 provide the details necessary to describe the specific research objectives given in section 1.5.

1.2 The Kidney

1.2.1 Structure of the Kidney

Kidneys serve numerous essential roles which include – regulating the urinary system, maintaining acid–base balance, regulation of blood pressure and producing different hormones necessary for the body. They serve as a natural filter of the blood and remove wastes which are sent to the urinary system. By this, the body gets rid of wastes, like urea and ammonium.

There are two kidneys placed one on either side of the spine under the lower ribs. On average, a person's kidneys process about 190 liters of blood to separate out about 1.9 liters of waste products and extra water at each day. The wastes and extra water turns into urine and flows to the bladder for disposal [3].

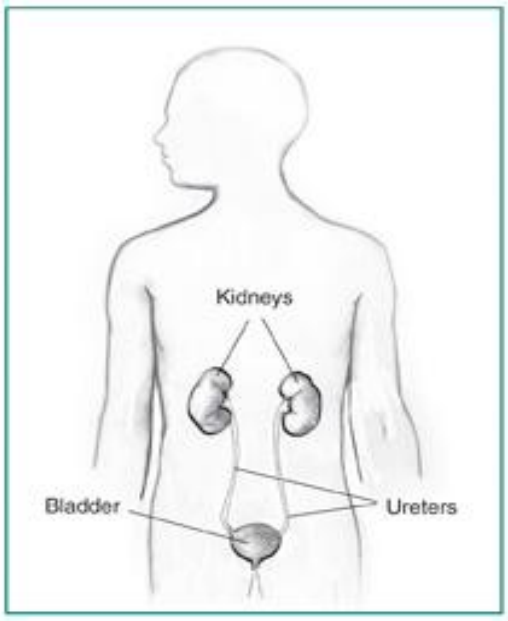

Figure 1.3 Position of kidneys inside human body [3]

The inner structure of a kidney is showed in Figure 1.4. The basic unit of a kidney is called nephron. There are millions of nephrons in one kidney. The removal process of toxins actually takes place inside these nephrons.

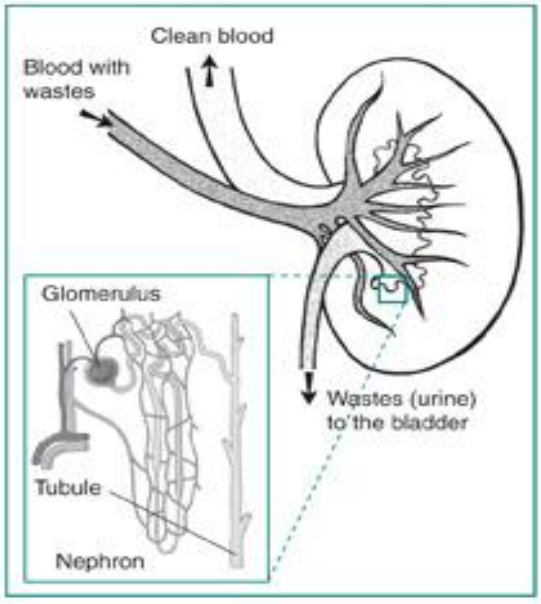

Figure 1.4 Inside the kidney [3]

As depicted in Figure 1.4, each nephron is made of glomerulus and tubule. The glomerulus retains the blood cells and proteins in the blood and at the same time allows the toxin molecules and extra water to pass through.

1.2.2 Kidney Failure

In order to understand the nature of hemodialysis, it is important to first describe the nature of kidney failure. In case of a renal or kidney failure the kidney's ability to remove toxins and waste products from the blood becomes reduced. It is detected by an elevated serum creatinine level [3]. Most of the time problems that are encountered in kidney malfunction include abnormal fluid levels in the body, increased acid levels and abnormal levels of Urea, Glucose, Endothelin, β2-Microglobulin, Complement Factor D [3, 4].

These molecules, which can cause complications to the patient, can be described as follows –

- **Urea:** The main role of Urea is to carry out the waste nitrogen out of the body. In case of kidney failure, the level of Blood Urea Nitrogen (BUN) rises in the human body and often leads to Uremia. Uremia can cause several kinds of complications starting from anorexia, lethargy, fatigue, nausea, bone pain, shortness of breath, seizures to mental acuity and coma [5].
- **Glucose:** Though Glucose is an important part of our metabolism, increased level of glucose causes serious problems like diabetes [6]. In case of a kidney failure when it cannot process the glucose out of the body through urine, dialysis is necessary.
- **Endothelin:** Endothelins are responsible for the growth of smooth vessels. At the same time they can restrict blood vessels and raise blood pressure. They are normally kept in balance by kidney functioning but in case of renal failure they become high in levels and contribute to high blood pressure and heart disease [7].
- **β2-Microglobulin:** β2-Microglobulin makes the peptide binding groove stable. But excess of it turns into amyloid fibers that agglomerate in joint spaces [8].
- **Complement Factor D:** Complement Factor D is elevated in the obese [9]. The exact cause of this elevation is not known. In case of a kidney problem, it cannot be removed from the blood stream.

Sometimes some useful molecules for the body, like Albumin, get removed by the hemodialysis process.

- **Albumin:** It is the main protein of human plasma. It transports fatty acids and hormones. Also it binds water, ions and other substances. Its main function is to regulate the osmotic pressure of blood. A big concern in dialysis process is to minimize the Albumin loss as much as possible [10, 11].

1.3 Hemodialysis

Hemodialysis system includes a blood circuit, a dialysate circuit and a dialyzer. The dialyzer membrane inside the dialyzer separates the two circuits. The blood circuit has a vascular access device, blood tubes, one or two blood pumps and pressure-air leak monitors. The dialysate circuit has one or two dialysis fluid pumps, ultrafiltration control system and dialysis fluid heating system. The whole process of dialysate flow including - flow rates, pressures, dialysis fluid composition and blood leakage are continuously monitored. The dialyzer membrane is the main component of the hemodialysis system because it basically ensures the removal of toxins, wastes and extra water and at the same time ensures the retaining process of blood molecules in the blood stream.

The principle of dialysis is - it involves diffusion of solutes across a semipermeable membrane. Hemodialysis utilizes counter current flow, where the dialysate is flowing in the opposite direction of blood flow.

1.3.1 Blood Circuit

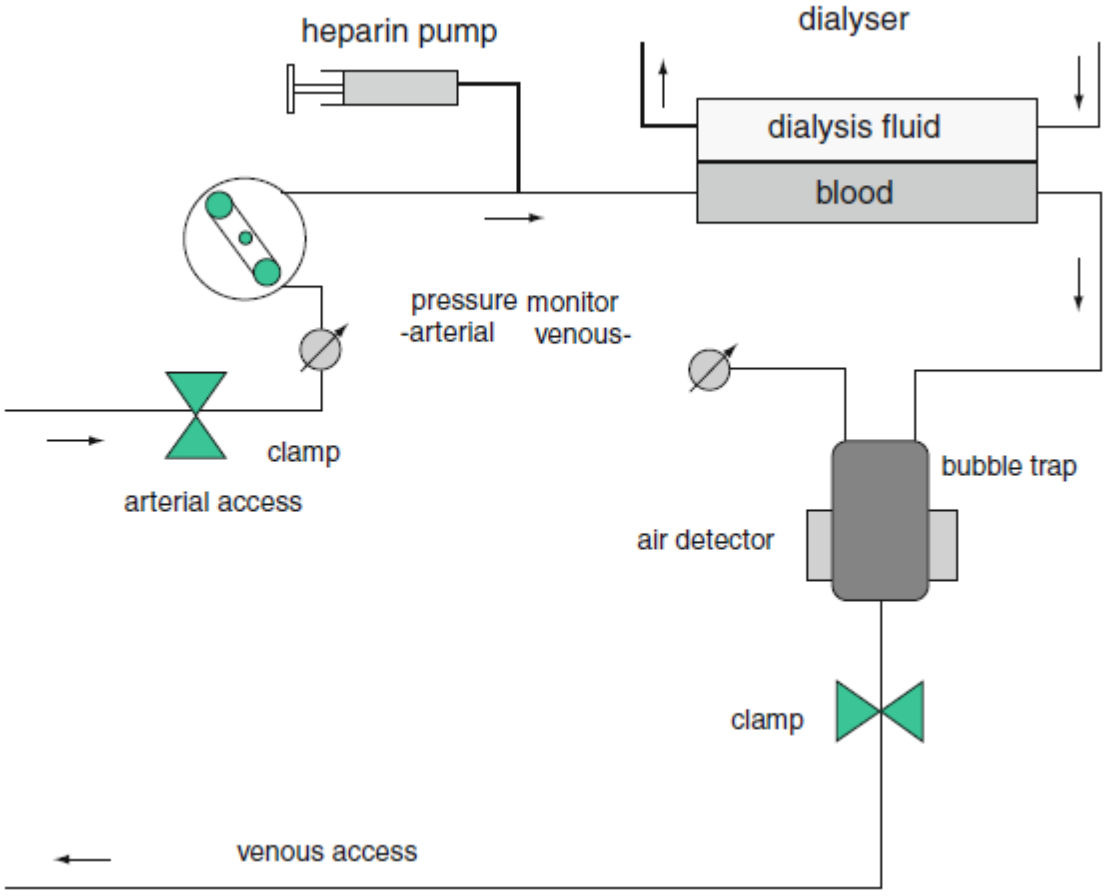

Figure 1.5 Blood circuit in hemodialysis [12]

The blood from the patient is pumped through the arterial (or vascular) access to the dialyzer. The purified blood or blood containing less amount of toxic from the dialyzer is recirculated to the patient after it is ensured that there is no air/bubbles present in the blood. This is done by passing the blood through an air trap. Ultrasound devices are used here to measure changes of ultrasound transmittance by air bubbles or foam. In the case of detecting foam or air, the whole system is stopped immediately.

The connection from the dialyzer to the patient is known as venous segment. Tubing systems made of polyvinylchloride and polycarbonate are used in both arterial and venous segments. Sterilization is an extremely important thing after every dialysis session even though one dialyzer is used for one patient only. Residues in the tubing from the last session for the same

patient can be seriously harmful for the next session. Two types of sterilization are used: steam sterilization and ethylene oxide. Steam sterilization is mostly used because ethylene oxide may induce antibody formation and cause allergic reactions [12].

1.3.2 Dialysate Circuit

A schematic diagram of the dialysate circuit is shown in Figure 1.6.

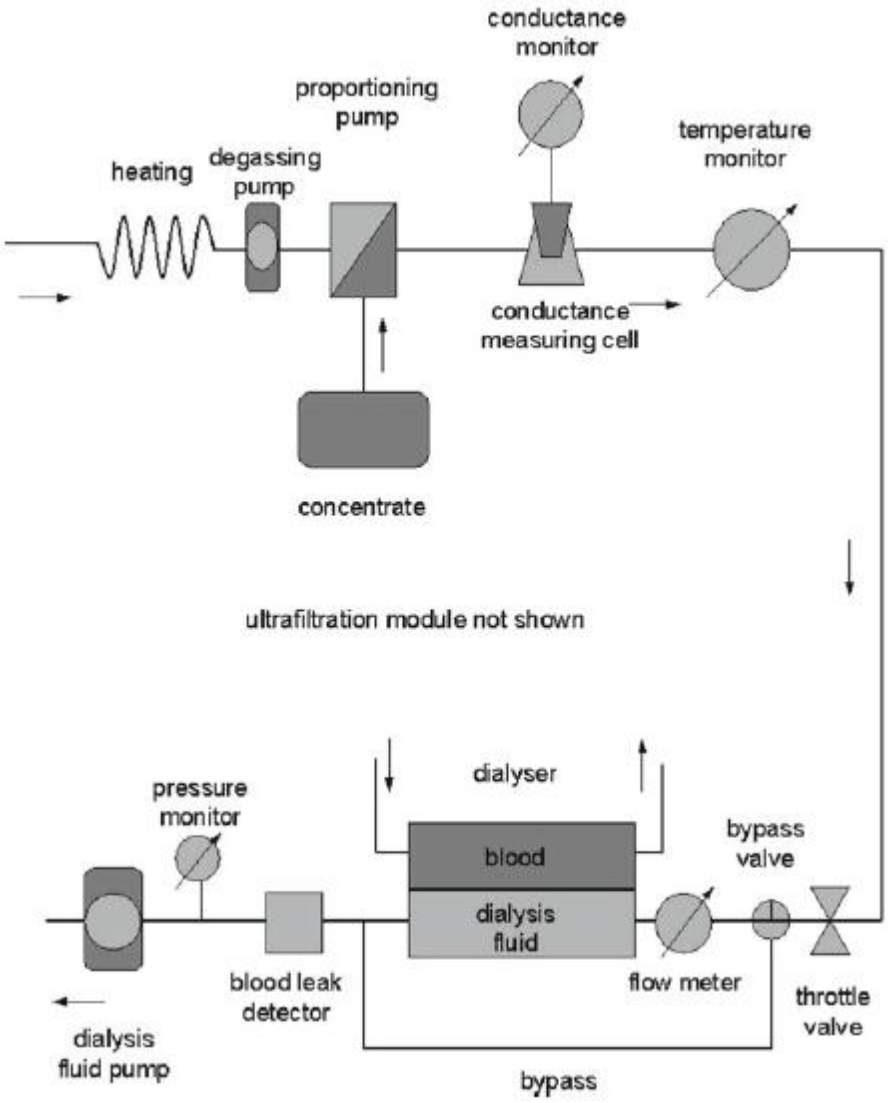

Figure 1.6 Dialysate circuit [12]

The temperature of the dialysate is always monitored to avoid hypothermic or hyperthermic incidents. In order to avoid formation of gas bubbles at the surface of the dialyzer membrane, regular degassing of the dialysis fluid is done. Dialysis efficiency can significantly reduce if proper degassing is not ensured. The quality of dialysis water is cautiously maintained by hospital authorities. For that, a standard water treatment device consisting of water softener, activated carbon filter, sediment filter and reverse osmosis system is used [12].

Sometimes in dialysis another system is introduced which is known as ultrafiltration control system which basically permits the removal of the desired amount of water from the blood.

1.3.3 Dialyzer

The dialyzer is the central component of the hemodialysis system simply because the blood purification is done inside it. Blood and dialysate flow on the two sides of the semipermeable membrane in a countercurrent manner. So dialyzer membrane basically decides which molecules are retained in the blood stream and which ones are diffused to the dialysate side. So the characterizations of the membranes are of utmost importance. This is done in terms of both permeability and morphological characteristics – clearance rate, sieving coefficient, ultrafiltration coefficient and membrane porosity. The dialyzer fibers are placed inside a cylindrical plastic casing. The number of these fibers inside a dialyzer varies depending upon the type of dialyzer. The casing along with the fibers makes a complete dialyzer.

Figure 1.7 A dialyzer defining its blood inlet and outlet, dialysate inlet and outlet

Two groups of membrane materials are used [12]:

- cellulose based membranes
- synthetic membranes

Cellulose based membranes are relatively inexpensive. One of the popular unmodified cellulosic membranes is Cuprophan which have many hydroxyl residues. These residues cause complications as they are involved in complement activation. To eradicate this problem, modified cellulosic membranes like Hemophan is introduced where most of the hydroxyl residues are esterified so that the interaction with complement factors can be reduced. But this kind of modified cellulosic membrane also has drawbacks as they cause higher activation of the coagulation cascade.

The various problems with the cellulosic membranes have led dialyzer manufacturers to use synthetic membranes. Synthetic membranes are made from various polymers which include polysulfone, polyamide, polyethersulfone, polyarylethersulfone/polyamide or polymethylmethacrylate (PMMA). This kind of membranes activates complement to a lower degree. At the same time their large pore size and thick wall structure ensures higher hemodialysis efficiency. But this poses the threat of losing Albumin also, which is an important molecule for the human body. So the real challenge in hemodialysis is to use such a dialyzer membrane that has an optimum balance between removing toxins as much as possible and at the same time ensuring minimum loss of useful molecules.

1.3.4 Polyflux 210H

Polyflux 210H is a dialyzer produced by Gambro Dialysatoren GmbH, Hechingen, Germany. In one dialyzer there are approximately 12,000 fibers. These fibers are made of Polyamix which is a blend of polyarylethersulfone, polyvinylpyrrolidone and polyamide. According to Gambro- “By using Polyflux H dialyzers you minimize the inflammatory effects of the dialysis treatment and you reduce the risk of membrane-induced clotting events” [13].

Figure 1.8 Polyflux 210H dialyzer [13]

In this thesis, the morphological characteristics of Polyflux 210H dialyzer membrane were evaluated and then these informations were used to develop a model in Finite Element software – COMSOL Multiphysics 4.3 to determine the effects of different parameters of a dialyzer on the dialysis performance.

1.4 Literature Review

A substantial amount of research has been performed regarding homogeneous dialyzer membranes. These homogeneous dialyzer membranes are mostly made of cellulose. These membranes have a uniform pore structure from the inner to the outer side of the membrane. As described in previous section, the surface of such membrane is not very biocompatible and activates complement in the blood [14]. That is why, now-a-days, dialyzer membranes are made from synthetic materials, especially polymers. These synthetic membranes activate complement in fewer amounts than cellulose membranes [15]. They have a structure which is known as asymmetric. This means that the shape of a pore gradually changes from inner to outer surface of

the membrane. Synthetic membranes are made in both low and high flux configuration. But most of them are high-flux dialyzer membranes. Polyflux 210H is such a high flux asymmetric polymer membrane.

There are not enough studies done on this kind of asymmetric membrane. Gastaldello et al. [16] showed the comparison between cellulose and polymer membranes in their study. This study was done using the two membranes for 53 patients. They got results which suggest better Urea and Vitamin B12 clearance can be achieved by polymer membranes than cellulose membranes. Sakai et al. [17] studied and captured the images of inner and outer surface images of such an asymmetric membrane. They calculated the surface porosity based on those photomicrographs. These give an idea of the surface porosity. But to what extend that porosity continues from one surface to another is not sure. Taking cross sectional image of the membrane and calculating the porosity from that image, give better details of it.

Experimental studies [18, 19] have been done to determine whether increasing the dialysate or blood flow rate leads to better clearance or not. But these studies did not consider the structure of the membrane. Also these studies were limited to clearance of Urea only. A reasonable concern for doctors these days are- whether the necessary elements like Albumin are diffused through the membrane during the dialysis or not [10, 11].

Most of the experimental studies are done with dialyzers which are commercially available. So they actually give a comparison between different dialyzers. But which parameters are really important to have a better overall clearance of toxin molecules and at the same time retain useful molecules is not clear. Also, how the change of those parameters can really affect the clearance is important. To the best of author's knowledge, this kind of parametric study has not yet been performed by other researchers.

1.5 Objectives

A cross sectional image of the asymmetric polymer membrane with details of the porosity is important. A multilayered membrane model with different porosity for each layer describes the actual structure of Polyflux 210H membrane. This model was developed using Finite Element Software- COMSOL Multiphysics 4.3. A blood flow containing - Urea, Glucose, Endothelin, β2-

Microglobulin, Complement Factor D and Albumin was introduced. For a certain blood flow rate the toxins diffuse through the membrane and on the other side of the membrane a dialysate flow removes the toxins. Two different definitions of effective diffusivity were considered for the phenomenon of the diffusion of the molecules in the membrane. Between the two, the better definition was found out by comparing the results with experimental data of the manufacturer of Polyflux 210H. Then for the chosen definition further analysis was done and the results were compared with another set of experimental data to validate the model. Then different parameters - magnitude and direction of both blood and dialysate flow, length and diameter of the fiber, pore sizes were changed to simulate how these changes affect toxin clearance and the removal of useful molecules.

So, the objectives can be summarized as -

- To characterize the morphology of Polyflux 210H dialyzer membrane. This study includes- outer and inner surface of the membrane, diameter and thickness of the fiber, cross section of the membrane, calculating porosity for different layers.
- To develop a model in Finite Element Software- COMSOL Multiphysics 4.3 consisting of –membrane with different layers of porosity, individual path for blood and dialysate flow. This model represents the process that takes place inside Polyflux 210H dialyzer.
- To validate the model using the manufacturer's data of the Polyflux 210H dialyzer.
- To determine the effects of changing the direction and magnitude of both the blood and dialysate flow.
- To determine the effects of changing the length and radius of the dialyzer fiber.
- To determine the effects of changing the pore size and porosity in different layers of dialyzer membrane.

1.6 Outline of Remainder of the Thesis

In the remainder of this thesis, chapter 2 provides the details of the experimental procedure that was conducted to obtain the morphological information about the Polyflux 210H dialyzer membrane. Then in chapter 3, the method and equations that were used to develop the FEM model is discussed. After that, chapter 4 describes the results that were obtained from simulation. Based on that, conclusions and recommendations are made in chapter 5.

CHAPTER 2

MORPHOLOGY OF POLYFLUX 210H DIALYZER MEMBRANE

2.1 Method for Observation

The dialyzer fibers were extracted from the Polyflux 210H dialyzer (obtained from Prof. Szpunar's previous research project) and prepared to observe under the Field Emission Scanning Electron Microscope (FESEM). Images of the outer and inner side of the membrane were taken to get an idea of the pore size and porosity. FESEM was used to get all these photomicrographs. Then to get a better idea of the porosity distribution, cross sectional images of the membrane were taken. These gave a clear idea of the porosity distribution along the thickness. The FESEM used here is a SU6600 Hitachi.

2.2 Details of the Method

The following steps had already been completed by N. A. P. Kiran Kumar from Prof. Szpunar's research group:

- At first the plastic casing of Polyflux 210H dialyzer was cut using a manual saw. During the cutting, care was taken so that the fibers inside the dialyzers remain untouched by the saw as much as possible. After that, a bunch of fibers were cut using scissors from an area which was not particularly affected from the cut of saw.
- A mixture of 2.5% gluterdehyde and 2% paraformaldehyde was taken in a petri dish and the fibers were soaked and thoroughly washed to ensure that there is no form of pathogen. Then the fibers were dehydrated using a series of ethanol and distilled water mixtures. Finally the fibers were dried in air.
- Once the fibers were dried properly, some fibers were attached on a special type of adhesive tape used in FESEM. Then these fibers were observed under the optical microscope. At the same time dialyzer fibers were dissected longitudinally using a surgical scalpel.
- In order to get better images of the inner and outer surface of the membrane in FESEM, both the surfaces were coated with gold. Gold was used because it has very good electrical conductivity and makes the surface conductive enough for FESEM imaging. A gold layer having thickness of 250 Å was applied on both surfaces of the membranes.

The following steps were done by the author:

- After applying the gold coating, the membrane was placed in FESEM and images were taken. Magnified images were taken to get details – pore sizes and porosity of the different layers in the membrane. Several photomicrographs were taken from the same layer to be sure about the pore sizes and the porosity. The pore sizes on the inner and outer surfaces were measured. And then the porosity of the whole membrane thickness (from cross sectional image of dialyzer membrane) was calculated while dividing it into three different layers. For each layer, FESEM photomicrographs were printed on a paper. Then for each photo the number of pores and their sizes were calculated. In the next step, the total area of pores was calculated and divided by the overall area. In this way the porosity of that particular layer can be determined. This whole procedure was done for all the three layers of the membrane to obtain the porosity value for each layer.
- In order to calculate diameter and thickness of the dialyzer fibers, images were also taken using FESEM. Measurements were taken on several areas and then averages were taken for each one of them.

2.3 Morphology

Polyflux 210H fiber has a porous structure. A single fiber has a length of 270 mm.

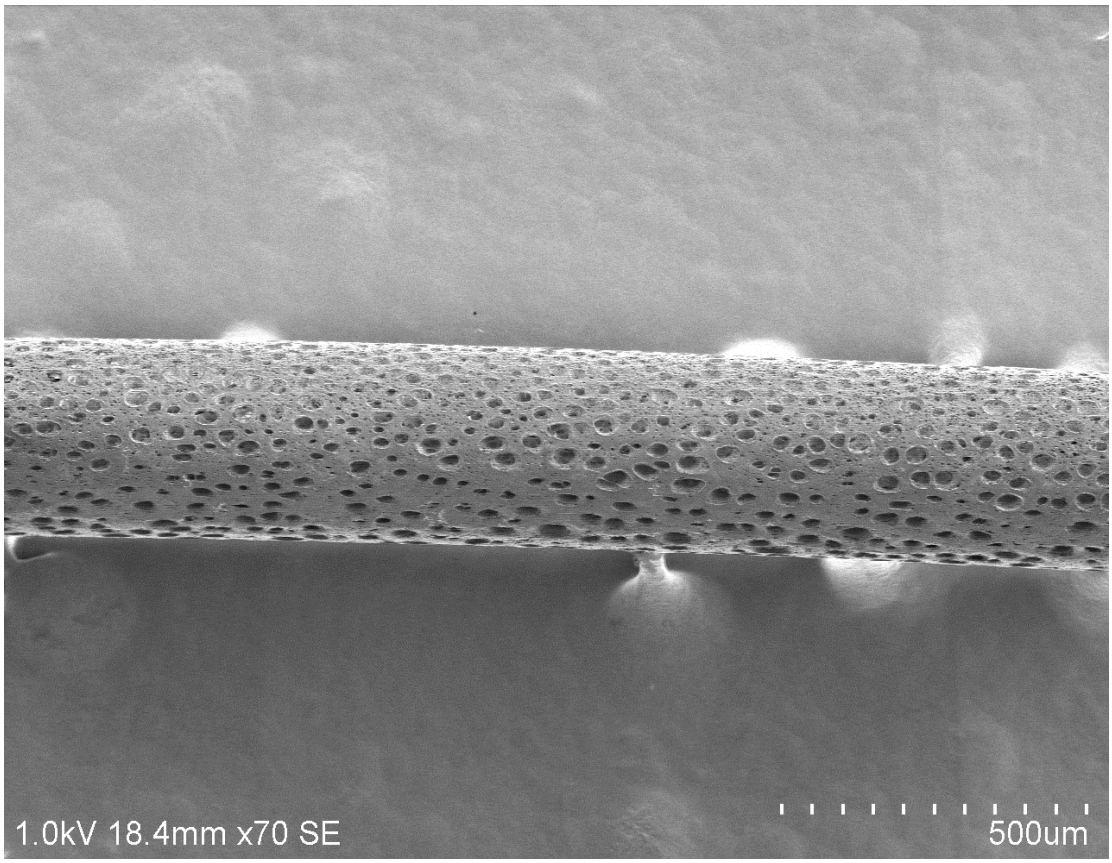

Figure 2.1 Longitudinal image of a fiber

The outer surface has a range of pore size which varies between 0.45 μm to 20.40 μm. But for the inner surface the range is between 34 nm to 45 nm.

