CSUMS Final Report, Spring 2011
Nanofiber Filtration System

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Abstract

Contaminated water is a largely growing problem worldwide. Many of the contaminants within the water sources can cause serious health problems for consumers. Using a nano-fiber filtration system to filter these contaminants has been shown to work well. The filter system works by exchange of the contaminant ion by the nano-fiber, and an exchange concentration of a benign, non-toxic ion is stripped out from the fiber. This project will numerically simulate a moving boundary model of the ion exchange of the fibers in cylindrical coordinates.

Contents

1 Introduction

Water sustainability is an up and coming problem facing the world. Water has always been thought of as an unlimited, clean source that will always be available. Although this has been true for a long time, this era of unlimited water is coming to an end. The water sources that have been available have become contaminated and or now gone. There are many programs now started by the EPA to help manage, protect, and restore natural water sources.

Typically water is treated at a water treatment plant in the US and the EPA has a list of standards and requirements for the water leaving the plant to the public. The water goes through a series of screenings, flocculation and coagulation, sedimentation, filtration and finally disinfection. The water goes through many series of settling basins, sand filters and disinfection systems to remove and clean water. A large amount of people use wells which are not regulated and the well users are required to maintain the quality of water.

WIth water sources becoming increasingly more contaminated it is a problem, since treatment is not designed to treat chemicals and metals to be removed from the water.

Although, the US is starting to face many water problems many countries have never had such water treatment systems to begin with. problems are worldwide issues and many sustainability options are available to clean and treat contaminated water. Some of these options include reverse osmosis, filtration methods, and ion exchange methods.

My project will focus on the innovative nanofiber filtration system. Nanofibers will be covered by a non-beign covering on the fiber which will be how the ion exchange will occur. When these covered fibers are placed into a contaminated water source the non-beign will release a non toxic ion such as chlorine, and the contaminate will be absorbed into the fiber.

2 Motivation Behind the Project

When I first started CSUMS I started working with finite elements and began learning basic Matlab coding and commands. The past few semesters I have started getting involved into Environmental Engineering classes and took a strong interest in the topic of study. I wanted a project that had some sort of meaning for me behind it but as well as a computational based project. When I learned about this project I was very excited to learn more about it. The project was very much independent based and fit a topic of study of interest. I learned a lot about the water treatment method. I was very interested in the methods that this method is all ready

3 Methodology

$$\frac{\partial \bar{c}}{\partial} = \frac{\partial^2 \bar{c}}{\partial \gamma^2}$$

3.1 Boundary Conditions

$$1. t = o, \bar{c}(0, \gamma) = 0$$
$$2. \gamma = \gamma_o, \frac{\partial \bar{c}}{\partial \gamma}(0, \gamma_o, t) = 0$$
$$3. \gamma = R_o, \bar{D}\frac{\partial \bar{c}}{\partial \gamma}(R_o, t) = K_f(c(t) - \frac{\bar{c}}{k}(R_o, t)))$$

Where:

$\bar{D}$=diffusivity of fiber K_f=Mass transfer coefficient of the film at the interface

c(t)=bulk concentration

$\bar{c}(R_o, t)$=concentration at $\gamma = R_o$ at the surface of the fibers

k=Partition coefficient

R_o=Outer radius

r_o=Inner radius

γ= undefined

γ_o=undefined

3.2 Method of Lines

The method of lines is a technique for solving PDEs in which all but one dimension is discretized, often used for solving time dependent parablolic PDEs. The method first discretizes the spatial derivative and only leaving the time variable continuous. In this case the procedure of solving the time dependient parabolic PDE numerically was used. When the spatial derivaties are no longer in explicite terms of the spatial independent variable only time remains and the system is able to be solved numerically.

3.3 ODE Solver

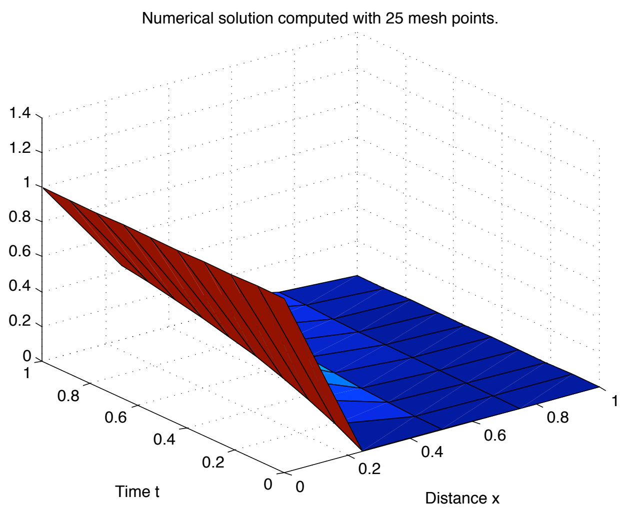
The code has many different commands used to fully write the code. One of the commands was an ODE solver which I looked into. The code was using an ODE45 to solve the ordinary differential equation given above. When I looked into these different solvers there are a lot of different solver methods available. I was curious as to why ODE 45 was used in the code opposed to other available.
The ODE given in the original problem is a non-stiff equations which could use the following ODE Solvers:
ODE 23 Low Accuracy
ODE 45 Medium Accuracy
ODE 113 High Accuracy (13th order)

These ODE solvers have different levels of accuracy depending on the ODE that is being used. Most of the time ODE 45 will work accuracy for the method needed for this problem. ODE 45 implements a version of Rung-Kutta(RK) 4th/5th order method. More advance ODE solver such as ODE 113 are multistep solvers, which work well if a stringent error tolerance or solving a computationally intensive ODE file. ODE 113 uses variable order Adams-Bashforth Moulton solver.