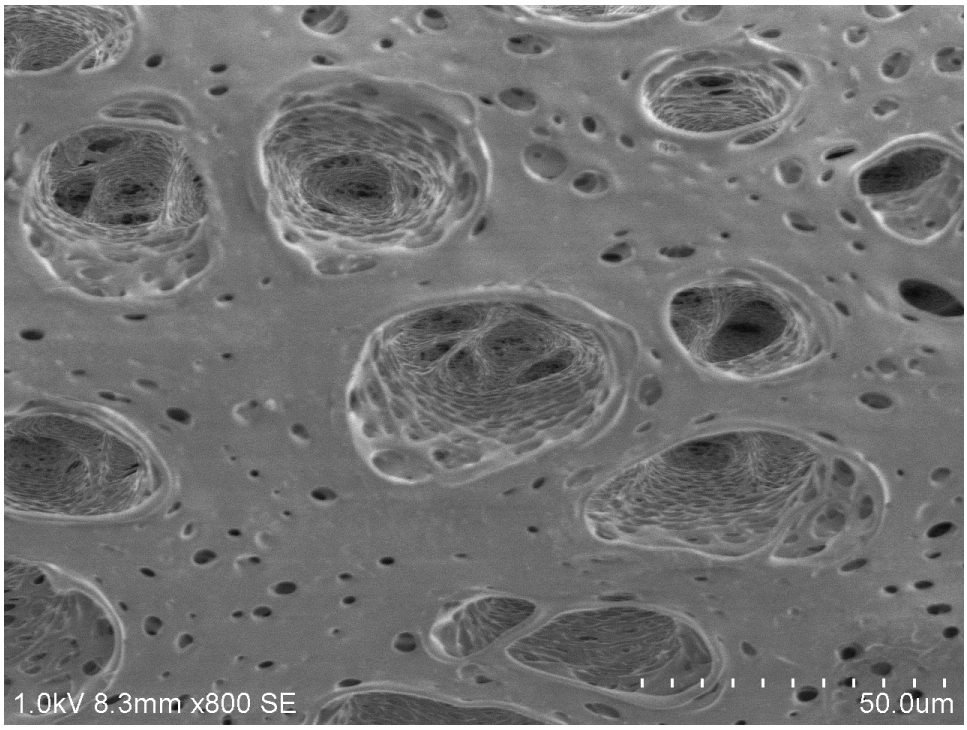

Figure 2.2 Outer surface of the dialyzer membrane (taken by N. A. P. Kiran Kumar)

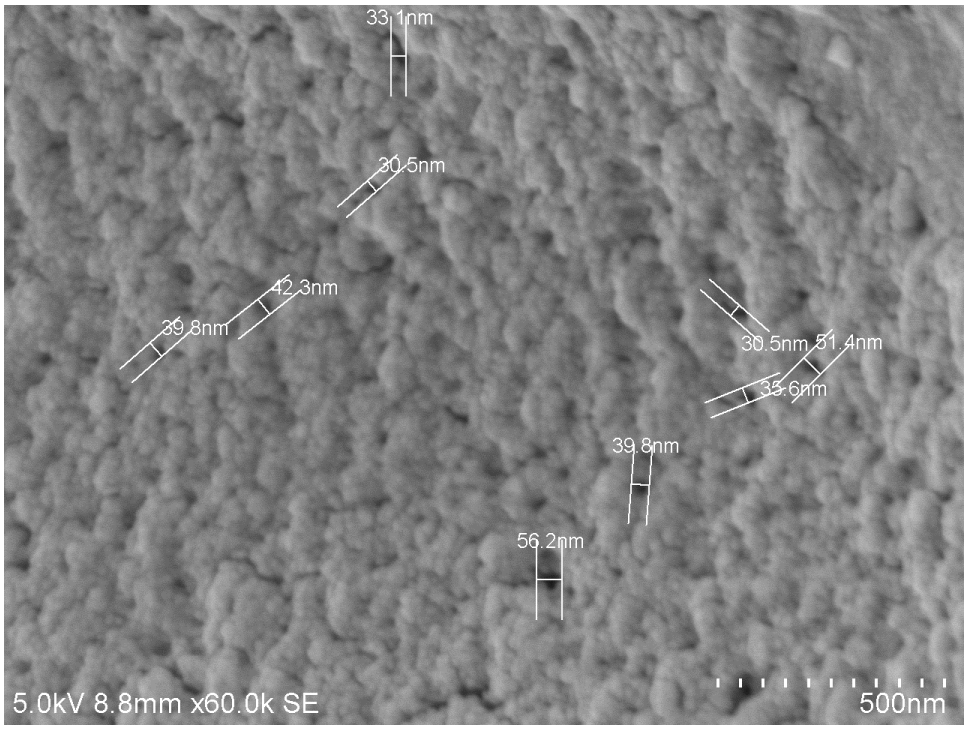

Figure 2.3 Inner surface of the dialyzer membrane (taken by N. A. P. Kiran Kumar)

The inner surface of the membrane is the most important because this side of the surface actually allows the diffusion of the toxin molecules but repels the proteins and blood cells. Because the range of the inner surface pore size (34 to 45 nm) ensures that the toxin molecules which has a size range of around 0.5 to 5 nm gets diffused through the inner surface. And once the toxin molecules can get through the inner surface, it does not get any hindrance from there on as the outer surface pore sizes (0.45 μm to 20.40 μm) are much bigger than the toxin molecules. Also, at the same time, because of the size of the blood cells (i.e. Red Blood cells – size approximately 6-8 μm) [20], they don't get diffused through the inner surface. So the blood cells are successfully retained in the blood stream.

From these images it is also evident that pore sizes are largely different from inner to the outer surface, in fact it changes from nanometer to micrometer level. So, to understand the pore distribution, a cross sectional image is necessary. Figure 2.4 is such a cross sectional image (taken by author).

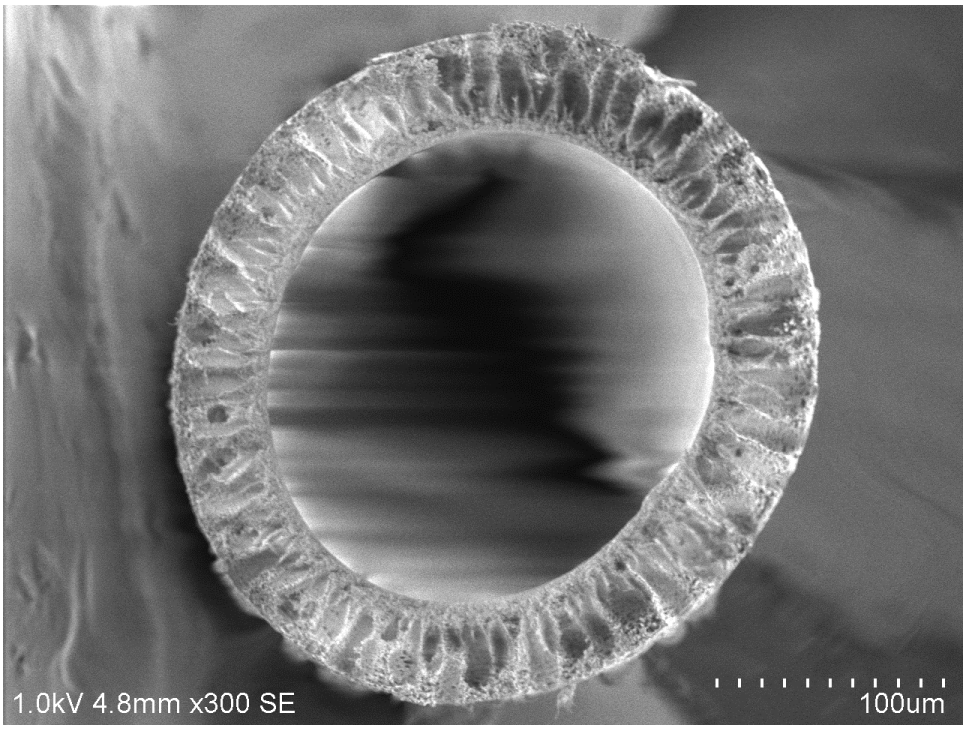

Figure 2.4 Cross section of the fiber

The inner diameter of the fiber is 200 μm with a thickness of 45 μm. To understand the pore distribution a magnified image of the cross section was taken.

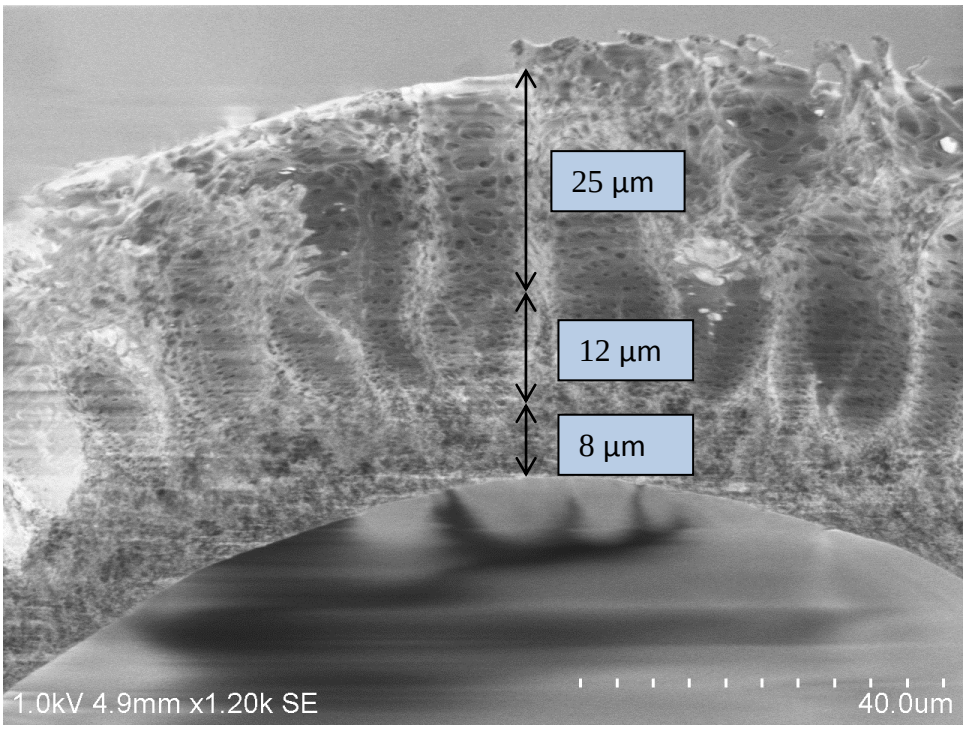

Figure 2.5 Cross section of the membrane

In figure 2.5, a dialyzer membrane having a total thickness of 45 µm was divided into three different layers to calculate the porosity (using the method described in the "Procedures" section) for each of the layer. First layer (thickness of 8 µm) has a porosity of around 0.1, second layer (thickness of 12 µm) has a porosity of around 0.27 and third layer (thickness of 25 µm) has a porosity of around 0.4

CHAPTER 3

FINITE ELEMENT MODEL

3.1 COMSOL Multiphysics 4.3

COMSOL Multiphysics 4.3 was used for developing and simulating the model of Polyflux 210H dialyzer. COMSOL Multiphysics is a finite element analysis and simulation software for various physics and engineering applications especially when there are different phenomena coupled together in one process. That is why the word "Multiphysics" is used to represent these coupled phenomena.

In this thesis, the COMSOL module that had been used was- **Chemical Species Transport**. Under this module the two interfaces are-

- Transport of Diluted Species
- Species Transport in Porous Media.

Transport of Diluted Species interface was used for both the blood and dialysate flow. Species Transport in Porous Media interface was used for different layers of the dialyzer membrane. All the interfaces were coupled together to simulate the process that goes on inside the Polyflux 210H dialyzer.

3.2 Developing Model

In this thesis, the modeling was done based on the assumption of steady state diffusive flux of toxins across the dialyzer's membrane because of the presence of the concentration gradients across it. It simulated the diffusion of toxin molecules through the dialyzer membrane so that it could demonstrate how the diffusion lowers the concentration of toxins in the blood stream.

The inner structure of a dialyzer is shown in Figure 3.1. In this figure the cross sectional view along the longitudinal direction is showed to illustrate the details inside a dialyzer. Basically the outer shell is made of plastic and inside the shell there is a bundle of dialyzer fibers. The blood flows through these hollow fibers while the dialysate flows over the dialyzer fibers from an opposite direction.

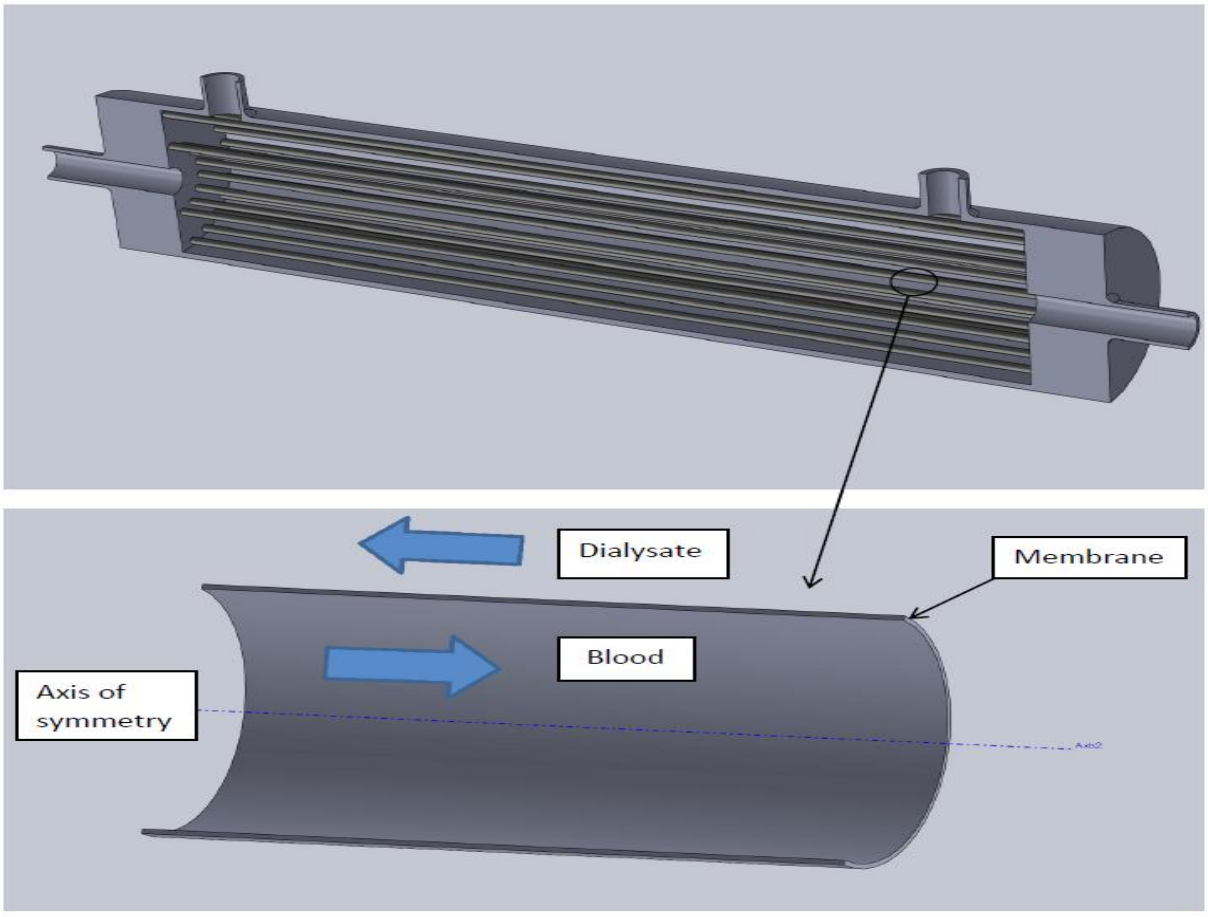

Figure 3.1 Diagram of dialysis hollow-fiber dialyzer

Here an axisymmetrical estimate for the dialyzer fiber was used to develop the model so that the computational efforts could be reduced. An axisymmetrical 2-D model developed in COMSOL Multiphysics 4.3 is shown in Figure 3.2.

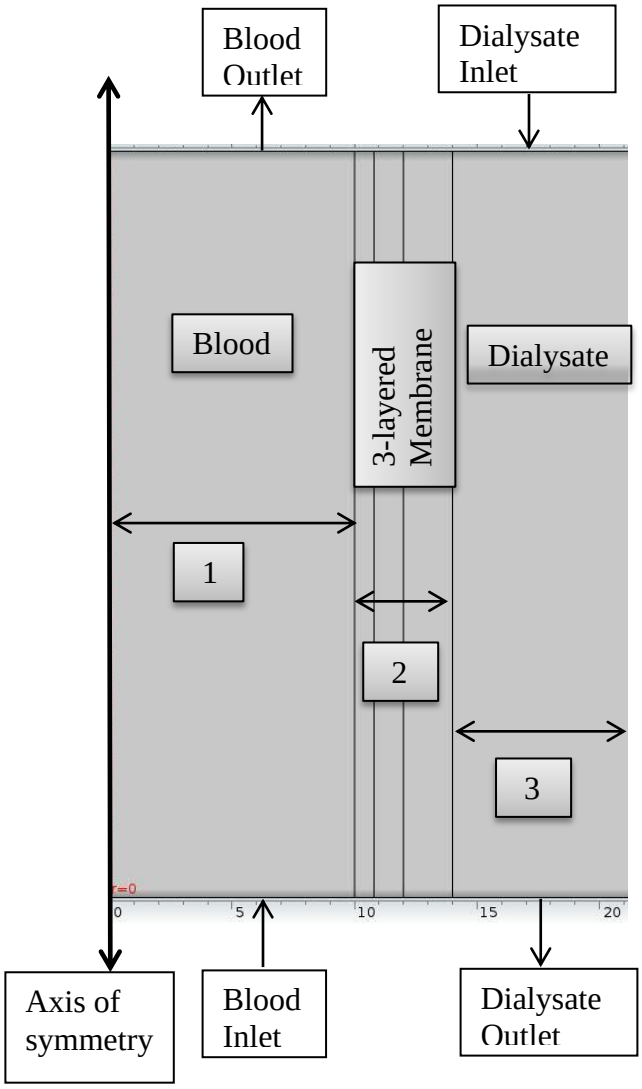

Figure 3.2 2-D axisymmetric model of the dialysis process where -

1: Inner radius of the dialyzer fiber
2: Thickness of the dialyzer membrane
3: Width of path for dialysate flow

As figure 3.2 suggests, there are basically three domains –

- Blood
- 3-layered membrane
- Dialysate

3.1 Model dimensions

The values that were used in the model for inner radius and thickness of the dialyzer fiber were obtained from FESEM (as described in section 2.2).

But to calculate the width of path for dialysate flow, the following equation was used [21] –

$$W = R_{ext}\left(\sqrt{\frac{\pi}{2\sqrt{3}\Phi}} - 1\right) \qquad (1)$$

where W is the width of path for dialysate flow, Φ is the fiber packing density and R_{ext} is the outer radius of the fiber.

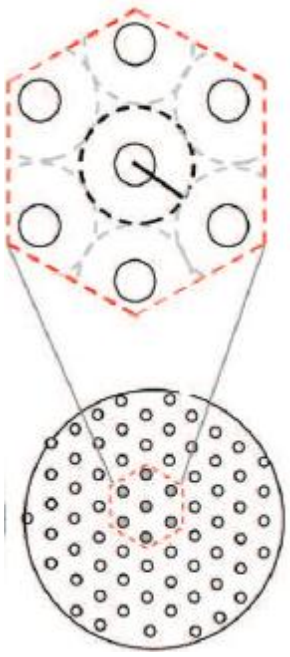

Figure 3.3 Hexagonal stacking of the fibers in packing density calculation [21]

For Polyflux 210H dialyzer the packing density is 45% and the R_{ext} was already known from the FESEM. So equation (1) provided the width of path for dialysate flow, W.

Here, fiber packing density is the percentage of area occupied by the hollow fiber in the cross sectional area of the dialyzer.

3.2 Equations

- **Transport of Diluted Species**

The Transport of Diluted Species interface has the equations for modeling mass transport of species in mixtures and solutions. This particular interface was chosen because it can simulate chemical species transport which involve diffusion (Fick's Law) and convection (in case of coupling to a fluid flow). The following simplified PDE (Partial Differential Equation) describes the convective and diffusion processes in the blood and the dialysate.

$$\nabla \cdot (-D_i \nabla c_i + c_i u) = 0 \qquad (2)$$

where c_i denotes the concentration of the toxin (mol/m^3) in the respective phase, D_i denotes the diffusion coefficient (m^2/s) in the liquid phase and u denotes the velocity (m/s) in the respective liquid phase.

For different toxins, the diffusion coefficient is different and it was calculated from [22] -

$$D = 1.62 \times 10^{-4} (MW)^{-0.552} \qquad (3)$$

where MW is the molecular weight of the respective toxin.

Table 3.1 Diffusivity for different molecules

Molecule	**Diffusivity (x 10^{-12} m^2/s)**
Urea	1690.346
Glucose	921.732
Endothelin	160.251
β2-Microglobulin	91.587
Complement Factor D	61.893
Albumin	35.410

Both the blood and dialysate flow were considered to have laminar flow because the Reynolds number calculated from –

$$Re = \frac{\rho v L}{\mu} \qquad (4)$$

where ρ is the density of blood or dialysate, v is the blood or dialysate velocity, L is the length of the dialyzer fiber and μ is the dynamic viscosity, suggests that for blood and dialysate flows inside the dialyzer they are 0.31 and 2.02 respectively. Both of the Reynolds numbers are well below 2300 which is the cut off limit between laminar and turbulent flow.

For an inlet velocity of blood along the axial direction [23],

$$v_B = \left(\frac{2Q_B}{\pi R_1^2 n}\right)\left[1 - \left(\frac{r}{R_1}\right)^2\right] \qquad (5)$$

where Q_B is the volume flow rate of blood, R_1 is the inner radius of the hollow fiber, r is the radial coordinate and n is the number of fibers in a dialyzer.

For an inlet velocity of dialysate along the axial direction [23],

$$v_D = \frac{2Q_D}{\pi\left(\frac{3R_3^4}{4}+\frac{R_2^4}{4}-R_2^2R_3^2-R_3^4\ln(\frac{R_3}{R_2})\right)n}\left[r^2 - R_2^2 - 2R_3^2\ln(\frac{r}{R_2})\right] \qquad (6)$$

where Q_D is the volume flow rate of dialysate, r is the radial coordinate and n is the number of fibers in a dialyzer.

The definitions of R_1, R_2 and R_3 are given in Figure 3.4.

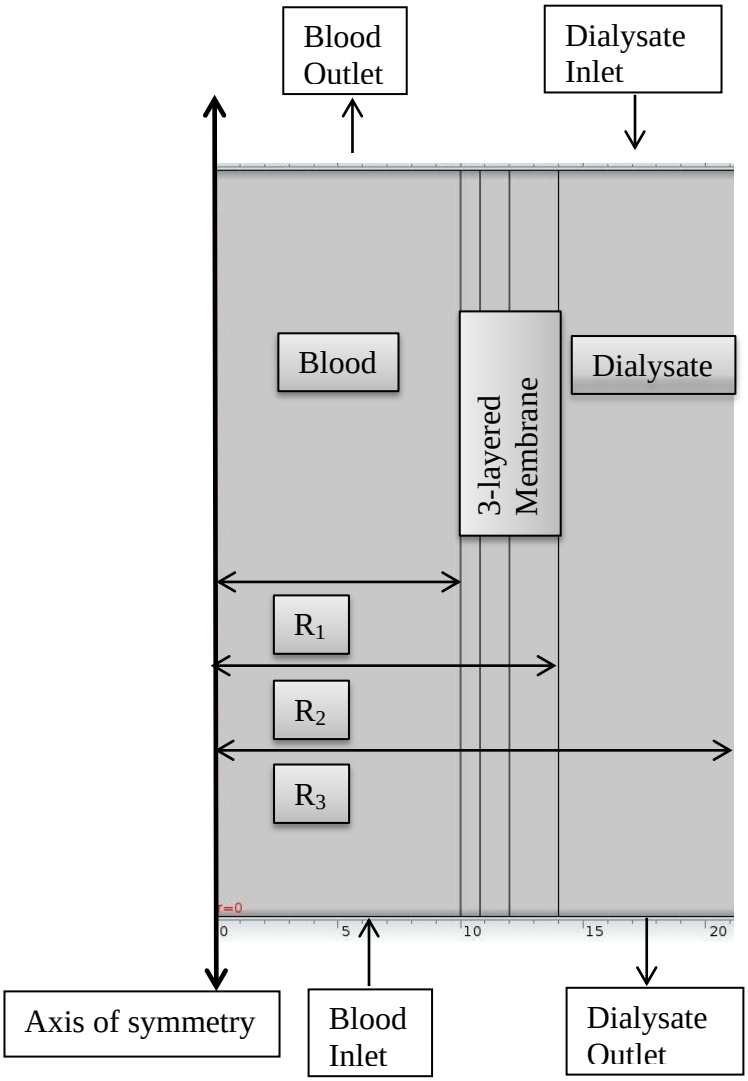

Figure 3.4 Model Geometry with R_1, R_2, R_3

- **Species Transport in Porous Media**

The Species Transport in Porous Media interface was chosen because it simulates species transport through completely or partially fluid filled voids in a solid porous medium. The interface has the equations to represent the phenomenon through the porous media.

For the phenomenon of diffusion through the membrane, the following equation has been used-

$$\nabla \cdot (-D_{e,i} \nabla c_i) = 0 \qquad (7)$$

where c_i denotes the concentration of the molecules (mol/m^3) in the respective phase, D denotes the diffusion coefficient (m^2/s) of the molecules and D_e denotes the effective diffusion coefficient of the molecules in the porous media.

As mentioned earlier, two different definitions were considered for the term - effective diffusivity. The first one being [24]-

$$D_e = \varepsilon D \qquad (8)$$

where D_e denotes the effective diffusion coefficient in the porous media while ε defines the porosity of that media. The porosity values of the three layers of the membrane were used for ε.

This will be regarded as **Case 1** in the rest of the thesis.

And for the second case [25] –

$$D_e = Df(q)S_D\varepsilon \qquad (9)$$

$$q = \frac{r_s}{r_p} \qquad (10)$$

$$f(q) = \frac{1-2.1050q+2.0865q^3-1.7068q^5+0.72603q^6}{1-0.75857q^5} \qquad (11)$$

$$S_D = (1-q)^2 \qquad (12)$$

where D is the diffusion coefficient of molecule, $f(q)$ the friction coefficient, S_D the steric hindrance factor at the pore inlet in diffusion, A_k the membrane porosity and q is the ratio of solute radius (r_s) to pore radius (r_p) [25]. Here also, the porosity values of the three layers of the membrane were used for ε.

This will be regarded as **Case 2** in the rest of the thesis.

So, from the definitions of both the effective diffusivity, it is clear that the second one considers the effects of both the solute and pore radii along with porosity whereas the first one only considers the effect of porosity. The comparison of the two definitions is shown in Chapter 4.

Table 3.2 Six molecules which were considered in the simulation with their molecular weight [26] and diameter [4]

Molecule	Molecular weight (Da)	Diameter (nm)
Urea	60	0.48
Glucose	180	1.0
Endothelin	4282.8	2.60
β2-Microglobulin	11800	3.88
Complement Factor D	24000	5.12
Albumin	66000	7.8

- **Clearance rate**

After developing the model, coupled with necessary modules in COMSOL, blood with different toxin molecules - Urea, Glucose, Endothelin, β2-Microglobulin, Complement Factor D and Albumin was introduced. To determine the clearance of each molecule, Nephrologists and manufacturers of dialyzers use this equation [27]:

$$K = \frac{Q_B(c_{in} - c_{out})}{c_{in}} \qquad (13)$$

For instance, Urea with inlet concentration, c_{in} was introduced at the blood inlet and the outlet concentration, c_{out} was measured from the blood outlet and then equation (13) was used to calculate the clearance rate for Urea.

3.3 COMSOL Multiphysics 4.3 Equation Solver

A "Stationary" study node is basically a stationary solver which adds a solver to the "Model Builder" tree in order to solve a stationary problem.

Under this "Stationary" study node, a model is solved by computing a "Solver Configuration". A "Solver" node has a sequence of sub nodes specifying the procedure to compute the solution. Also a solver configuration contains information about physics, geometry and variables.

In this dialysis problem, the two sub nodes that were used include –

- Fully Coupled
- Direct

3.3.1 Fully Coupled

The **Fully Coupled** is a node that processes parameters for a fully coupled solution approach like the dialysis process where there are different physics (or multiphysics) like – diffusion of the molecules, blood and dialysate flow. The Fully Coupled node uses a damped version of Newton's method [28].

3.3.2 Direct

The **Direct** node is a node that processes settings for direct linear system solvers. The method it uses for solving is known as **MUMPS** (**MU**ltifrontal **M**assively **P**arallel **S**parse). **MUMPS** is a parallel solver used to increase the computational efficiency. This basically works on general sparse linear systems in the form of $Ax = b$. It does **LU** factorization on the matrix A to compute the solution, x. For that a pre-ordering algorithm is used which permutes the columns of A to minimize the number of non-zeros in the L and U factors [28]. So it allows the solution of large linear systems with reduced computational efforts.

CHAPTER 4

RESULTS & DISCUSSIONS

4.1 Simualtion results from COMSOL Multiphysics 4.3

The model was developed in COMSOL Multiphysics 4.3 with necessary inlet, outlet and boundary conditions. Then the problem was solved using the **Solver** nodes. This whole process was repeated every time for changes of different parameters.

A typical concentration profile for Urea along the dialyzer membrane on both blood and dialysate side is shown in Figure 4.1. The velocity field on the blood side domain is shown in Figure 4.2.

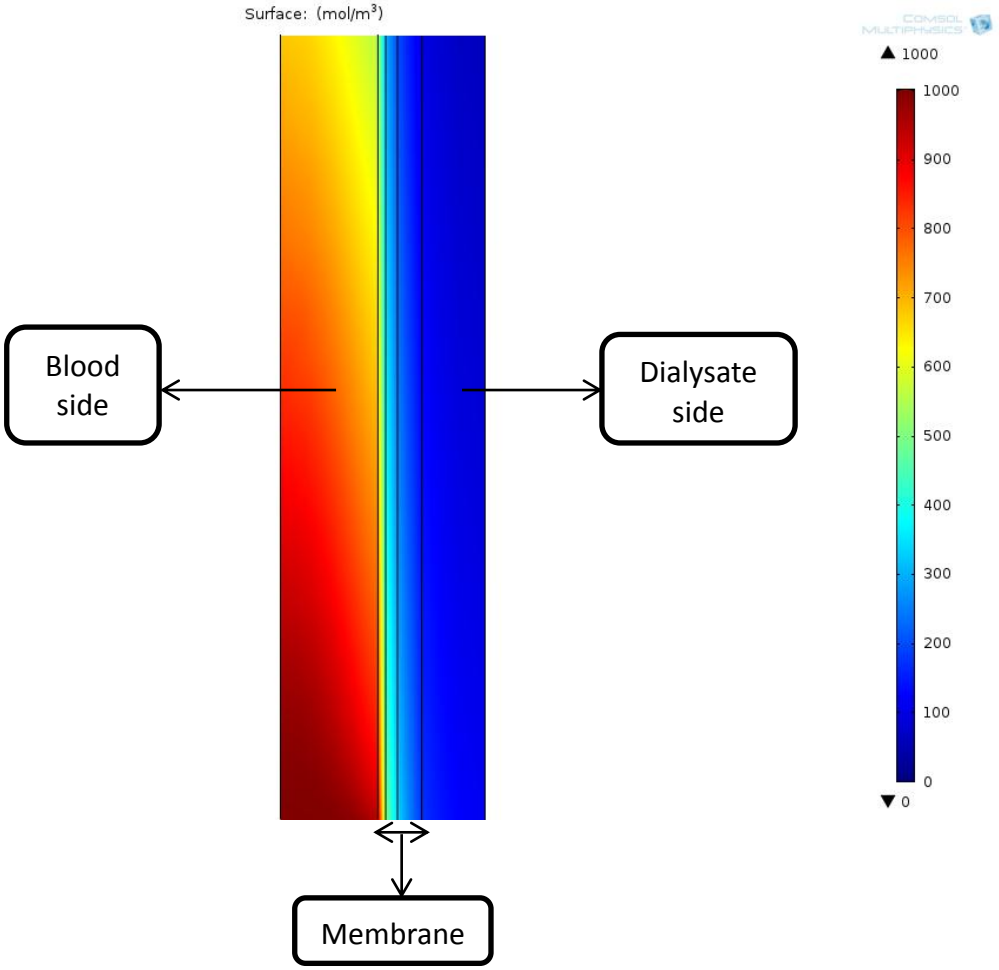

Figure 4.1 Concentration of Urea at both blood and dialysate side along the membrane (axisymmetric)

In Figure 4.1 the color legend corresponds the variation of concentration of Urea.

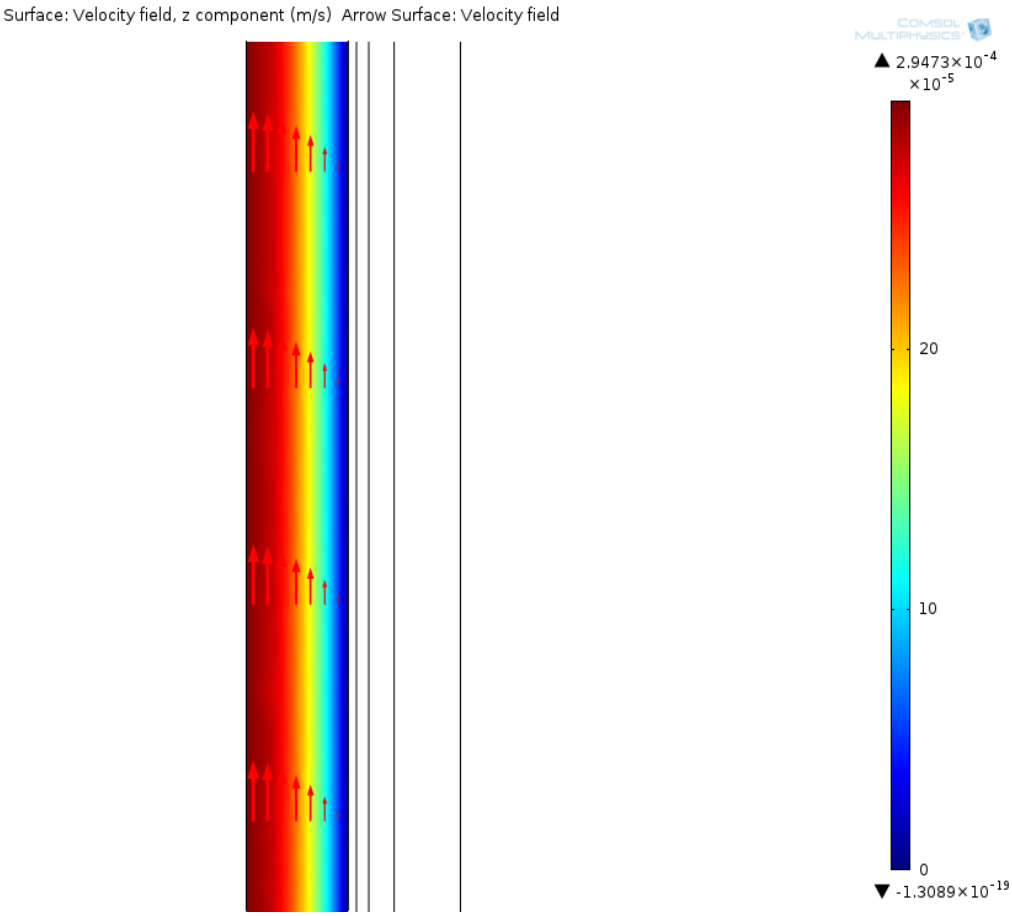

Figure 4.2 Velocity field on the blood side (color legend showing the variation of the velocity)

The red arrows in Figure 4.2 represent the direction of the velocity on the blood side. The velocity is at minimum in the vicinity of the membrane. Further away from the membrane, the velocity increases.

The velocity field on the dialysate side domain is shown in Figure 4.3.

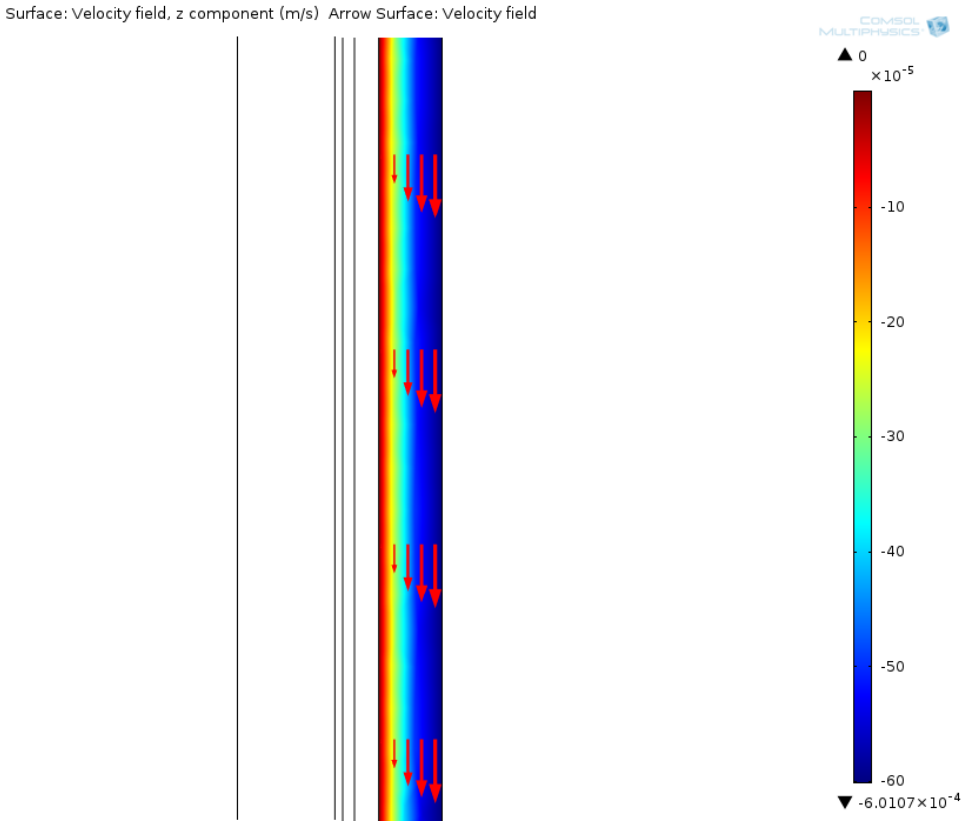

Figure 4.3 Velocity field on the dialysate side (color legend showing the variation of the velocity)

The red arrows (in Figure 4.3) represent the direction of the velocity on the dialysate side. The velocity is at minimum in the vicinity of the membrane. Further away from the membrane, the velocity increases.

After solving the problem in 2-D axisymmetric model, a 3-D representation can be generated from the post-processing results. Such a 3-D representation is shown in Figure 4.4.

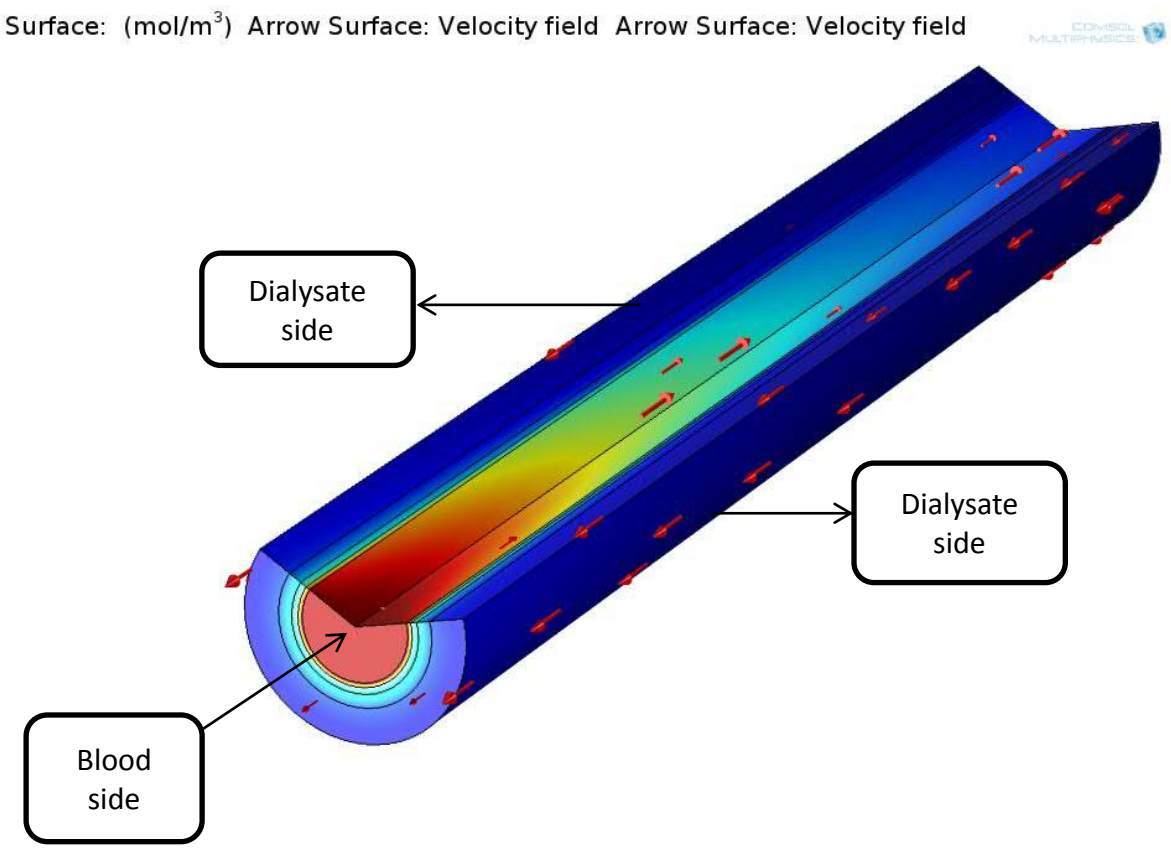

Figure 4.4 A 3-D representation of Figure 4.1 showing blood flow inside the fiber and dialysate flow surrounding the fiber

In Figure 4.4, the arrows from down to up represent the blood flow direction inside the fiber and the arrows from opposite direction represents the dialysate flow surrounding the fiber. The color differences show the change of concentration of Urea along the membrane on both sides of blood and dialysate side.

4.2 Validation of the model

The validation of the model was done in two ways. At first, the better definition between the two diffusivity definitions was chosen. This was done by comparing "Sieving coefficient" for both the cases with Polyflux 210H manufacturer's and individual researchers' experimental results. And then for the chosen definition, the "Clearance rate of Urea" was compared with Polyflux 210H manufacturer's data.

4.2.1 Comparing the two diffusivity definitions: Case 1 vs. Case 2

For the blood flow rate of Q_B = 200, 300, 400, 500 and 600 ml/min and dialysate flow rate of Q_D = 500ml/min, the clearance rate for six molecules was calculated for both the cases (shown in Figure 4.5 and 4.6). In Figure 4.5, '1' and '2' denotes the first and second case. For instance, 'Urea 1' means clearance rate of Urea using first definition of effective diffusivity (**Case 1**) and 'Urea 2' means clearance rate of Urea using second definition of effective diffusivity (**Case 2**).

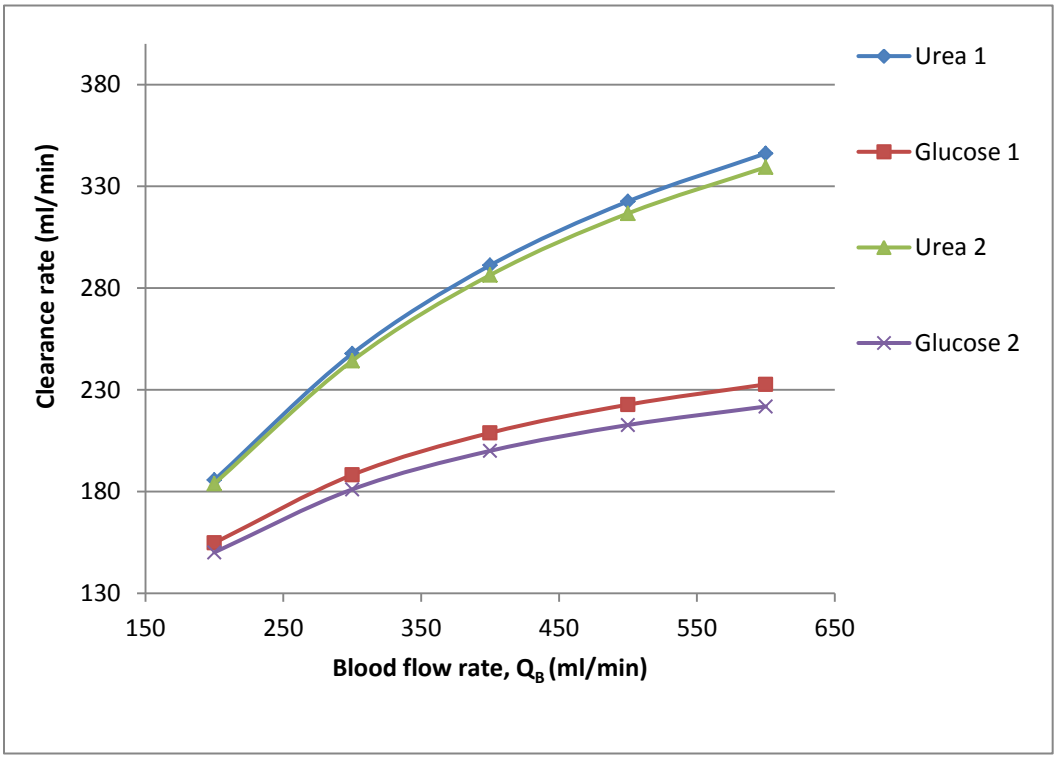

Figure 4.5 Clearance rate of Urea and Glucose at different blood flow rates when Q_D = 500ml/min for both cases

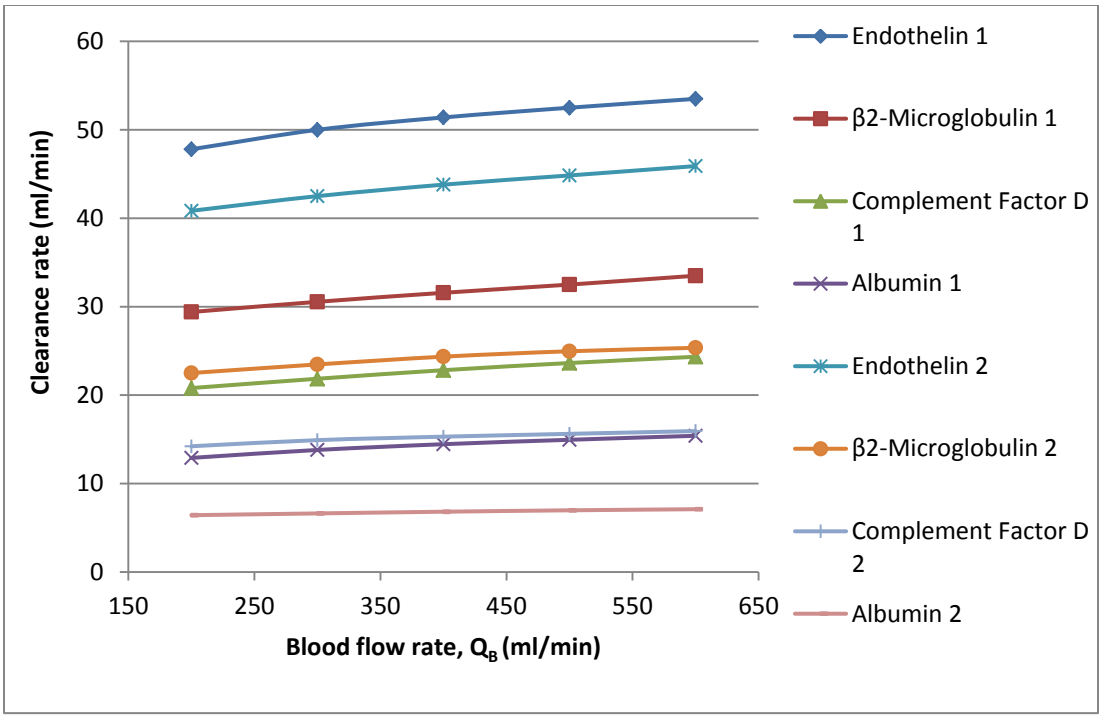

Figure 4.6 Clearance rate of Endothelin, β2-Microglobulin, Complement Factor D and Albumin at different blood flow rates when Q_D = 500ml/min for both cases

As it can be seen from Figure 4.5, with the increasing blood flow rate, the clearance rate of both Urea and Glucose increase rapidly. Specially, for Urea, when the blood flow rate increases from 200 to 600 ml/min, the clearance rate gets almost doubled. It is true for both the cases. And from Figure 4.6, it is evident that the clearance rate of Albumin remains almost constant for both the cases.

The difference between the clearance rates of Urea for two cases is negligible. It is also true for Glucose. But as the sizes of the molecules get bigger, the difference between the two cases becomes more noticeable. For instance, for blood flow rate of 200 ml/min, the clearance rate of Albumin for first case is 12.9 ml/min whereas for the second case it is 6.42 ml/min. This suggests that for smaller molecules both the definitions indicate more or less the same level of clearance. But for bigger molecules, there are obviously significant differences.

In order to determine which definition corresponds to the actual phenomenon, the sieving coefficient of Albumin was calculated for both the cases. Sieving coefficient S is calculated from [29] -

$$S = \frac{C_r}{C_d} \qquad (14)$$

where C_r is the mean concentration in the mass receiving stream and C_d is the mean concentration in the mass donating stream.

Table 4.1 Sieving coefficient for two cases

	Case 1	**Case 2**
Sieving coefficient of Albumin, S	0.012	0.0048

As experimented by the Polyflux 210H dialyzer's manufacturer, Gambro, the sieving coefficient of Albumin is well less than 0.01 [13]. The literatures [26, 30] also support this claim. So considering all these facts, the second case was chosen for further investigation in this thesis as the second definition represents the actual phenomenon relatively better than the first one.

4.2.2 Comparing Clearance rates of Urea

To further justify the choice of **Case 2** (or second case), the clearance rate of Urea, obtained from simulation, was compared with the experimental results provided by the manufacturer [13].

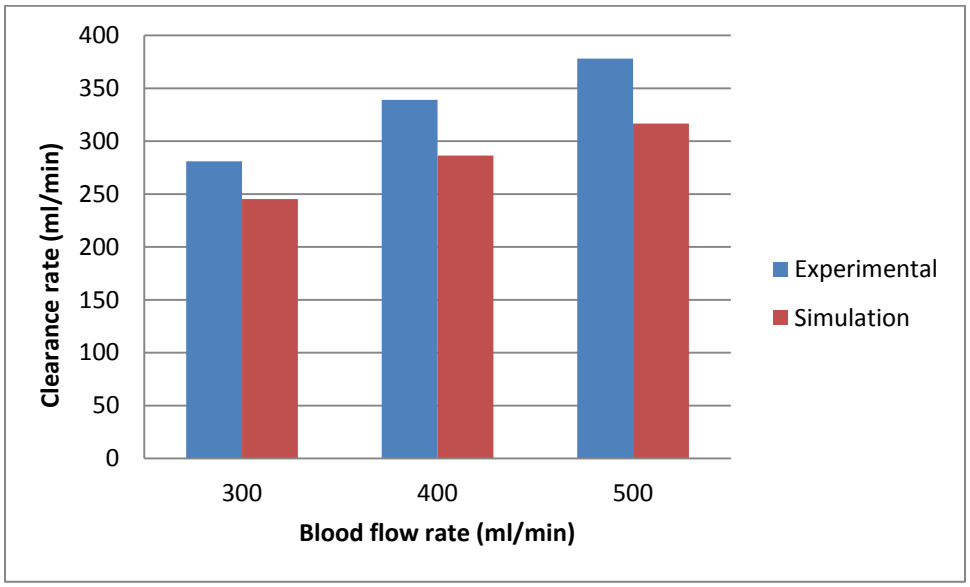

Figure 4.7 Clearance rate of Urea for both experimental and simulation cases at Q_B = 300, 400 and 500 ml/min whereas Q_D = 500ml/min for **Case 2**

From Figure 4.7, it can be concluded that the clearance rate of Urea at different blood flow rate is in good agreement with the data provided by the Polyflux 210H manufacturer.

Now this **Case 2** or second definition was used for the rest of the thesis to determine the effects of changing the magnitude and direction of blood and dialysate flow, length and diameter of the fiber, pore sizes of the membrane.

4.3 Effects of changing direction of blood and dialysate flow

The directions of both blood and dialysate flows were changed. For both counter-current and co-current flow the clearance rate of Urea, Glucose, Endothelin, β2-Microglobulin, Complement Factor D and Albumin was calculated (Figure 4.8 and 4.9).

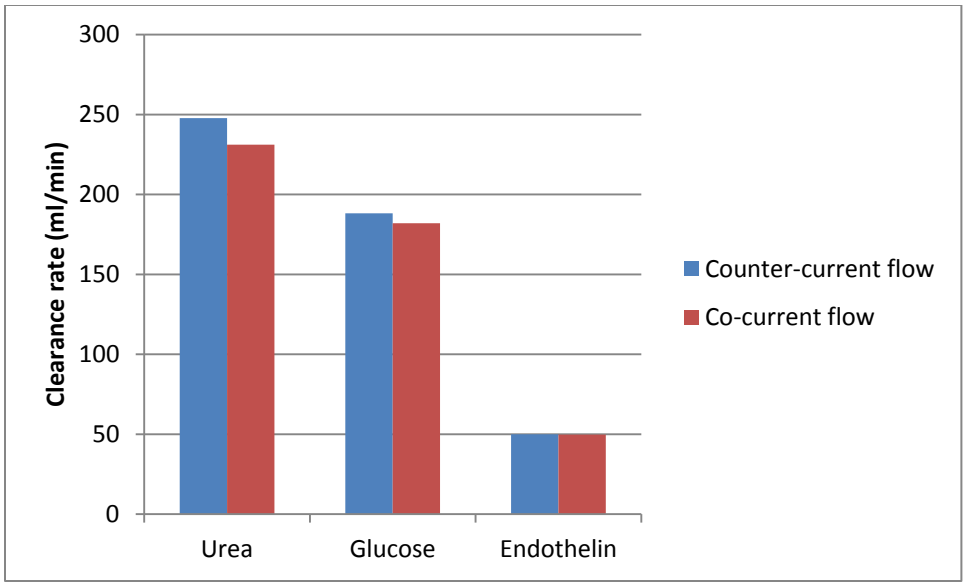

Figure 4.8 Clearance rate of Urea, Glucose and Endothelin at Q_B = 300 ml/min and Q_D = 500 ml/min

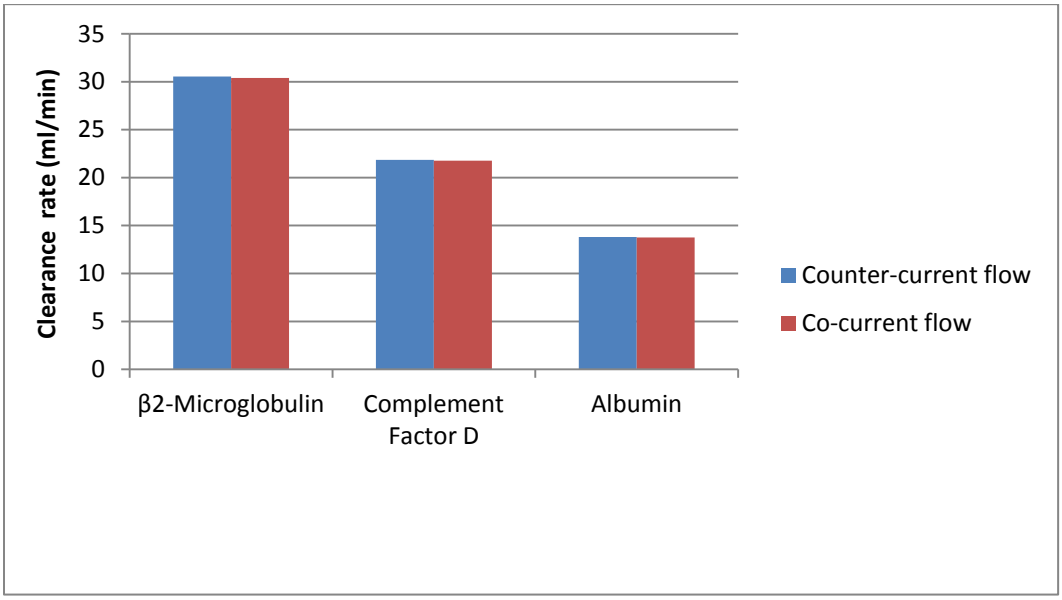

Figure 4.9 Clearance rate of β2-Microglobulin, Compliment Factor D and Albumin at Q_B = 300 ml/min and Q_D = 500 ml/min

For Urea and Glucose, counter-current flow shows better clearance than co-current flow.

4.4 Effects of blood flow rate on clearance rate

The dialysate flow rate, Q_D = 500 ml/min was kept constant and the blood flow rate, Q_B was gradually increased from 200 to 600 ml/min (Figure 4.10 and 4.11).

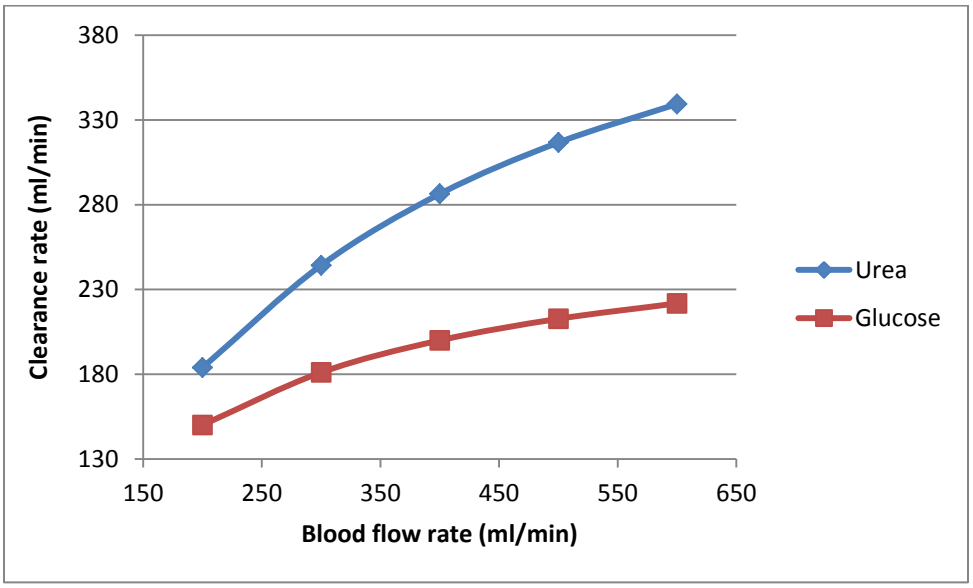

Figure 4.10 Clearance rate of Urea and Glucose at different blood flow rates when Q_D = 500ml/min

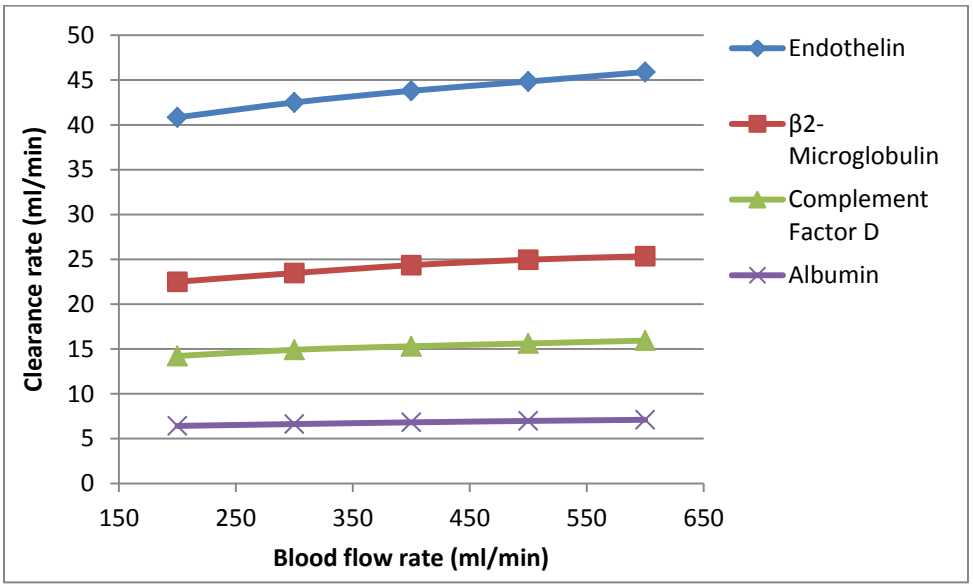

Figure 4.11 Clearance rate of Endothelin, β2-Microglobulin, Complement Factor D and Albumin at different blood flow rates when Q_D = 500ml/min

As it can be seen from Figure 4.10, with the increasing blood flow rate, the clearance rate of both Urea and Glucose increase rapidly. Specially, for Urea, when the blood flow rate increases from 200 to 600 ml/min, the clearance rate gets almost doubled. And from Figure 4.11, it is evident that the clearance rate of Albumin remains almost constant.

4.5 Effects of dialysate flow rate on clearance rate

The blood flow rate, Q_B= 400 ml/min was kept constant and the dialysate flow rate, Q_D was gradually increased (Figure 4.12 and 4.13).

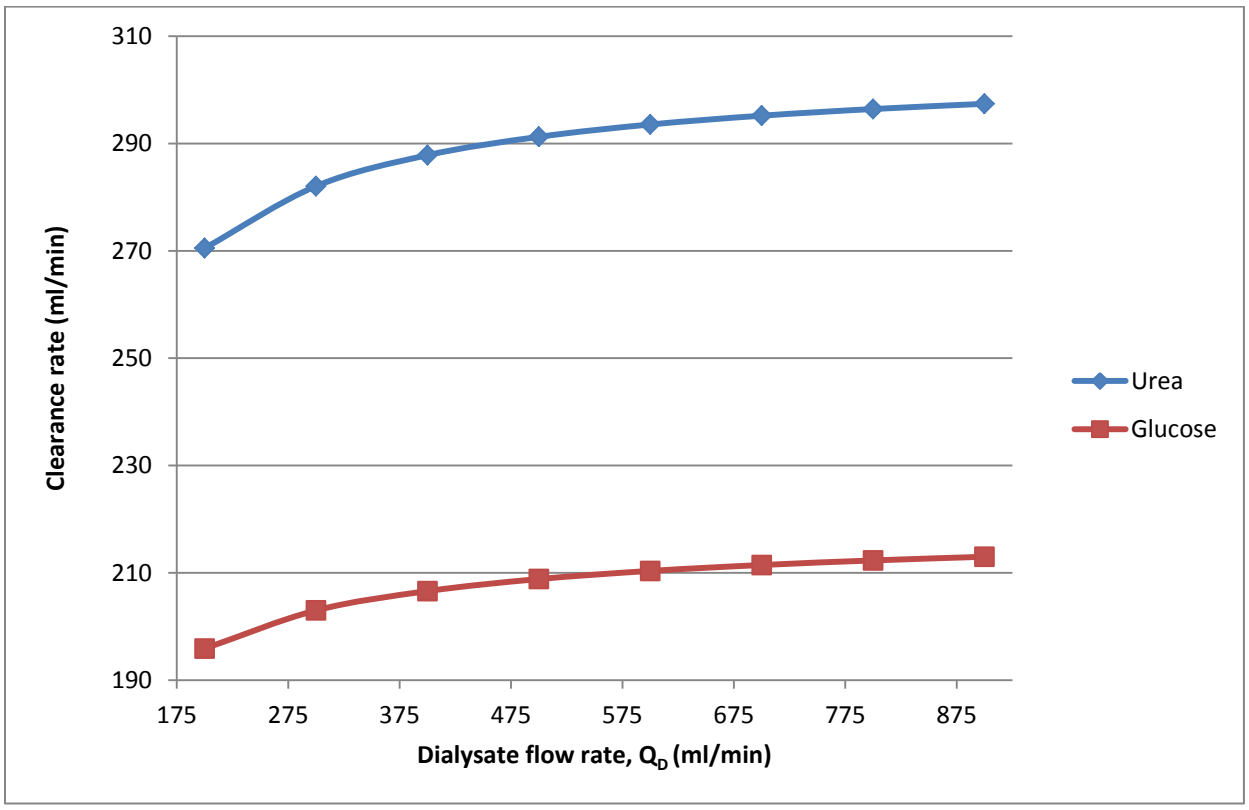

Figure 4.12 Clearance rate of Urea and Glucose at different dialysate flow rates when Q_B = 400ml/min

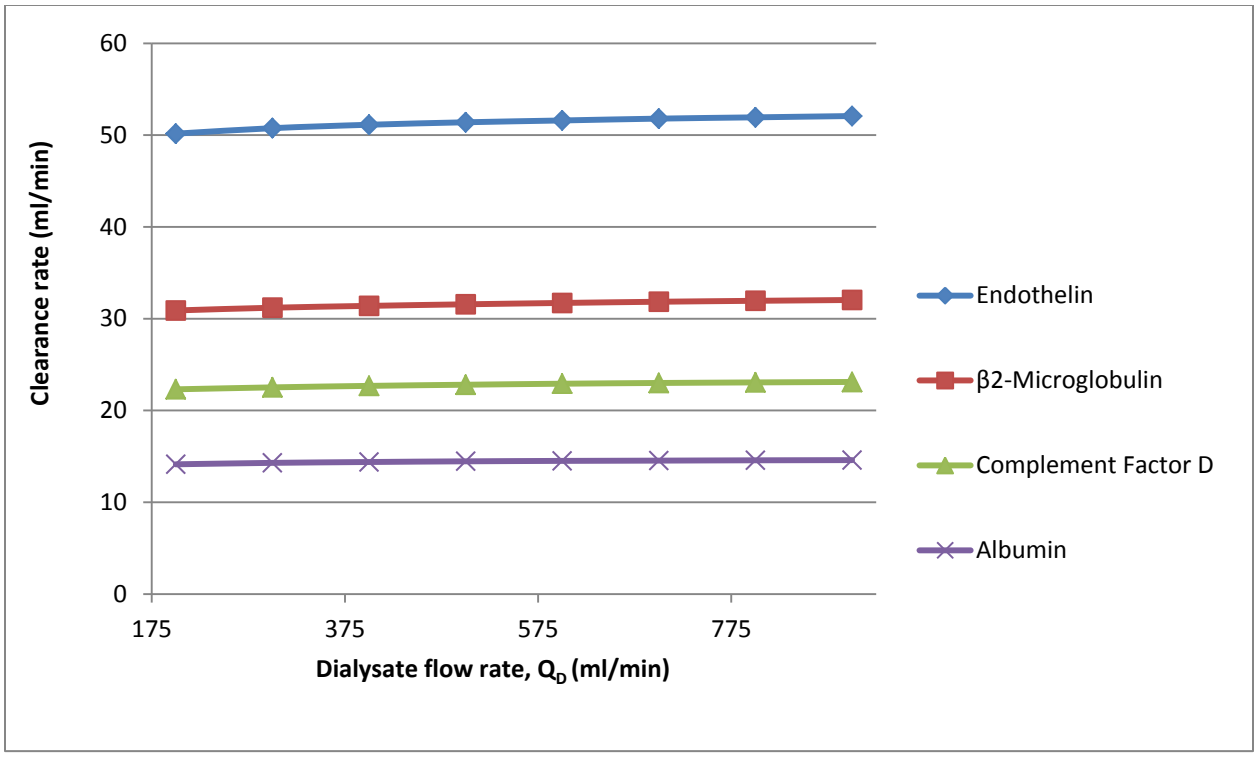

Figure 4.13 Clearance rate of Endothelin, β2-Microglobulin, Complement Factor D and Albumin at different dialysate flow rates when Q_B = 400ml/min

At a constant blood flow rate, the increasing dialysate flow rate ensures better clearance of Urea and Glucose.

Not for all patients increasing the blood flow rate is a good idea. For end stage renal failure patients, increasing the blood flow rate can be dangerous. In that case, a doctor or nephrologist can determine the maximum blood flow rate which is safe for a patient and then increase the dialysate flow rate to further increase the clearance rate of toxin molecules.

4.6 Effects of length of the dialyzer fiber on clearance rate

The length of the dialyzer fiber was varied from 270 to 540 mm when Q_B=300 ml/min and Q_D=500 ml/min (Figure 4.14 and 4.15).

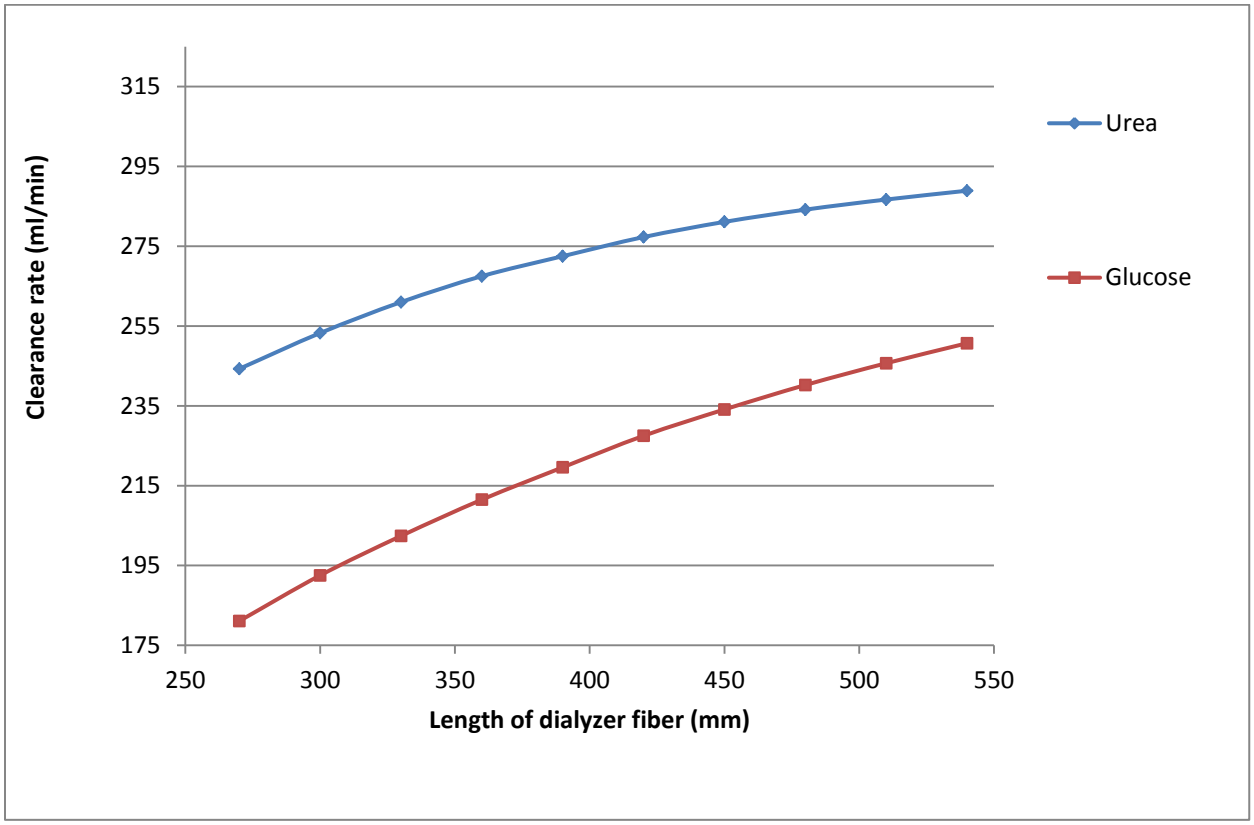

Figure 4.14 Clearance rate of Urea and Glucose at Q_B = 300ml/min and Q_D = 500ml/min

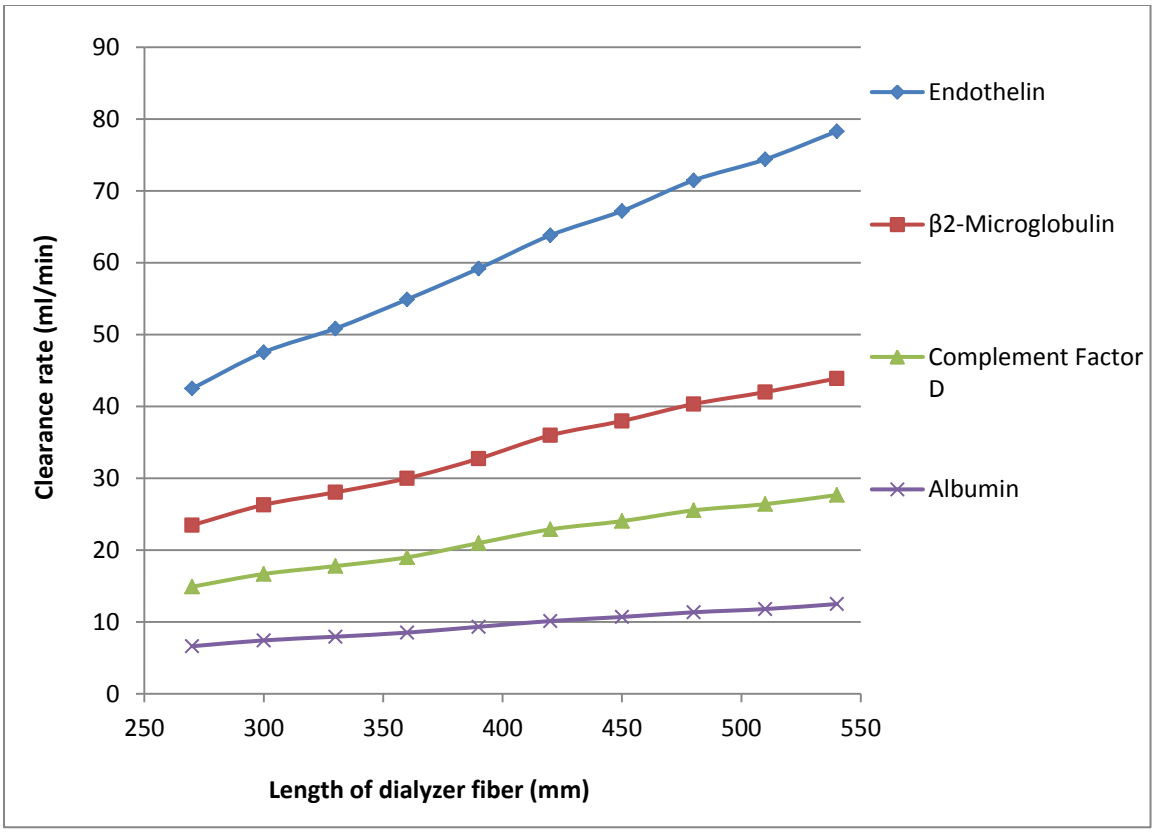

Figure 4.15 Clearance rate of Endothelin, β2-Microglobulin, Complement Factor D and Albumin at Q_B = 300ml/min and Q_D = 500ml/min

From Figure 4.14, it can be seen that if the length of the dialyzer fiber is increased, the clearance rate of Glucose increases more rapidly than the clearance rate of Urea. For Endothelin and β2-Microglobulin (Figure 4.15) the clearance rate increases twice compared to the initial condition. Meanwhile, the clearance rate of Albumin does not change that much.

4.7 Effects of radius of the dialyzer fiber on clearance rate

The radius of the dialyzer fiber was increased from 0.1 mm to 0.2 mm when Q_B=300 ml/min and Q_D=500 ml/min (Figure 4.16 and 4.17).

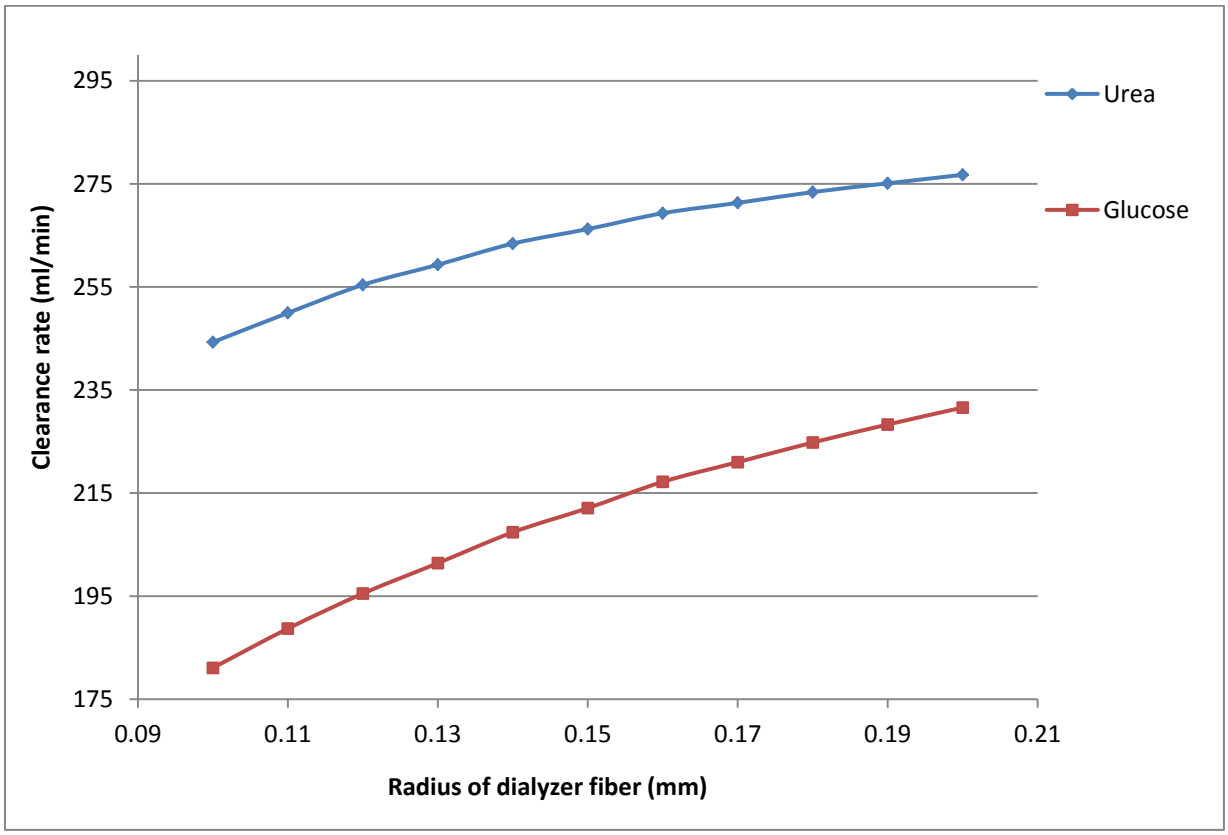

Figure 4.16 Clearance rate of Urea and Glucose at Q_B = 300ml/min and Q_D = 500ml/min

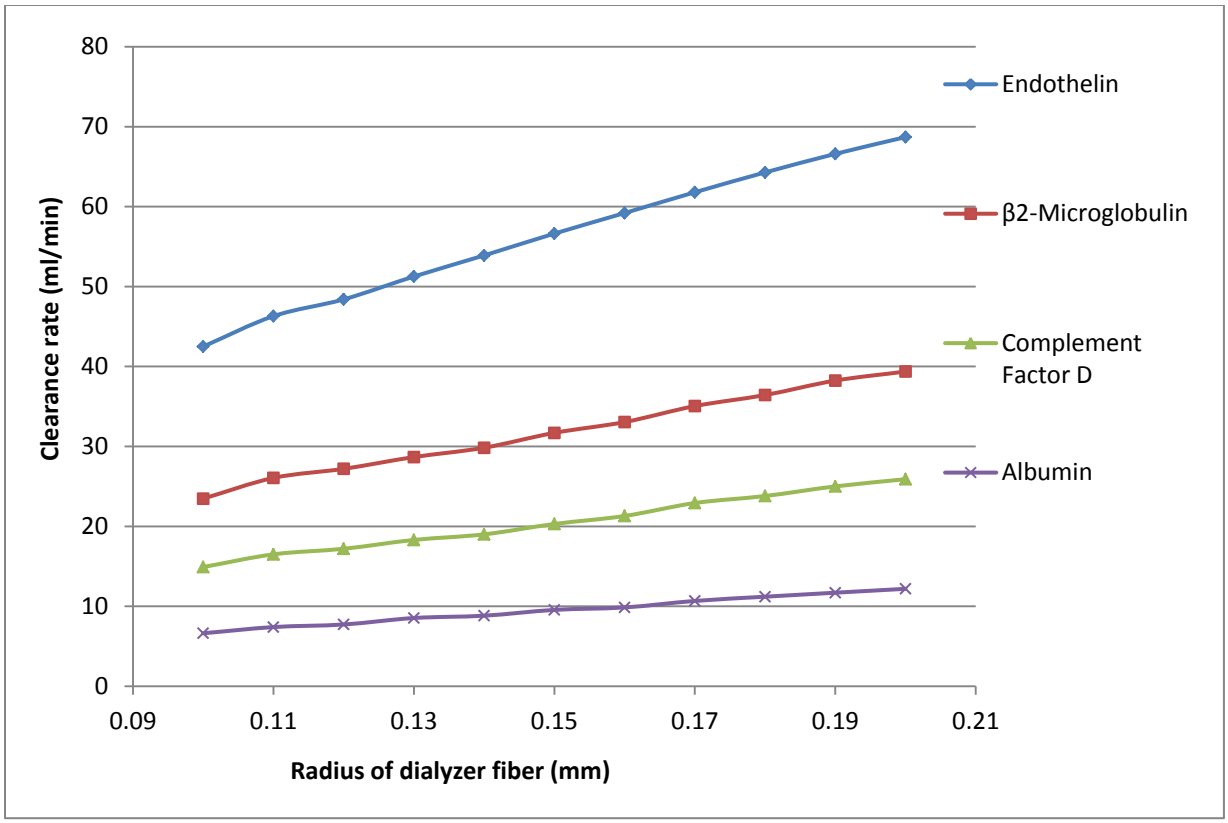

Figure 4.17 Clearance rate of Endothelin, β2-Microglobulin, Complement Factor D and Albumin at Q_B = 300ml/min and Q_D = 500ml/min

From Figure 4.16 and 4.17 it is evident that the effect of increasing radius of dialyzer fiber is similar to that of increasing the length of the dialyzer fiber. However, a case was considered where the clearance rate of Albumin is same for a dialyzer fiber with length = 450 mm, radius = 0.1 mm and a dialyzer fiber with length = 270 mm, radius = 0.17 mm.

Table 4.2 Clearance rate of different molecules for two dialyzer fibers consisting length = 450 mm, radius = 0.1 mm and length = 270 mm, radius = 0.17 mm

	Length = 450 mm, Radius = 0.1 mm	Length = 270 mm, Radius = 0.17 mm
Urea	281.1	271.3
Glucose	234.1	221
Endothelin	67.21	61.8
β2-Microglobulin	37.97	35.05
Complement Factor D	24.04	22.92
Albumin	10.67	10.7

From Table 4.2, it is evident that for the same level of clearance rate of Albumin (or loss of Albumin), the dialyzer fiber with relatively higher length and lower radius shows better clearance of Urea, Glucose, Endothelin, β2-Microglobulin and Complement Factor D than the dialyzer fiber with relatively higher radius and lower length.

4.8 Effects of changing pore's diameter in the first layer of the dialyzer membrane

As mentioned before, the first layer of the dialyzer membrane is the most important of all the three layers. Because if the toxin molecules can get through the first layer, they can easily get through the outer two layers because of their relatively bigger pore sizes. Increasing the porosity of the first layer of the dialyzer membrane can improve the clearance rate of Urea, Glucose, Endothelin, β2-Microglobulin and Complement Factor D. But at the same time it ensures the loss of Albumin. So it has a downside. But changing the pore diameter of the membrane has some significant positive effects (Figure 4.18 and 4.19).

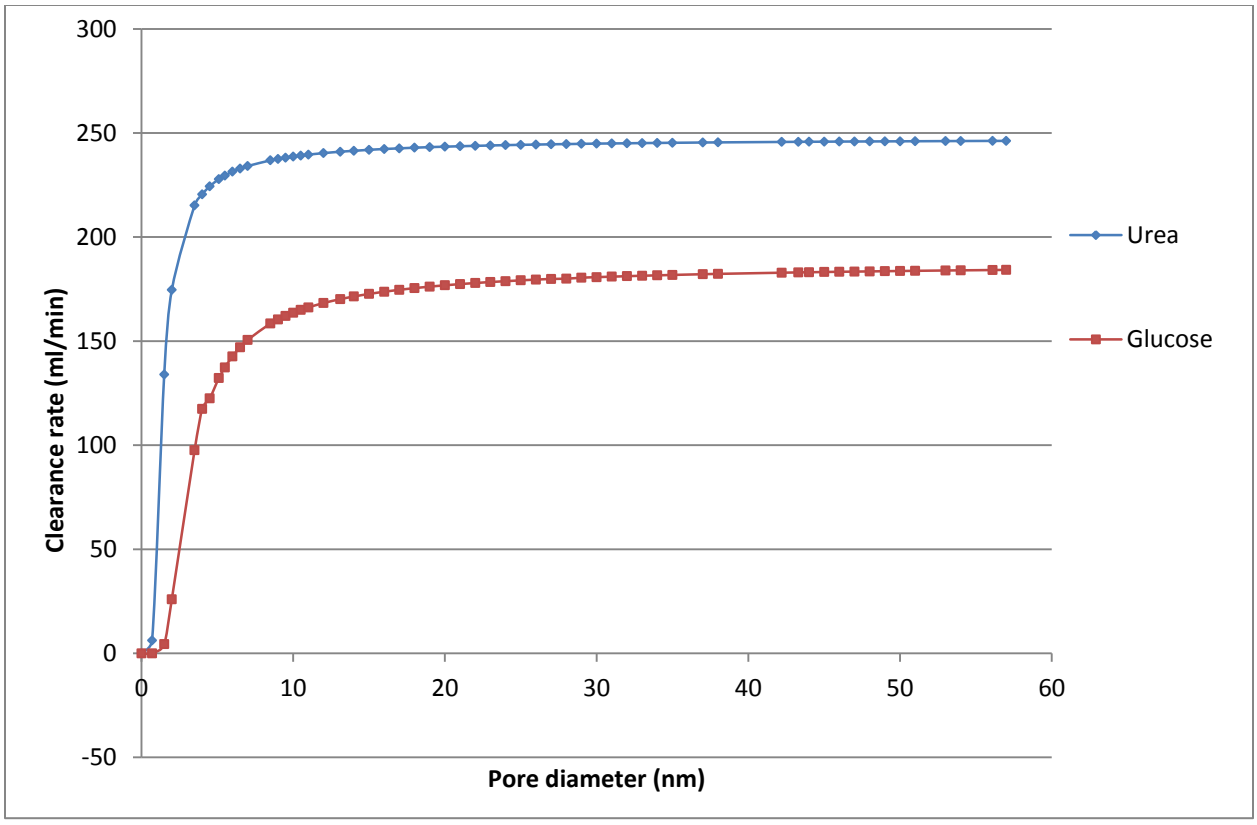

Figure 4.18 Clearance rate of Urea and Glucose while increasing the pore diameter in the first layer of the dialyzer membrane

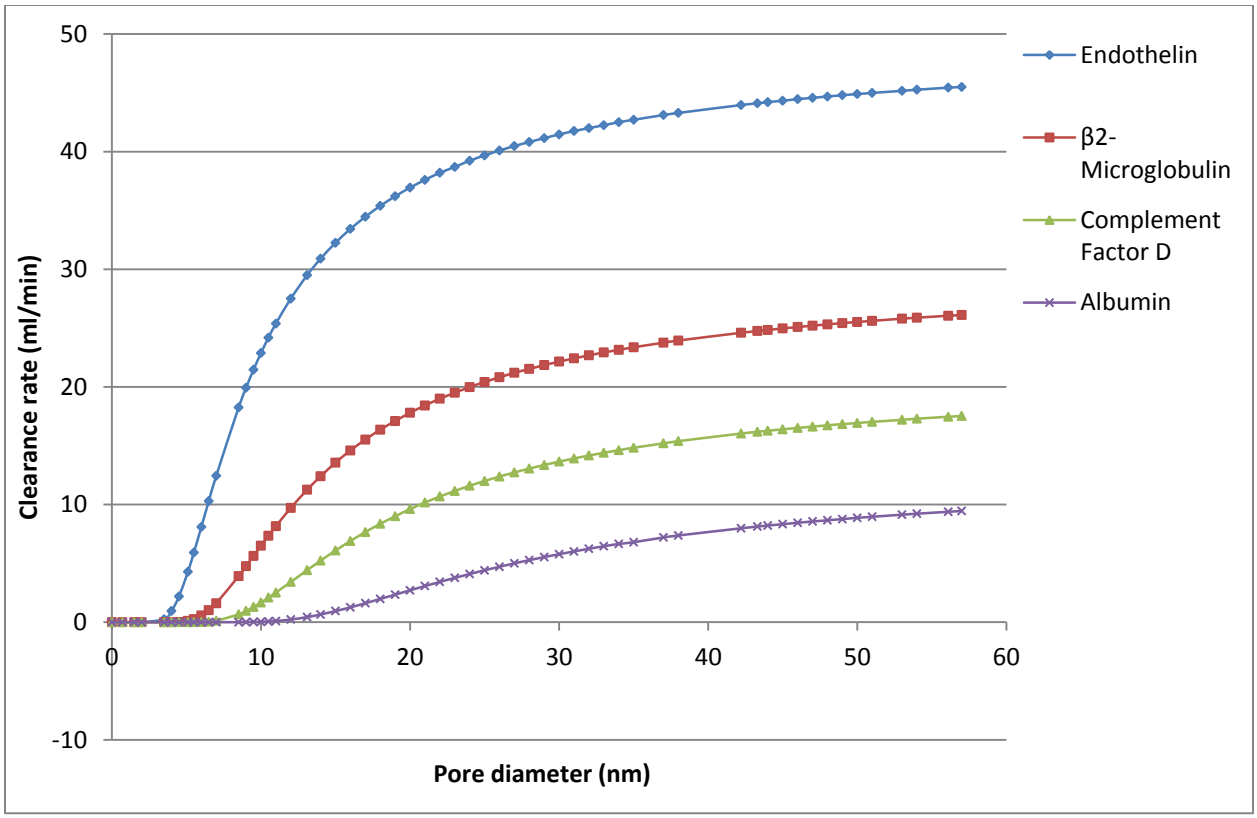

Figure 4.19 Clearance rate of Endothelin, β2-Microglobulinm, Complement Factor D and Albumin while increasing the pore diameter in the first layer of the dialyzer membrane

Figure 4.18 suggests that the clearance rate of Urea and Glucose rises significantly between the pore diameters of 1 to 10 nm. Then between 10 to 20 nm they increase a little bit. But after 20 nm it is almost constant. But Figure 4.19 suggests that if the pore diameter increases beyond 20 nm the Albumin clearance rate (or albumin loss) increases rapidly. In the range of 1 to 20 nm the Albumin loss is still very low and at the same time moderate clearance rate of the middle molecules can be achieved.

So all in all, if the pore diameter is increased up to 20 nm (but not higher than that), higher clearance rate of Urea and Glucose, moderate clearance rate of middle molecules and minimum loss of Albumin can be ensured.

CHAPTER 5

CONCLUSIONS & RECOMMENDATIONS

5.1 Conclusions

- The definition of effective diffusivity through the dialyzer membrane which considers the effects of both the solute and pore radius along with porosity (**Case 2**) is chosen over the one which only considers porosity (**Case 1**).
- The clearance rate of Urea at different blood flow rate is in good agreement with the data provided by the Polyflux 210H manufacturer.
- Counter-current flow in the dialyzer shows better clearance rate of Urea and Glucose.
- The clearance rate of both Urea and Glucose increase rapidly with the increasing blood flow rate. Specially, for Urea, when the blood flow rate increases from 200 to 600 ml/min, the clearance rate gets almost doubled. At the same time clearance rate of Albumin remains almost constant.
- When a maximum allowable blood flow rate is attained, increasing the dialysate flow rate can ensure better clearance rate for Urea and Glucose.
- In both the cases of increasing radius or length of the dialyzer fiber, the clearance rate of Glucose increases more rapidly than the clearance rate of Urea. For Endothelin and β2-Microglobulin the clearance rate increases twice compared to the initial condition. Meanwhile, the clearance rate of Albumin does not change that much.
- At the same level of Albumin loss, the dialyzer fiber with relatively higher length and lower radius shows better clearance of Urea, Glucose, Endothelin, β2-Microglobulin and Complement Factor D than the dialyzer fiber with relatively higher radius and lower length.
- Increasing the pore diameter up to 20 nm (but not more than that) can ensure higher clearance rate of Urea and Glucose, moderate clearance rate of middle molecules and minimum loss of Albumin.

5.2 Recommendations

- Now-a-days an important additional function to the hemodialysis process is the ultrafiltration. In fact, a hemodialysis process associated with an ultrafiltration system is known as hemodiafiltration. Polyflux 210H dialyzer is also used as a hemodiafiltration.

Ultrafiltration is the process of removing excessive water from blood during the dialysis process. For many of end stage renal failure patients, removing excessive fluid from the body is extremely important. This ultrafiltration is done by the trans-membrane pressure created by the arterial, venous and dialysis pressure fluids [12]. At the same time, a small amount of small and big sized toxin molecules get convected across the dialyzer membrane, even though the significant amount of toxin molecules is cleared by the diffusion process.

Since in this thesis the main focus was on the hemodialysis process, the equations which represent the diffusion process were used. If equations which represent the convection of the toxin molecules, removal of fluid from the blood stream along with the diffusion equations are used, the simulation of hemodiafiltration can be done.

- In this thesis, the dialyzer membrane was divided into three layers to calculate the porosity for simulation purposes. Higher number of layers can predict the characteristics of the membrane more precisely.

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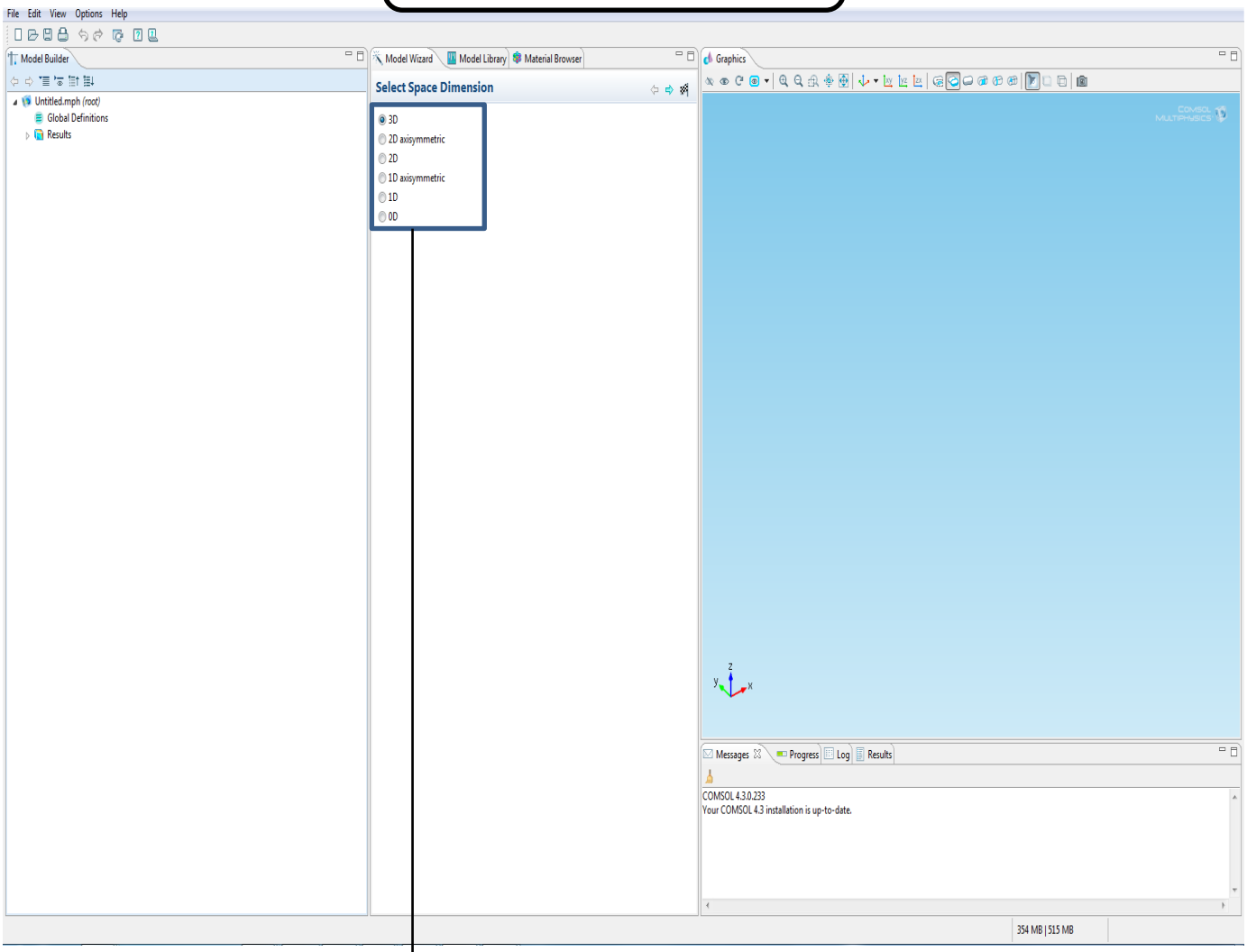
APPENDIX

How to do it in COMSOL Multiphysics 4.3?

- **Starting and Selecting the modules**

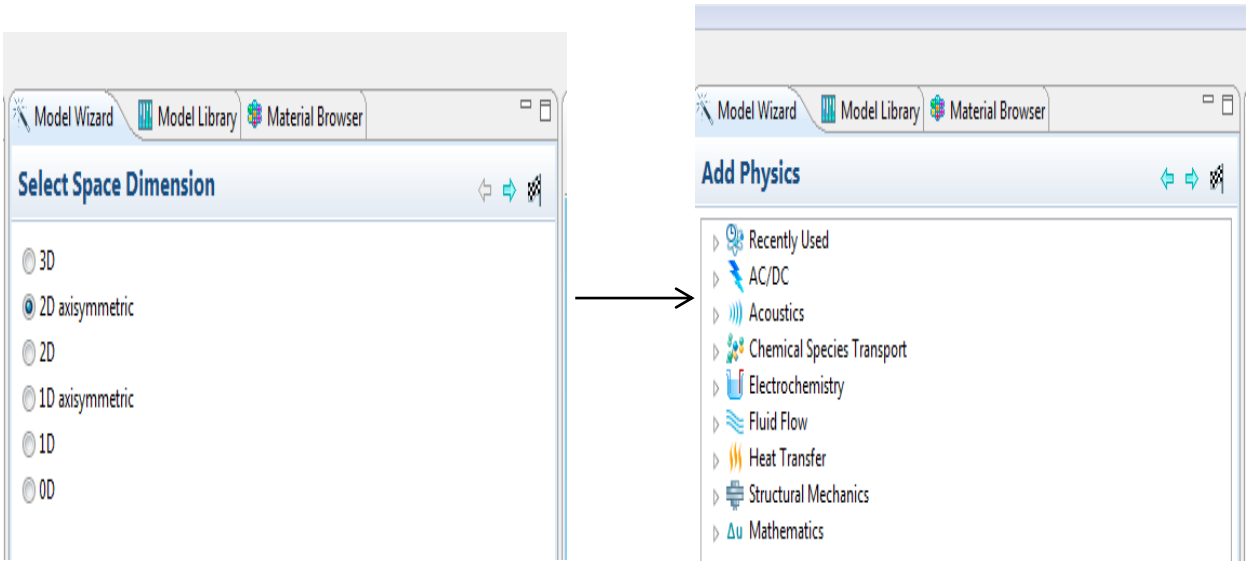
Start **COMSOL Multiphysics 4.3**



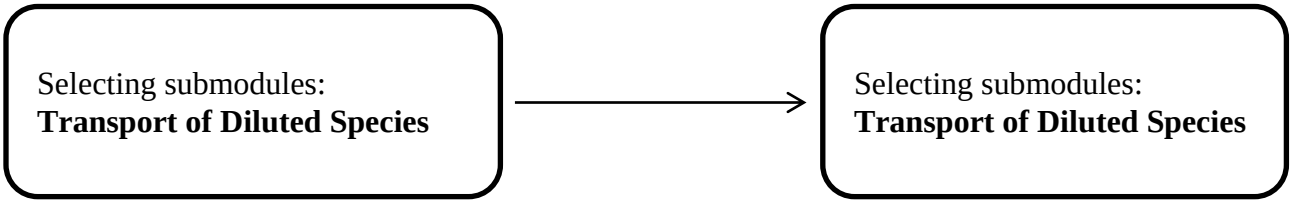
Selecting the space dimension: **2D axisymmetric**

→

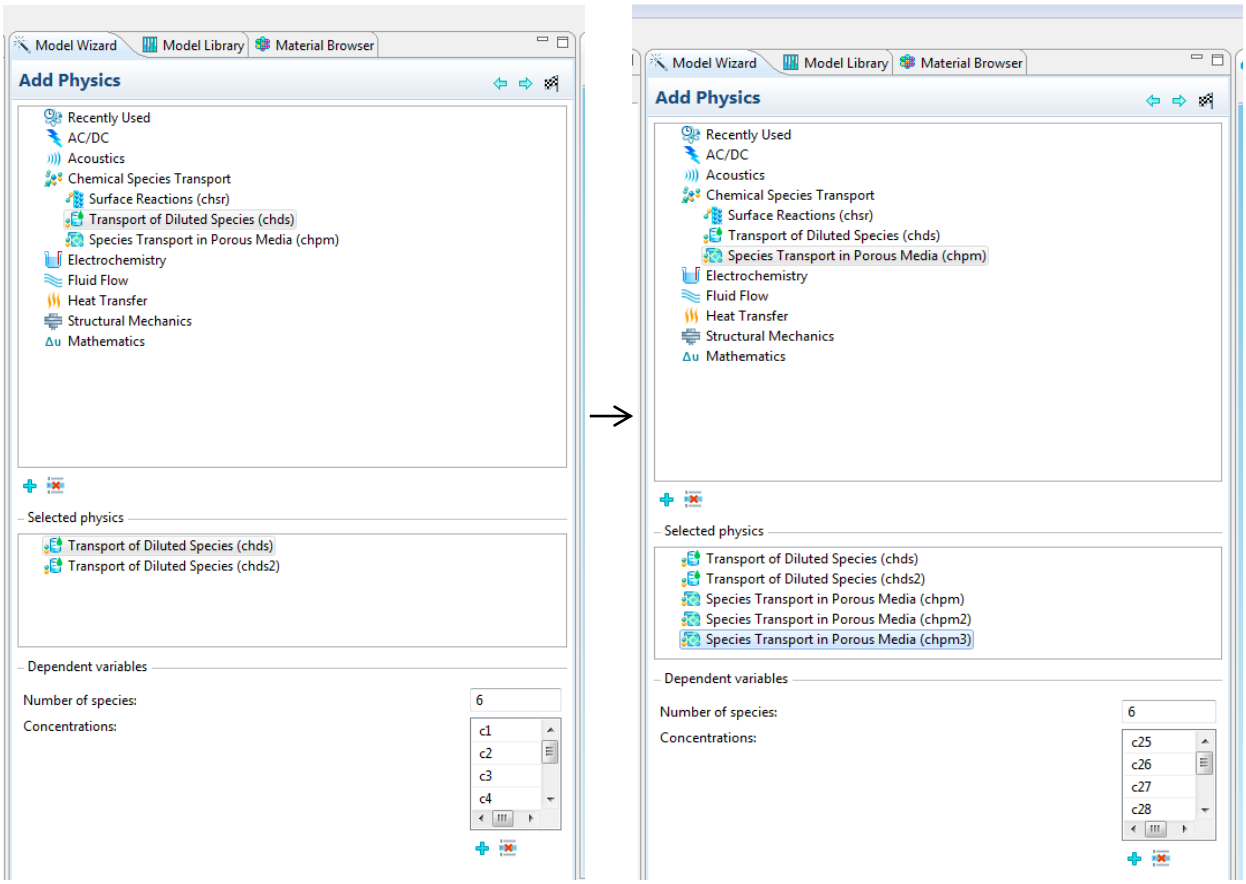
Adding physics (main module): Expand **Chemical Species Transport**



- **Selecting sub modules** : Two submodules (**Transport of Diluted Species**) for the blood and dialysate and three submodules (**Species Transport in porous Media**) for the three layers of the membrane



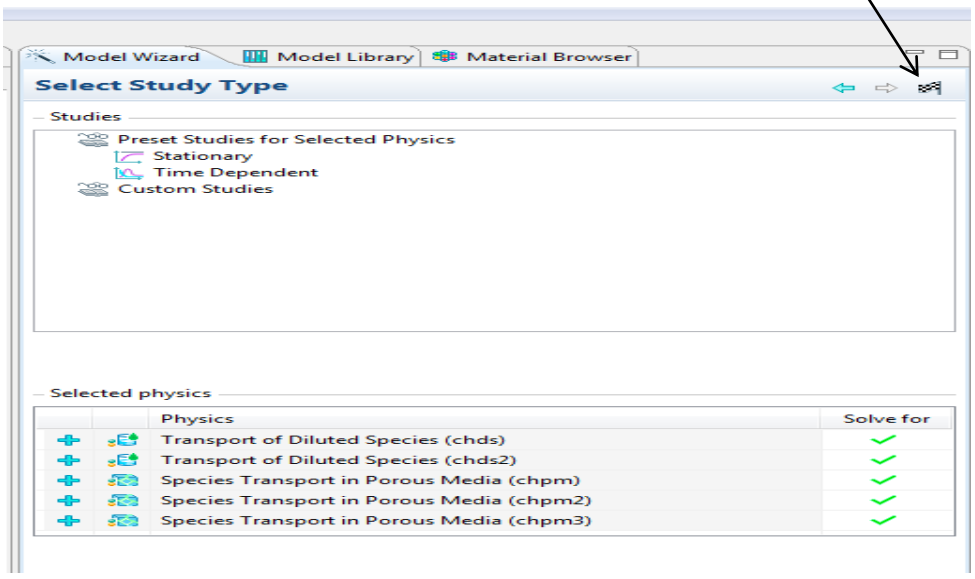
Note: Six species have been chosen for each submodule, since we have taken six molecules into consideration.



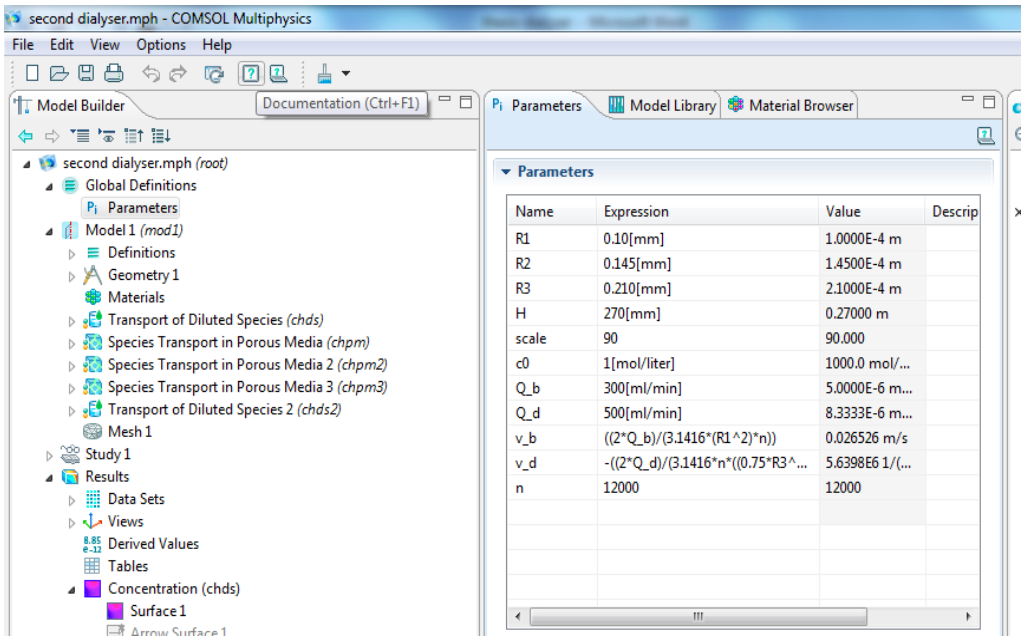
➢ Selecting study type

Selecting study type: **Stationary**

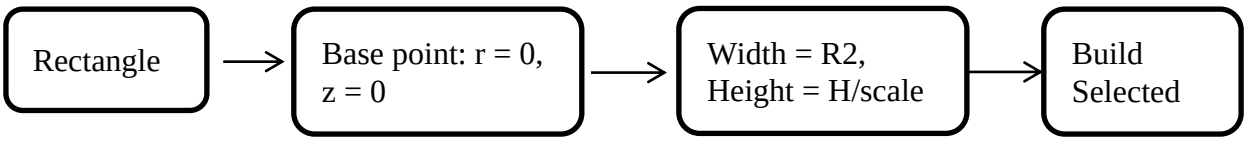
Select chequered flag to **Finish**

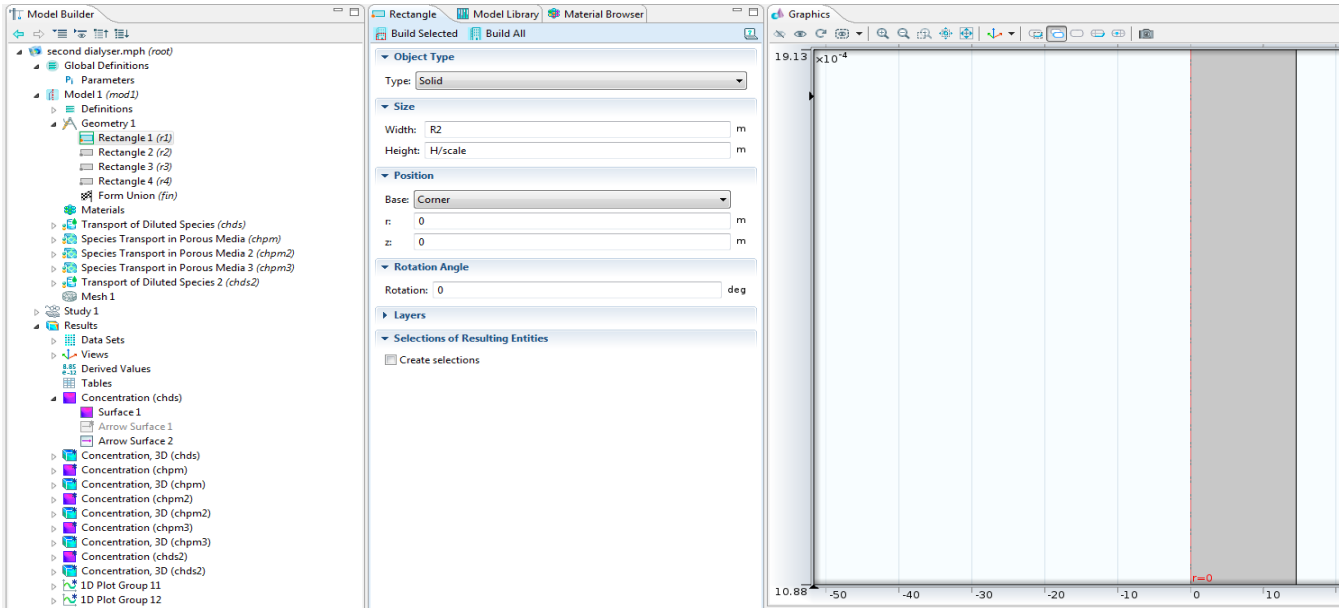


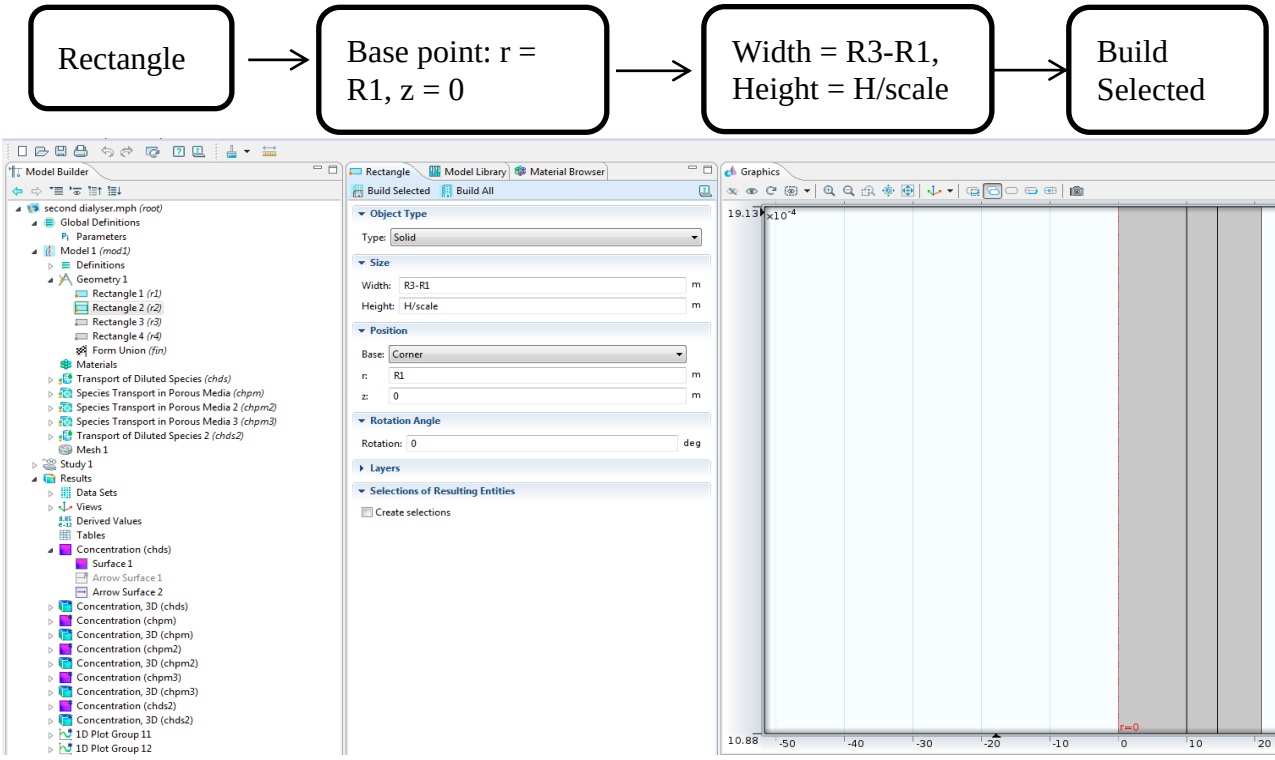
➢ Setting Global definitions by using “Parameters” option



➢ Drawing Geometry in 2-D



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Material Browser
Graphics
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Materials
Transport of Diluted Species (chds)
Species Transport in Porous Media (chpm)
Species Transport in Porous Media 2 (chpm2)
Species Transport in Porous Media 3 (chpm3)
Transport of Diluted Species 2 (chds2)
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Study 1
Results
Data Sets
Views
Derived Values
Tables
Concentration (chds)
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Arrow Surface 2
Concentration, 3D (chds)
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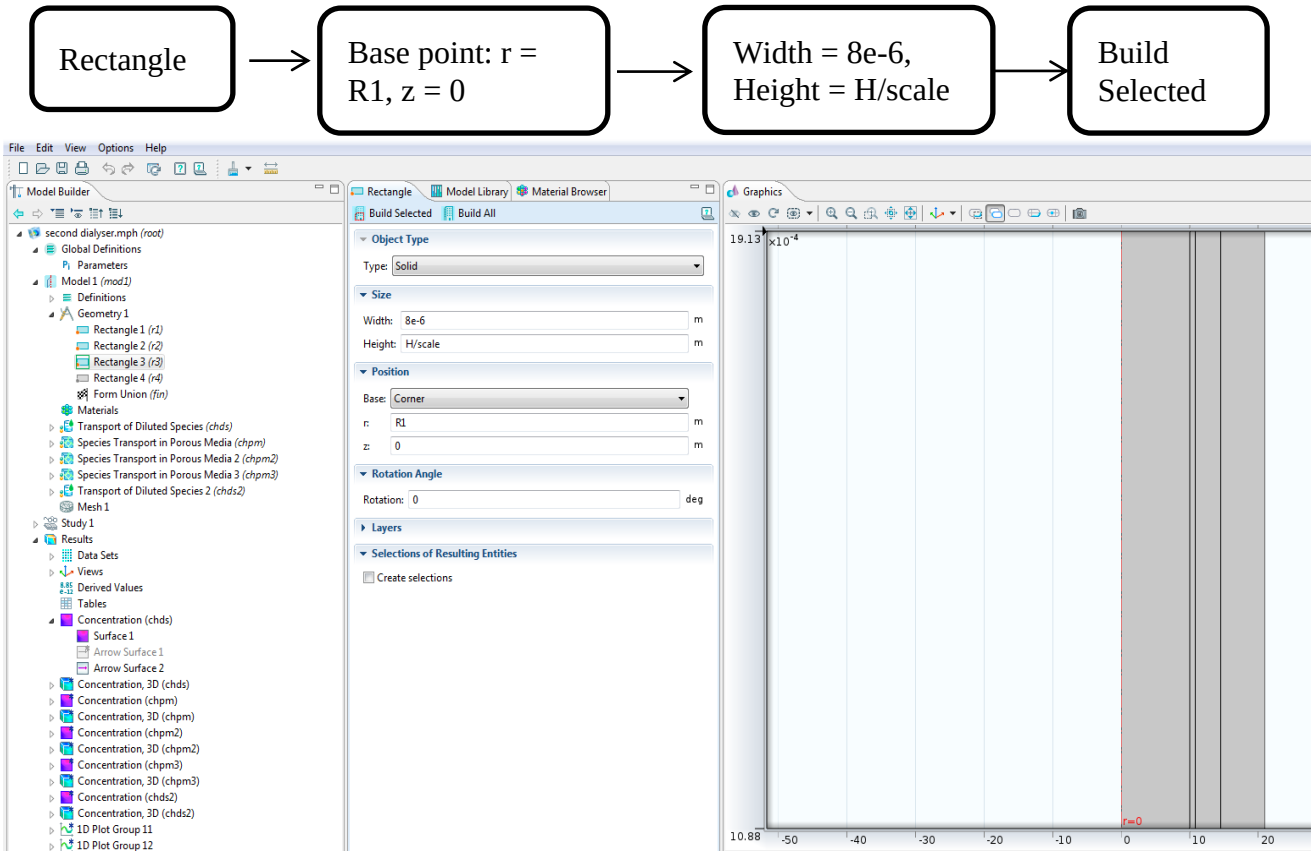
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Model Builder
Rectangle
Model Library
Material Browser
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Type: Solid
Size
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Base: Corner
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Geometry 1
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Rectangle 4 (r4)
Form Union (fin)
Materials
Transport of Diluted Species (chds)
Species Transport in Porous Media (chpm)
Species Transport in Porous Media 2 (chpm2)
Species Transport in Porous Media 3 (chpm3)
Transport of Diluted Species 2 (chds2)
Mesh 1
Study 1
Results
Data Sets
Views
Derived Values
Tables
Concentration (chds)
Surface 1
Arrow Surface 1
Arrow Surface 2
Concentration, 3D (chds)
Concentration (chpm)
Concentration, 3D (chpm)
Concentration (chpm2)
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Concentration (chpm3)
Concentration, 3D (chpm3)
Concentration (chds2)
Concentration, 3D (chds2)
1D Plot Group 11
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-40
-30
-20
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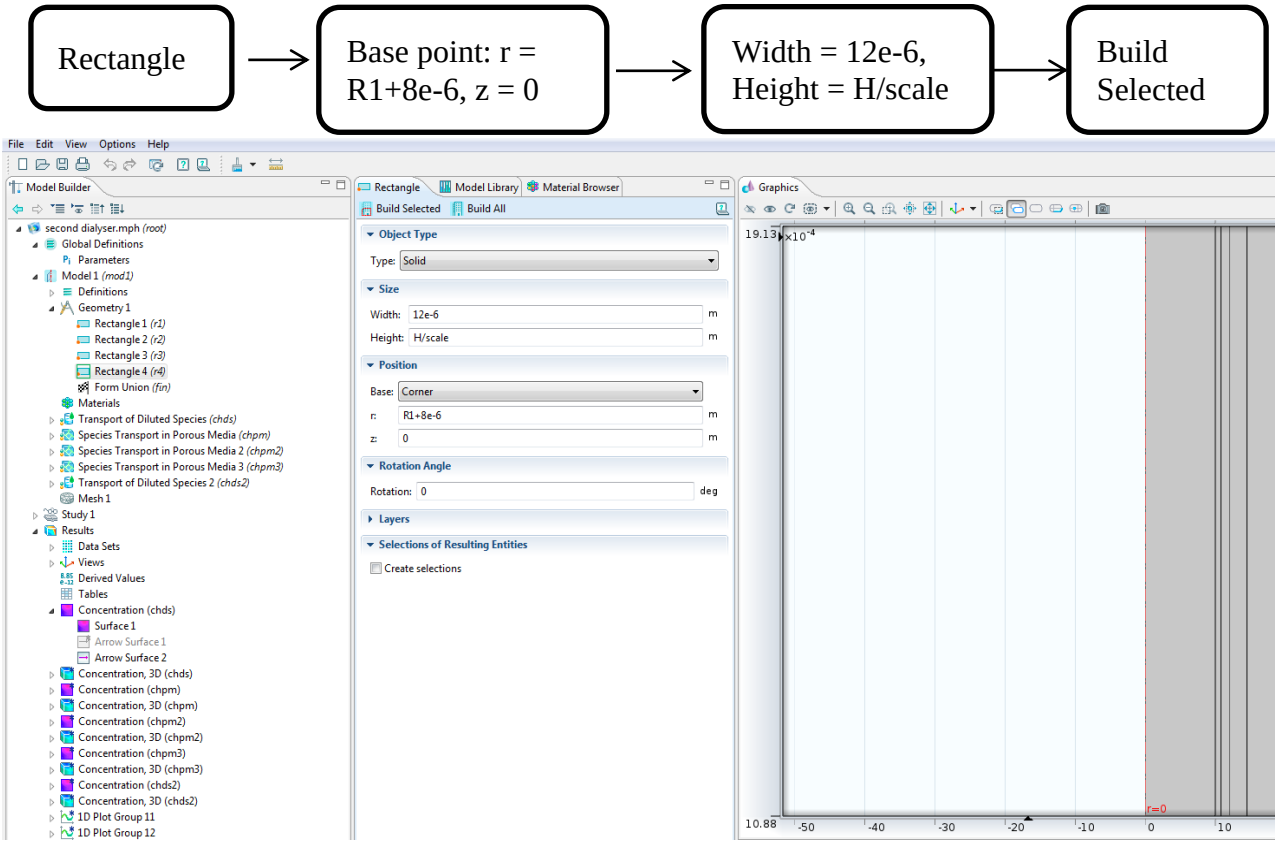
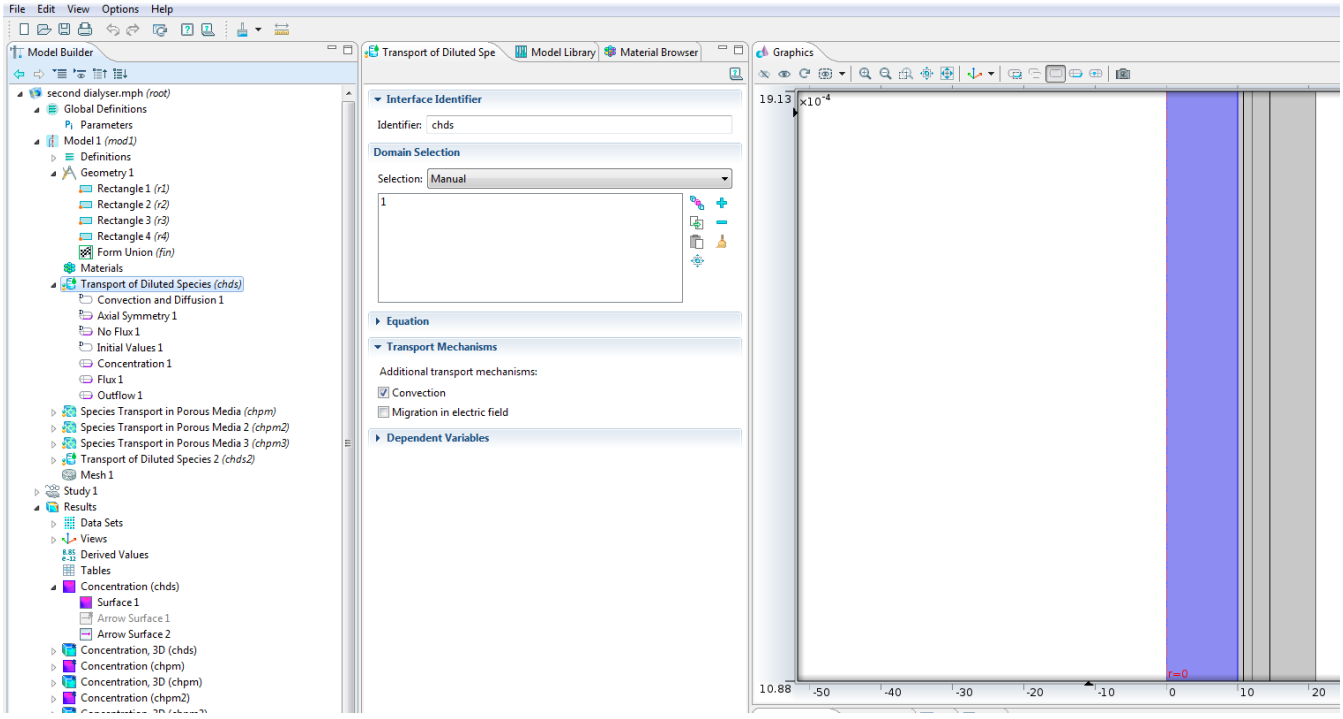
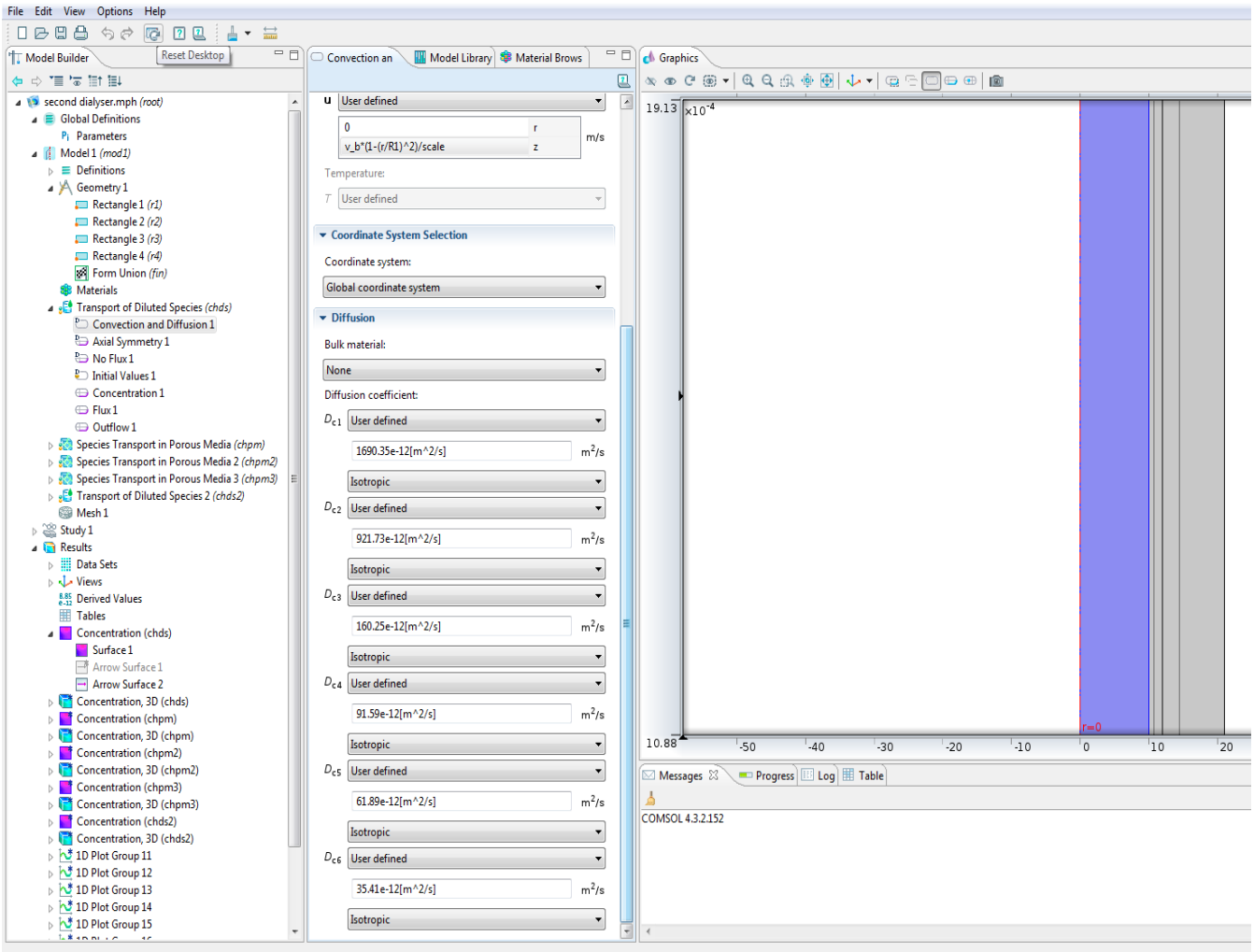
r=0



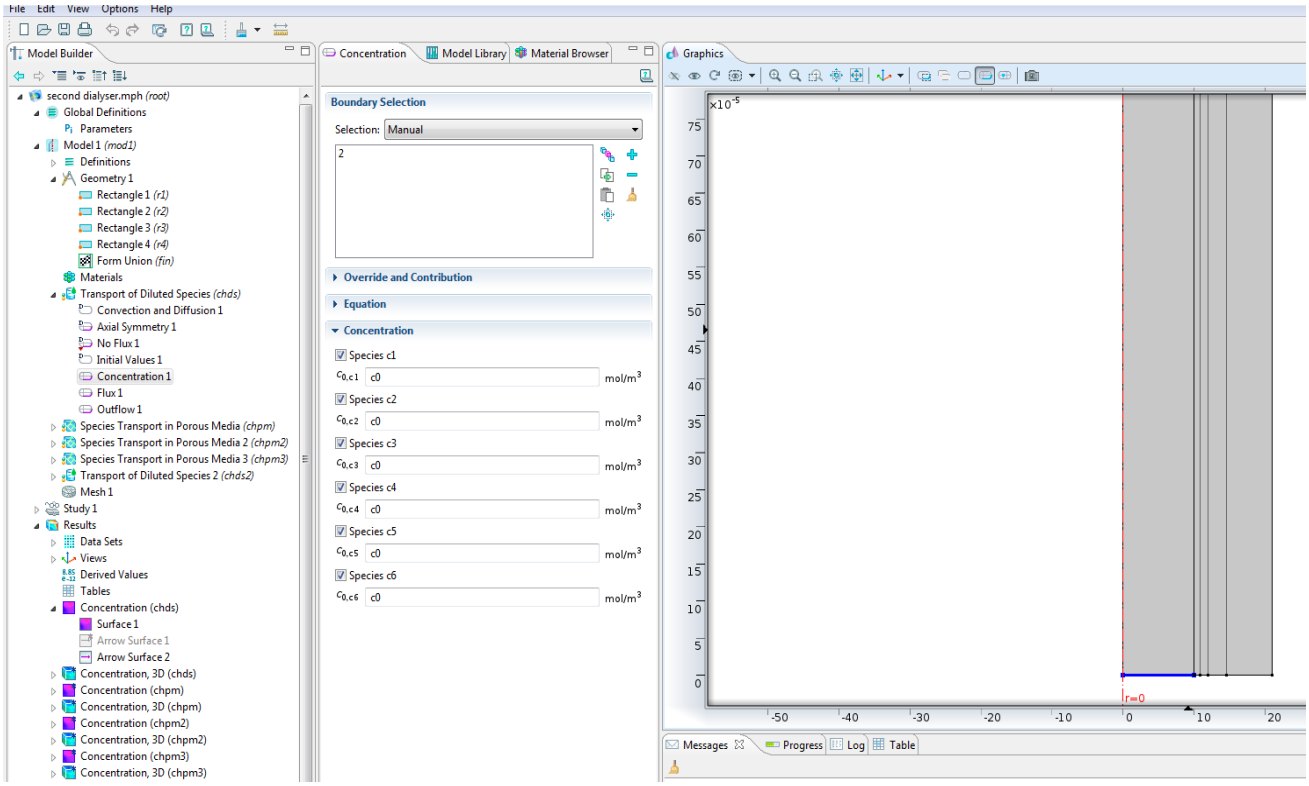
- **Transport of Diluted Species 1 (Blood domain):** Domain 1



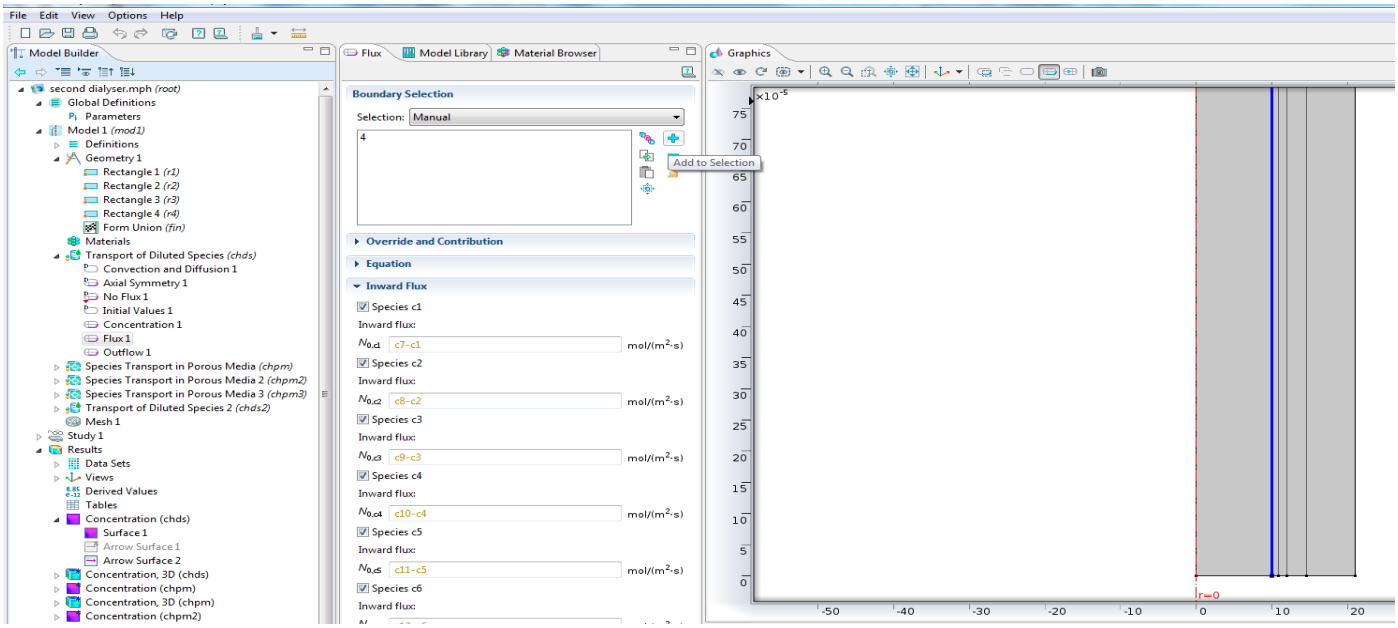
Convection and Diffusion → Velocity field (z component) = v_b*(1-(r/R1)^2)/scale → Values of diffusion coefficients (D_{C1}, D_{C2} ,D_{C3} D_{C4}, D_{C5}, D_{C6}) for six molecules



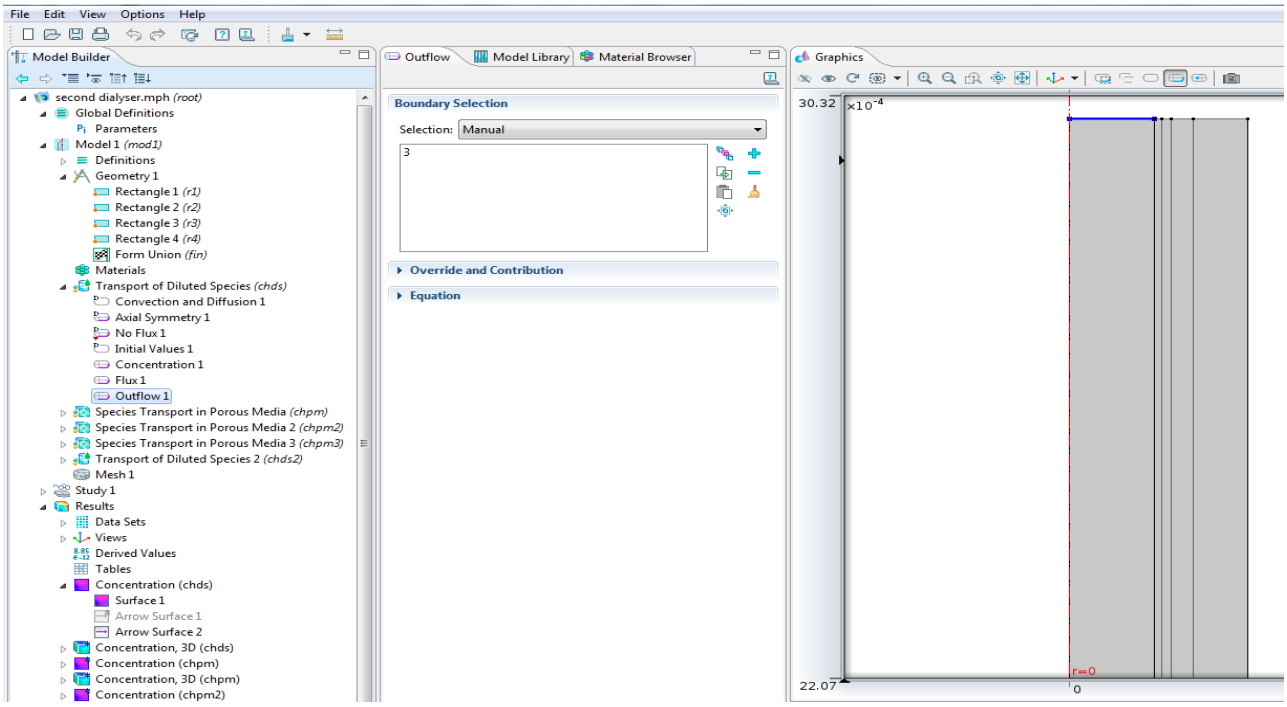
Select Boundary no. 2 as blood inlet → Concentration at inlet for six species is set to c0 = 1 mole/liter



Select Boundary no. 4 for outward flux → Expression for outward flux for each of the six species

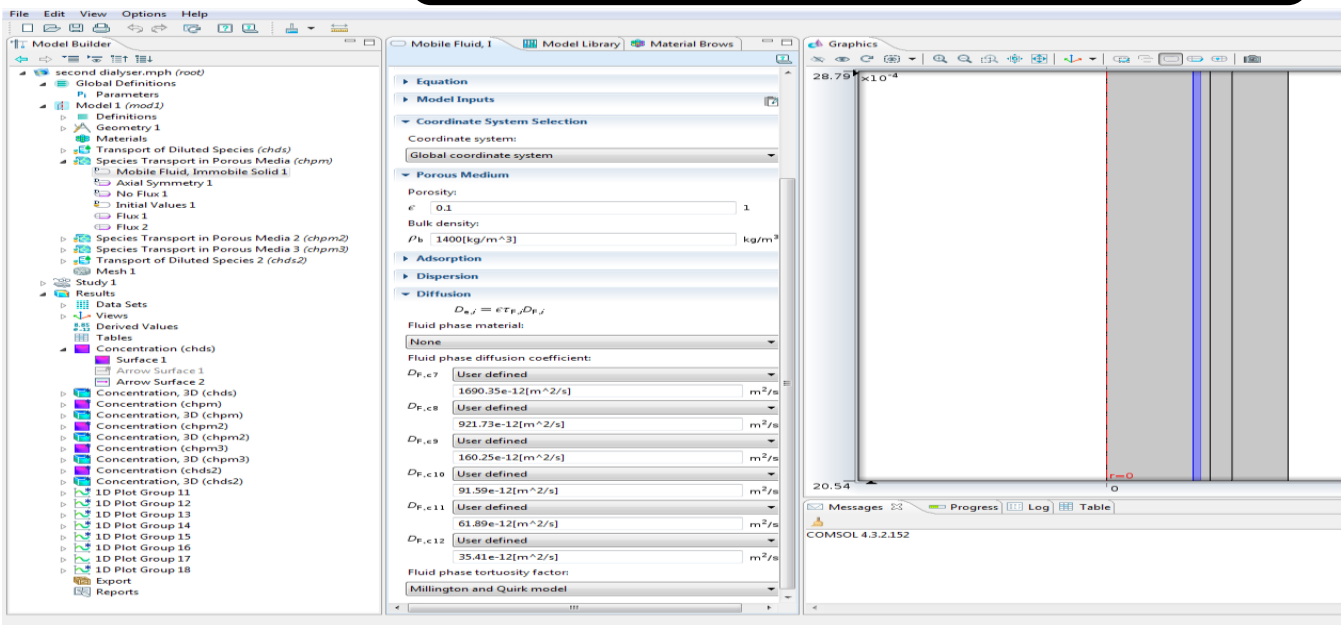


Select Boundary no. 3 for outflow of blood

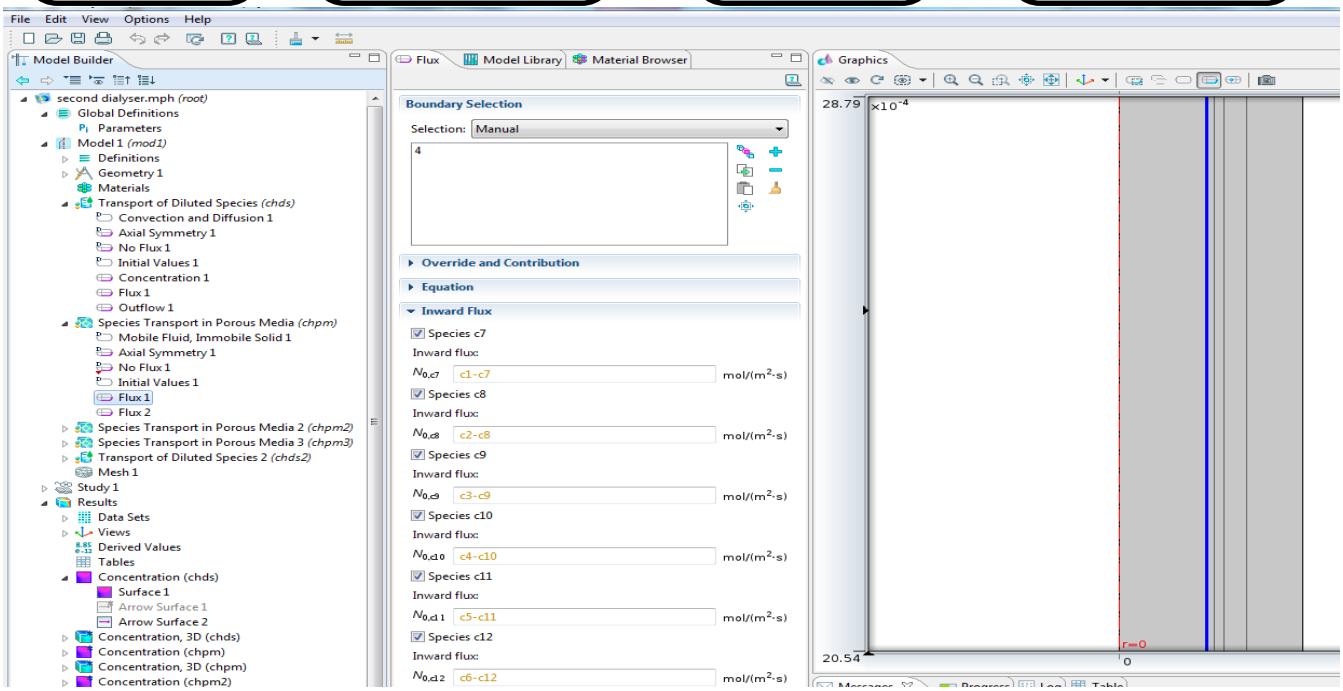


➢ **Species Transport in Porous Media 1 (First layer of dialyzer membrane):** Domain 2

Porosity, ε = 0.1 ⟶ Values of diffusion coefficients (D_{C7}, D_{C8}, D_{C9}, D_{C10}, D_{C11}, D_{C12}) for six molecules

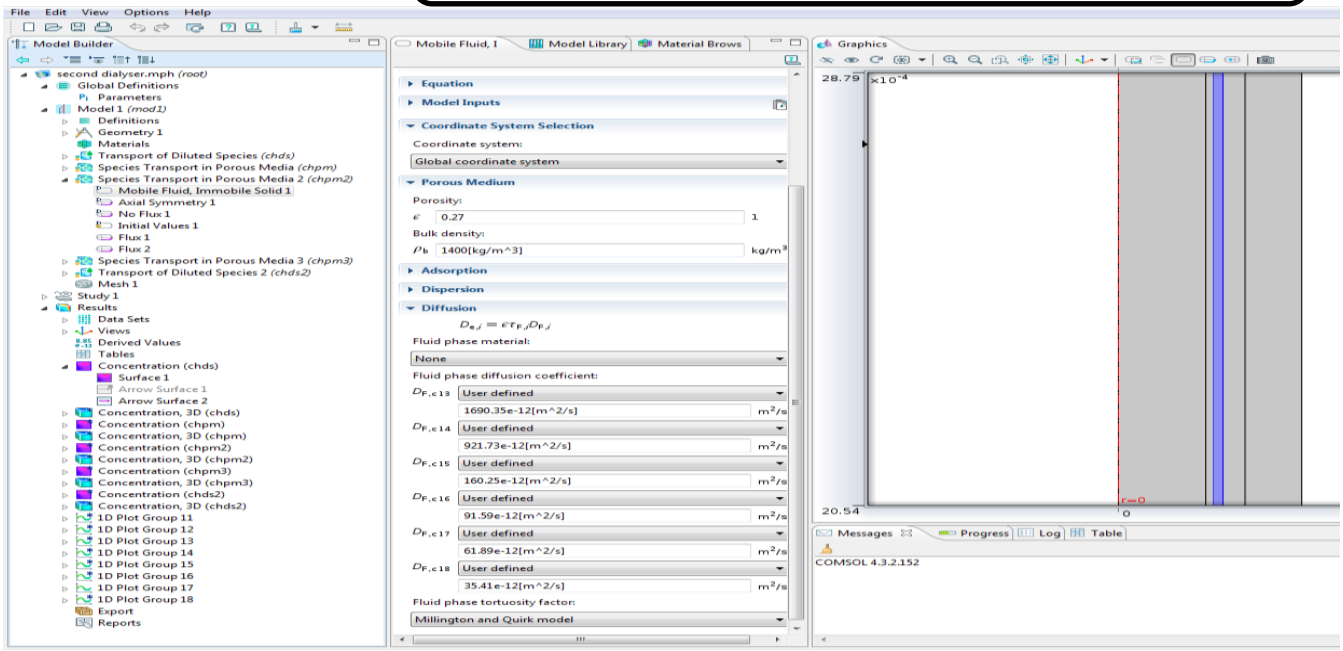


Select Boundary no. 4 for inward flux → Expression for inward flux for each of the six species → Select Boundary no. 7 for outward flux → Expression for outward flux for each of the six species

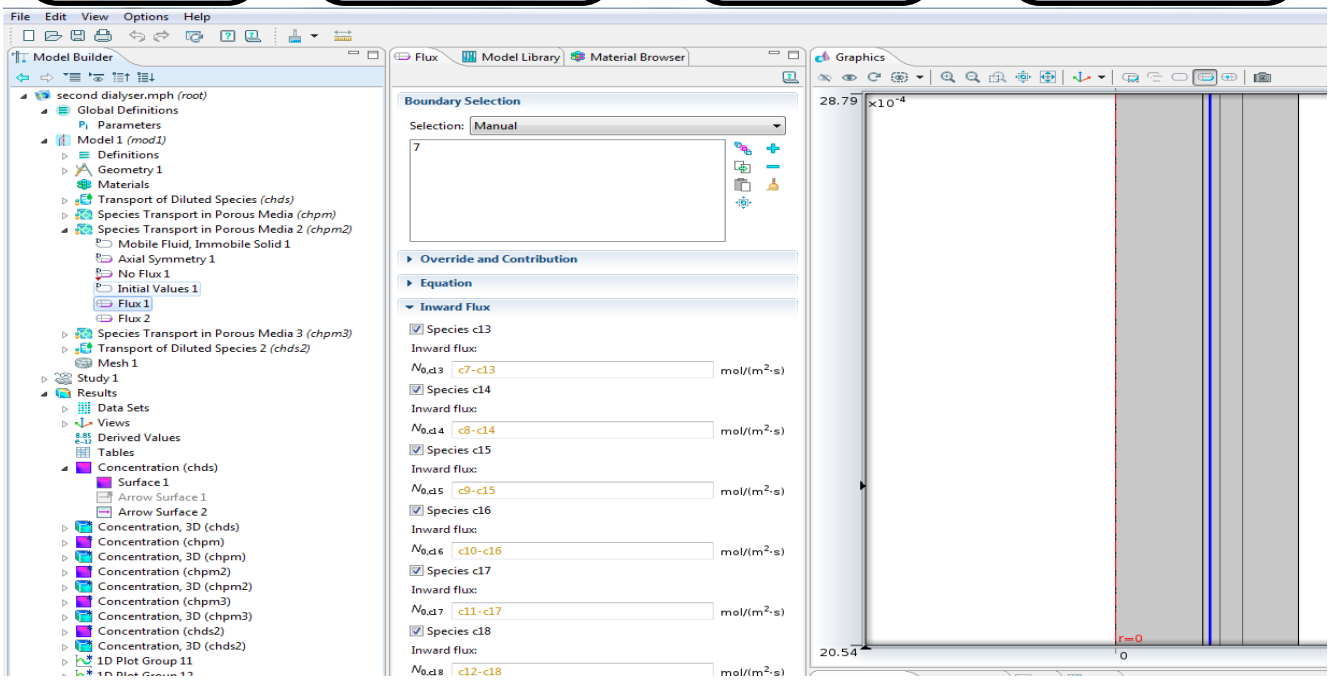


- **Species Transport in Porous Media 2 (2nd layer of dialyzer membrane):** Domain 3

Porosity, ε = 0.27 → Values of diffusion coefficients (D_{C13}, D_{C14}, D_{C15}, D_{C16}, D_{C17}, D_{C18}) for six molecules

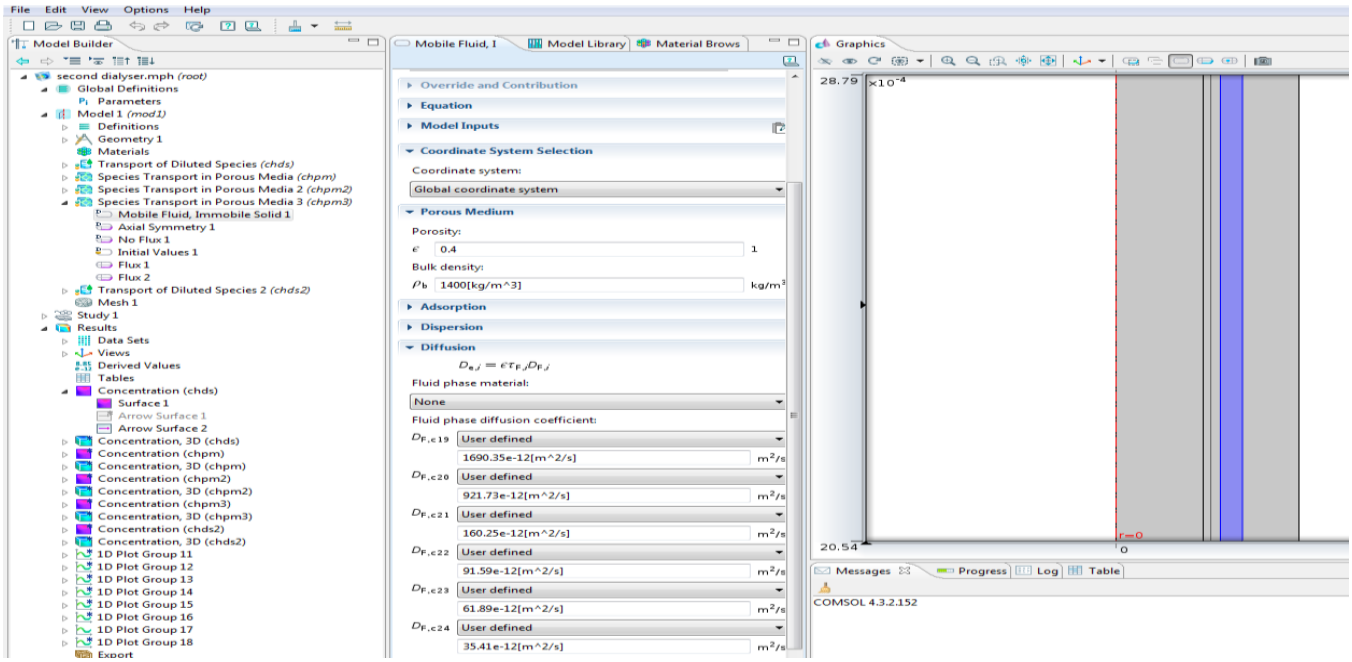


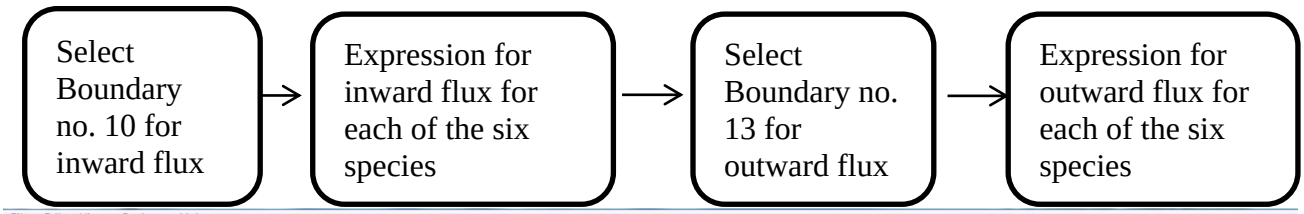
Select Boundary no. 7 for inward flux → Expression for inward flux for each of the six species → Select Boundary no. 10 for outward flux → Expression for outward flux for each of the six species

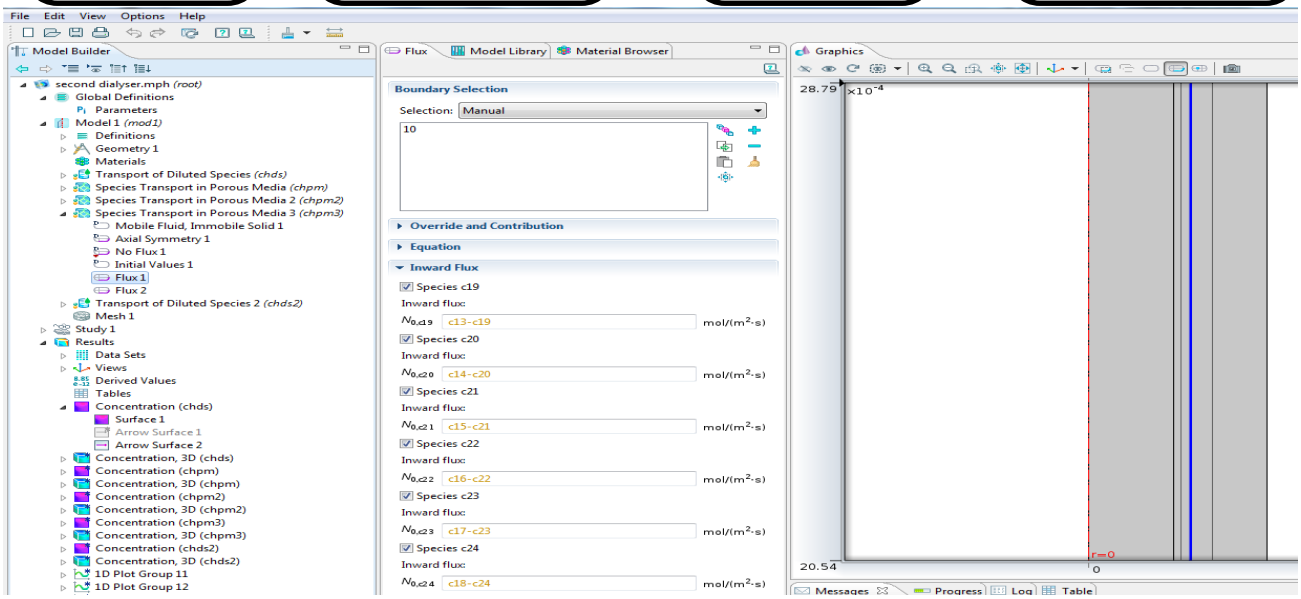


- **Species Transport in Porous Media 2 (Third layer of dialyzer membrane):** Domain 4

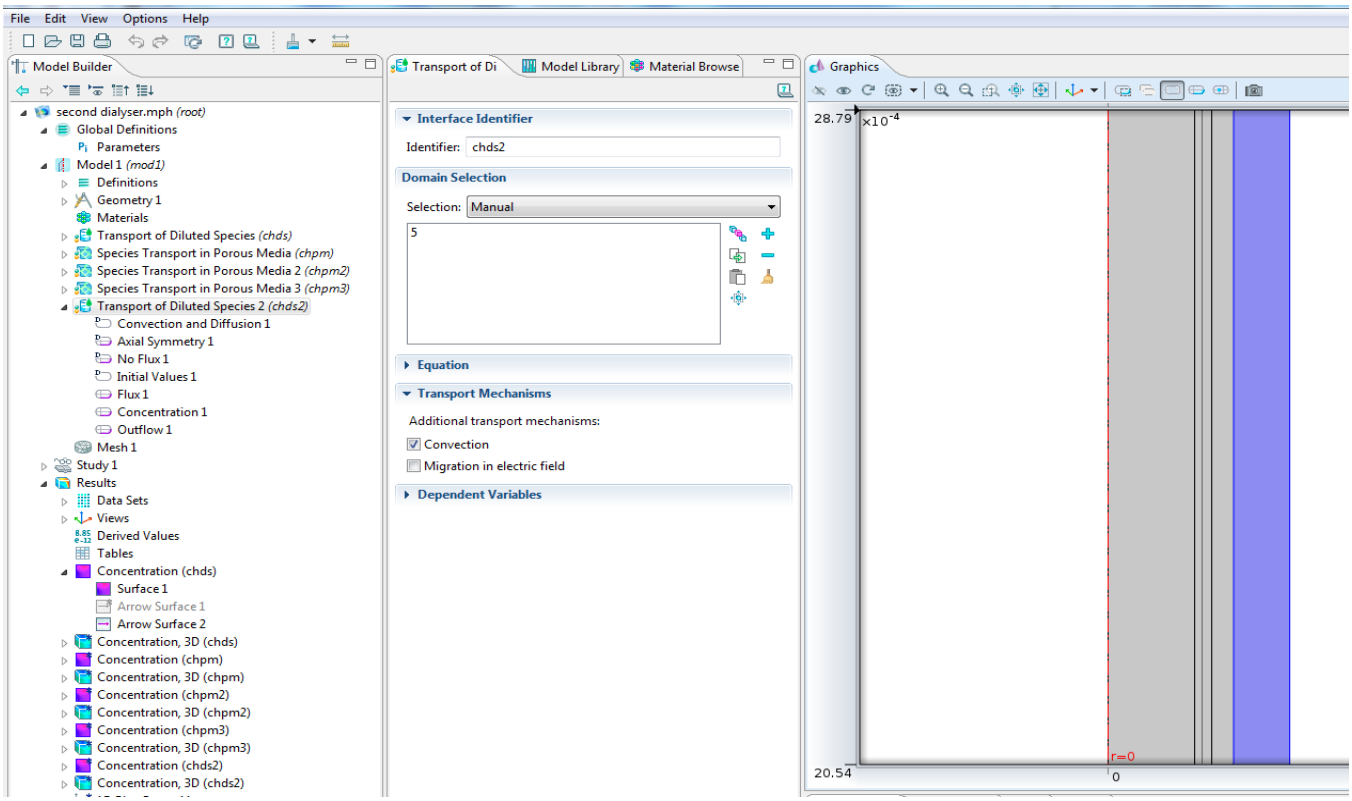
Porosity, ε = 0.4 → Values of diffusion coefficients (D_{C19}, D_{C20}, D_{C21}, D_{C22}, D_{C23}, D_{C24}) for six molecules



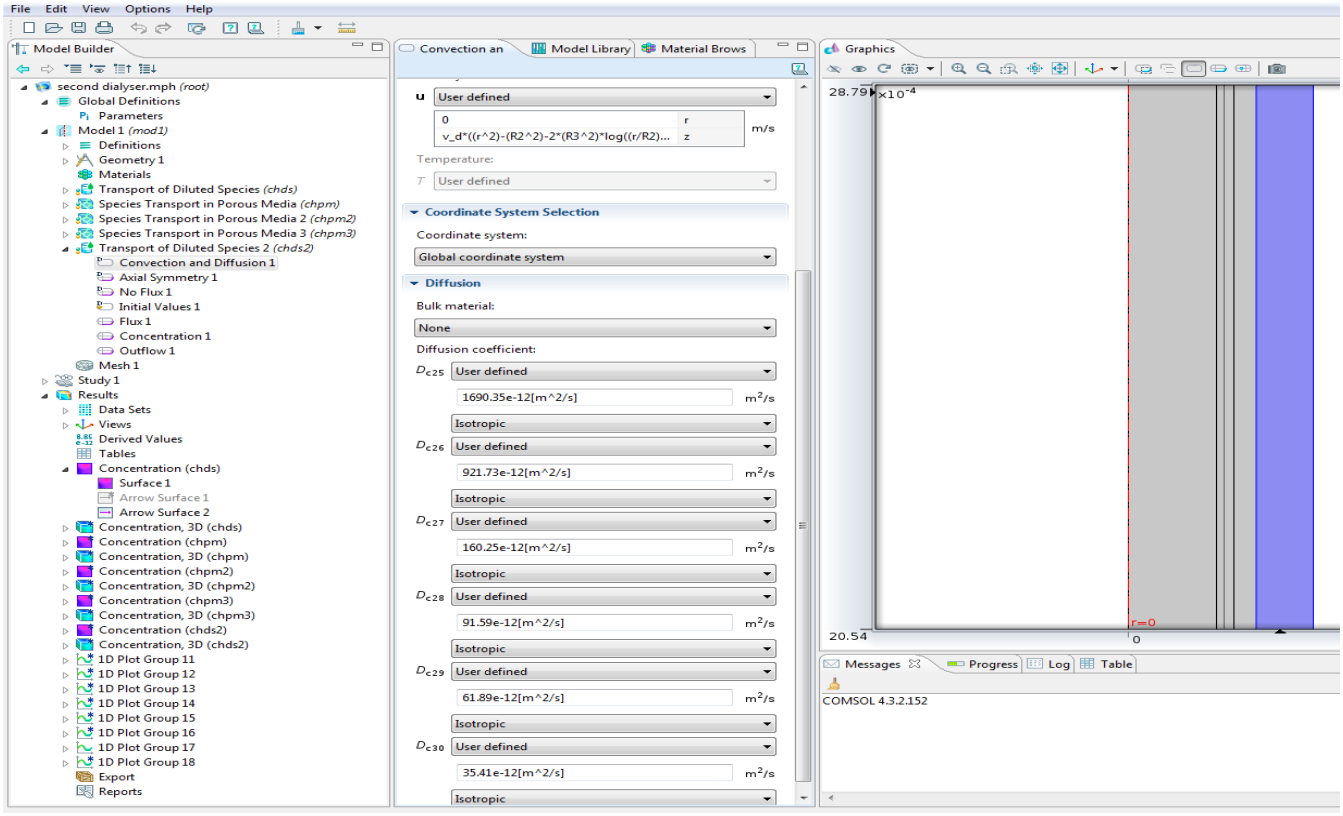




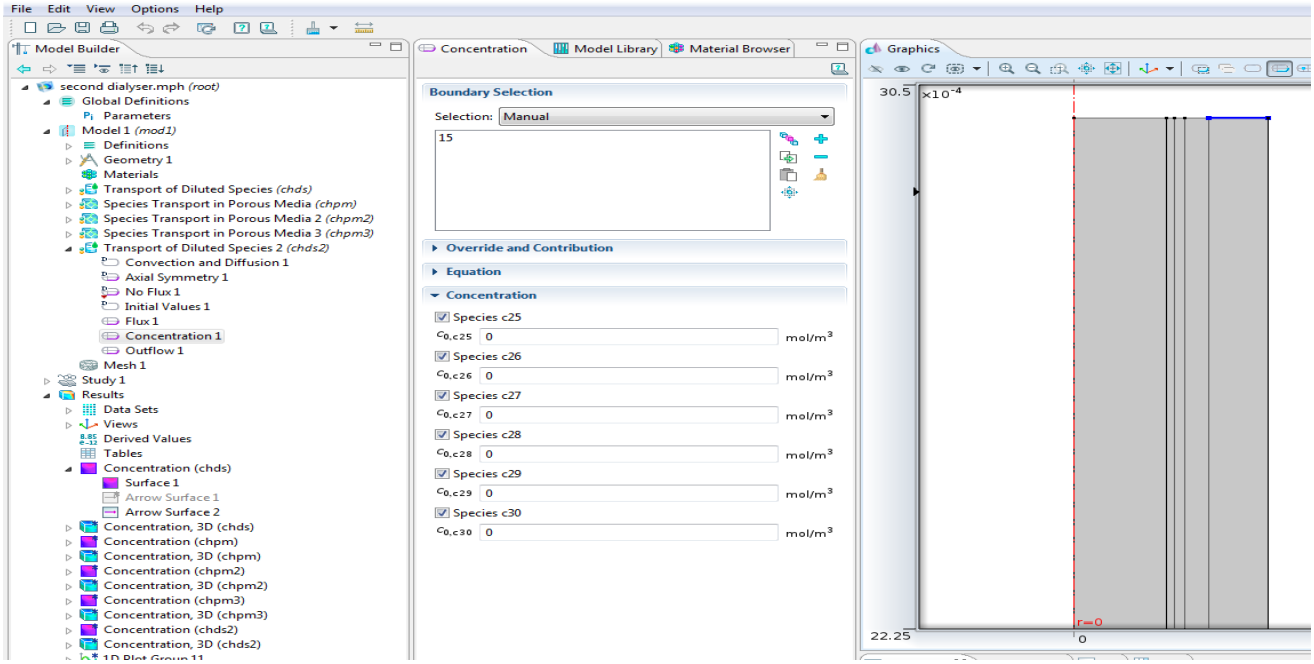
- **Transport of Diluted Species 2 (Dialysate domain):** Domain 5



Convection and Diffusion → Velocity field (z component) v_d*((r^2)-(R2^2)-2*(R3^2)*log((r/R2)))/scale → Values of diffusion coefficients (D_{C25}, D_{C26}, D_{C27}, D_{C28}, D_{C29}, D_{C30}) for six molecules



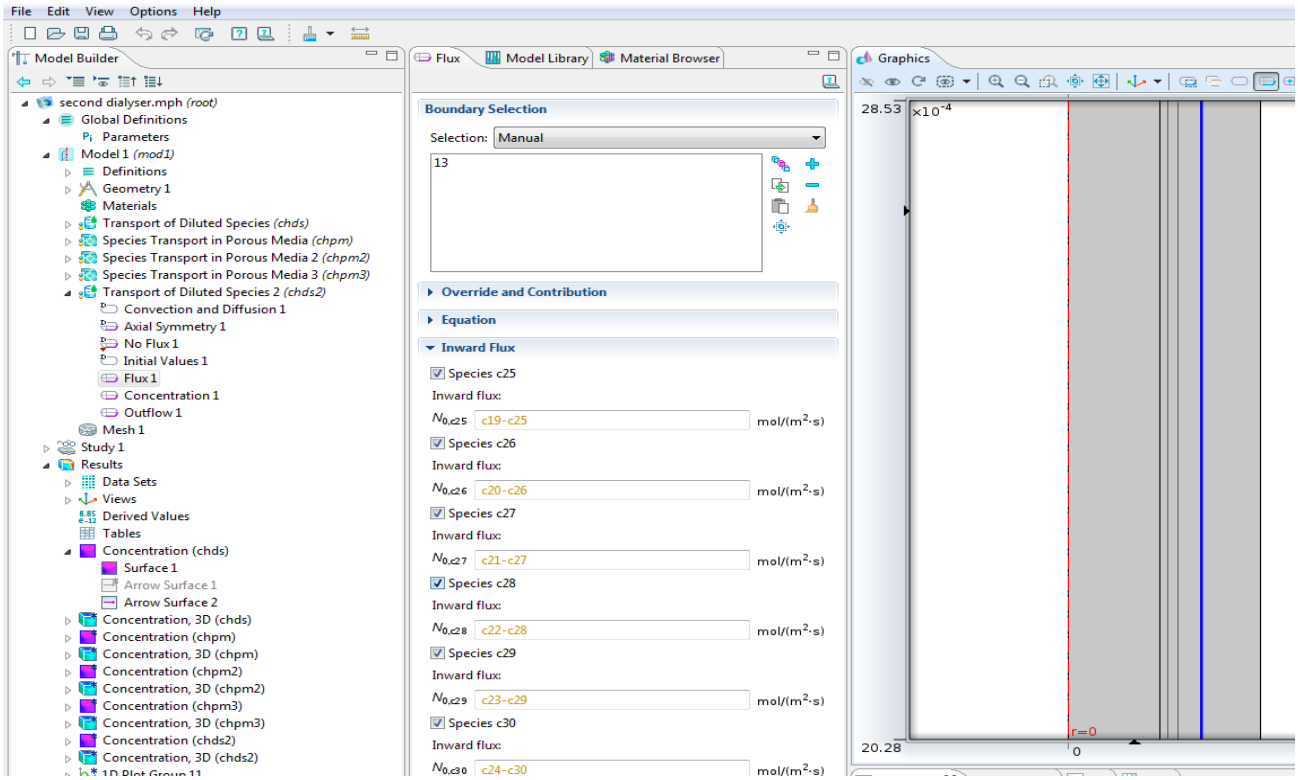
Select Boundary no. 15 as dialysate inlet → Concentration at inlet for six species is set to c0 = 0 mole/liter



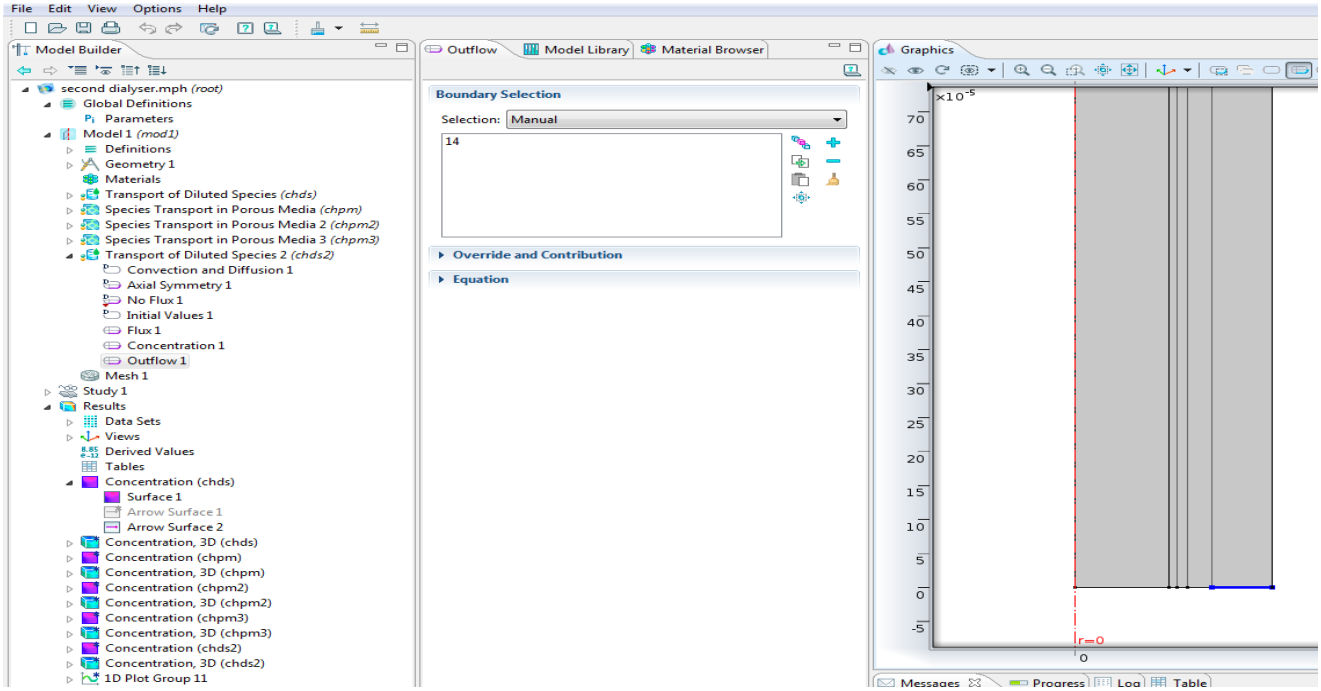
Select Boundary no. 13 for inward flux

→

Expression for inward flux for each of the six species

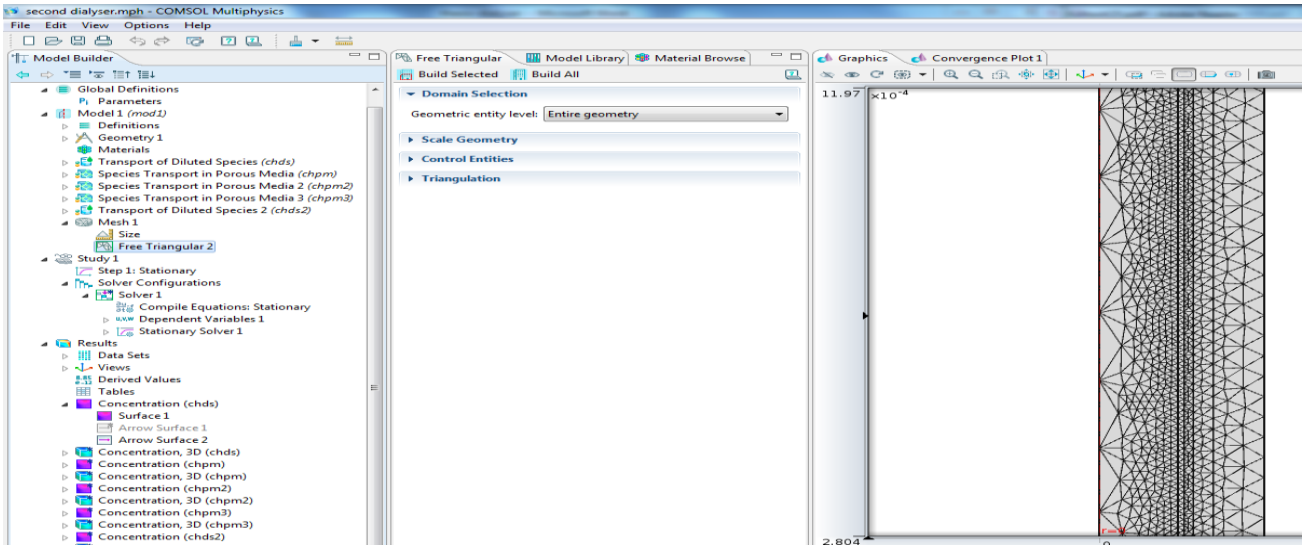


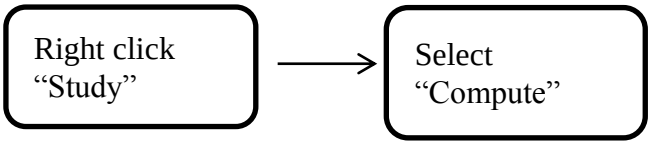
Select Boundary no. 14 for outflow of dialysate



- **Meshing and Solve**

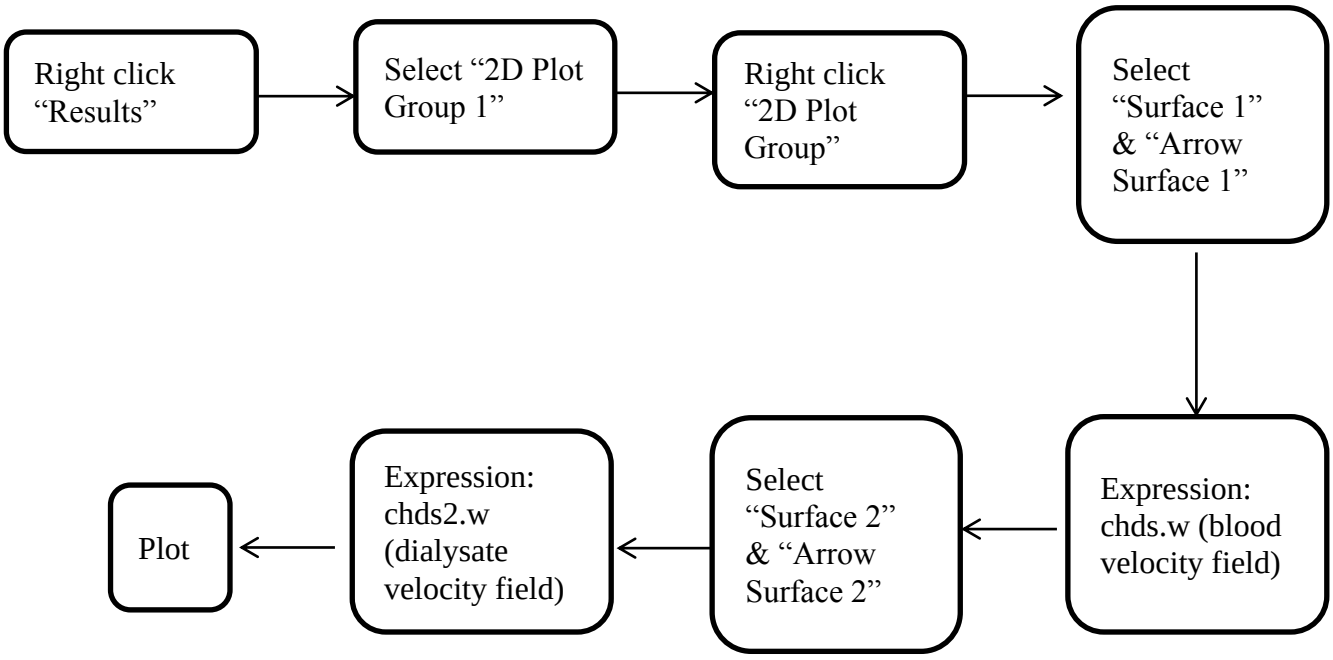
Right click "Mesh" → Select "Free Traingular" → Size: Normal

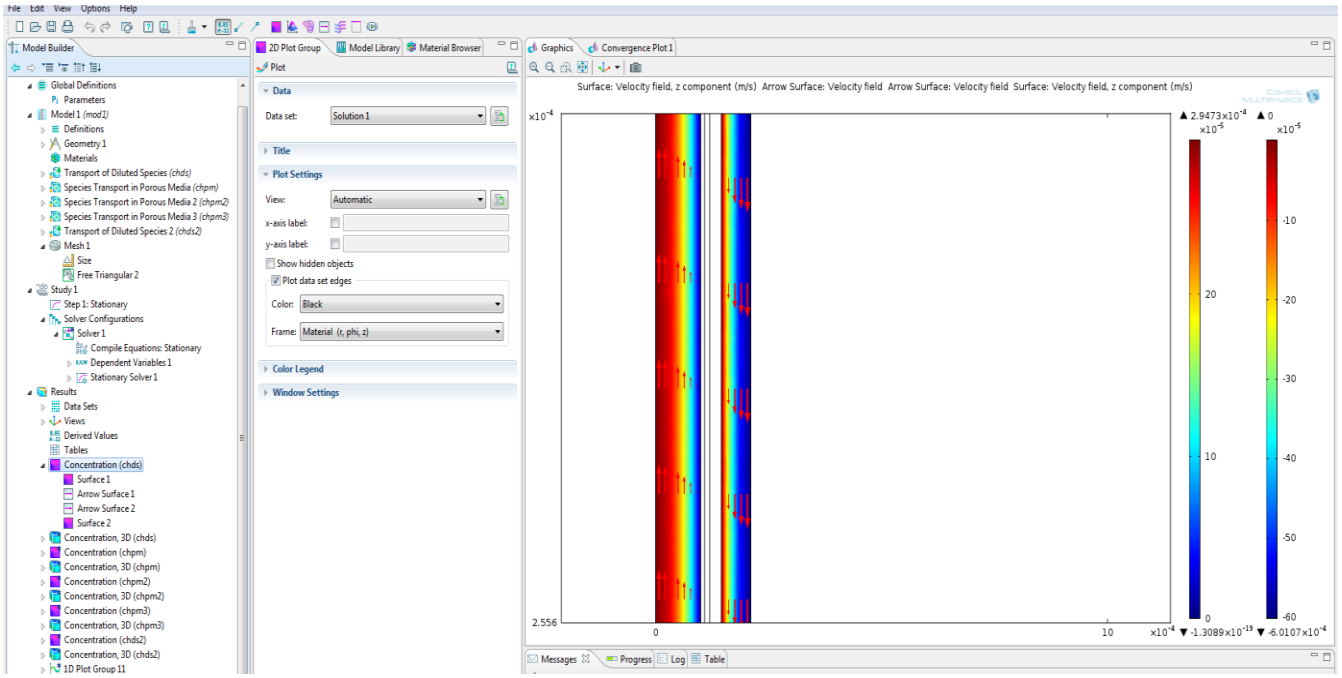




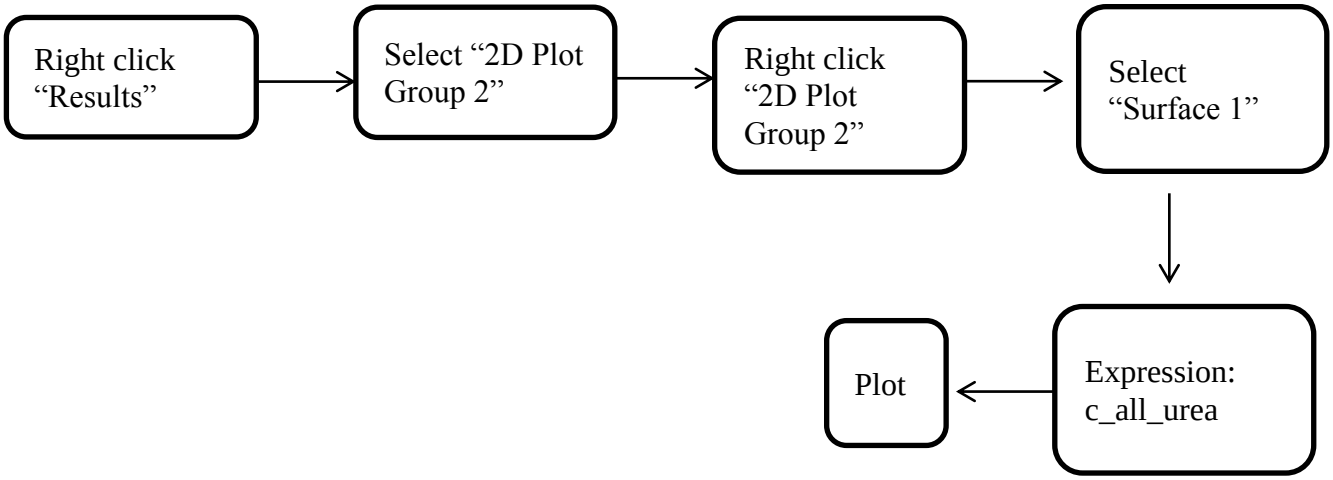
- **Post processing results**

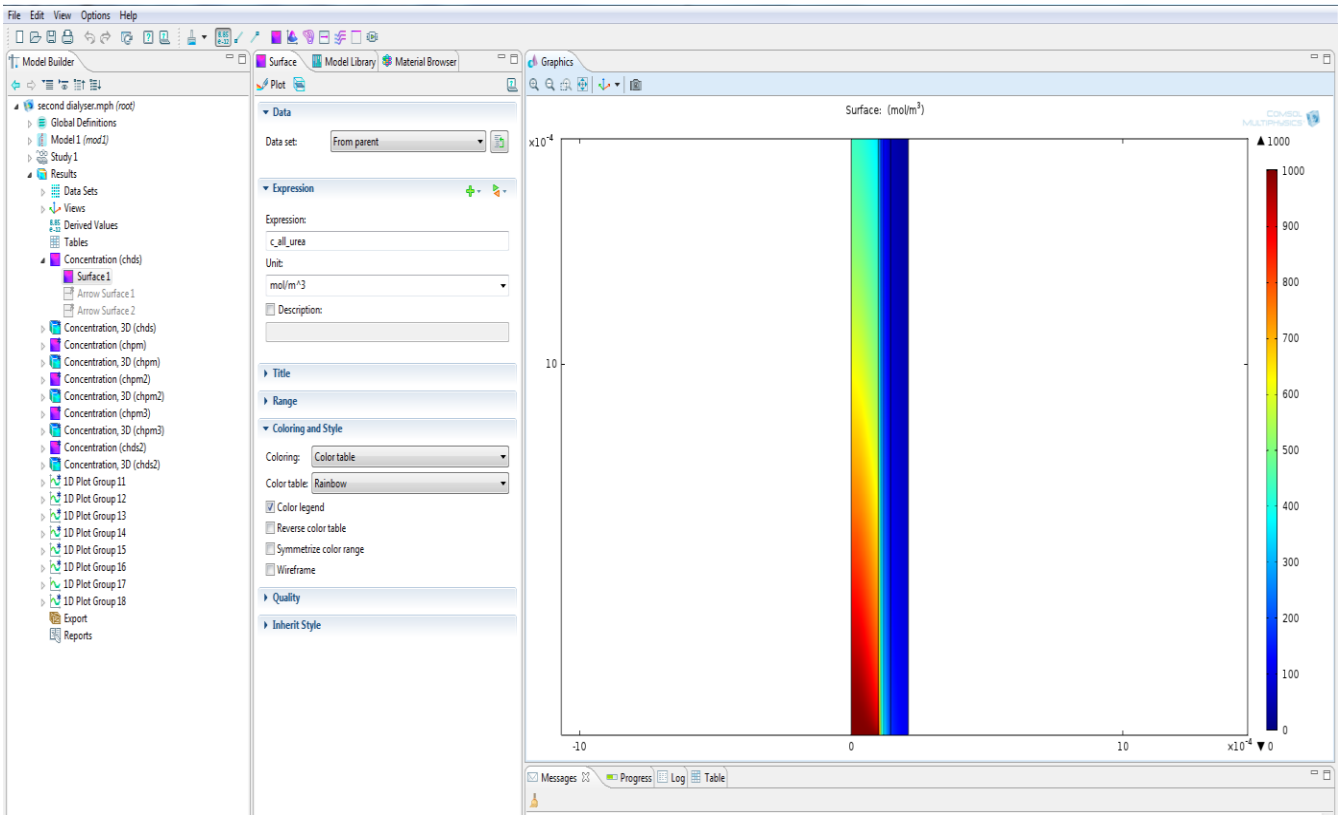
For velocity field:





For toxin (in this example Urea) concentration:





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