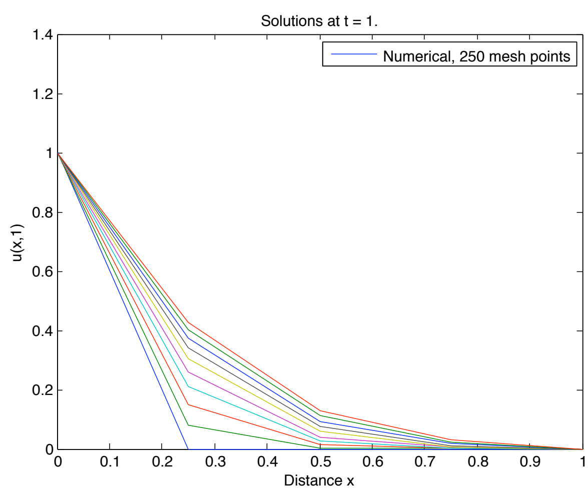
The ODE file I was given for my problem is for a non-stiff problem but there are also other solvers to solve stiff systems where the ODE numerical error compounds dramatically over time.

4 Numerical Results

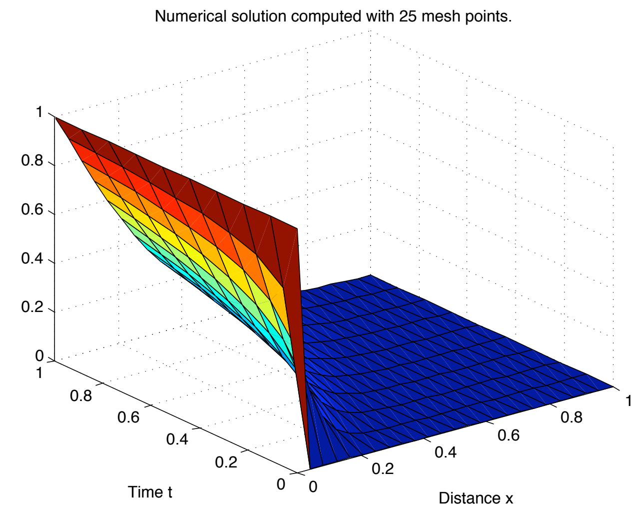
Graph 1.1



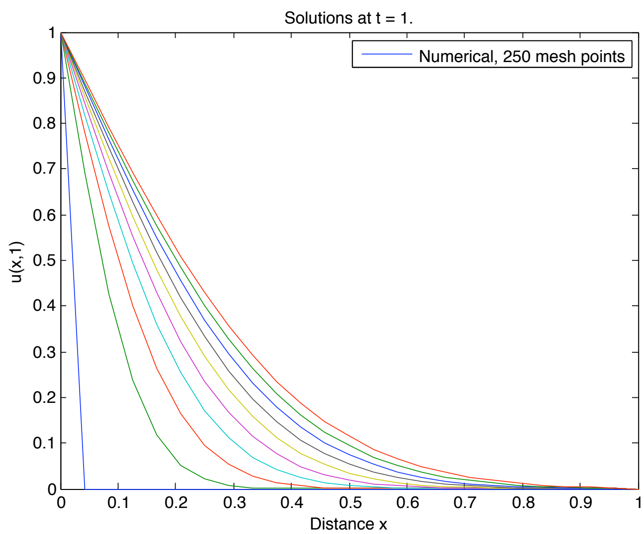
Graph 2.1



Graph 1.2

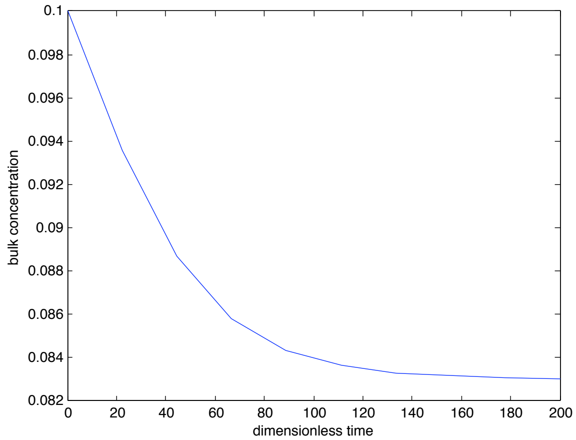


Graph 2.2

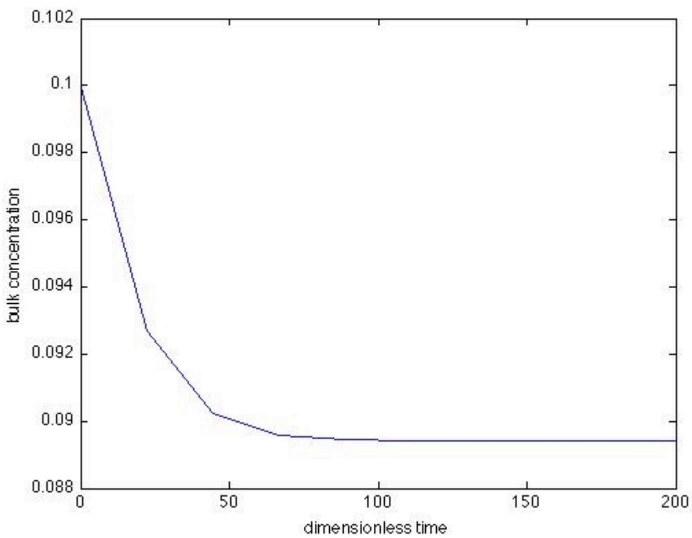


Graphs 1.1 and 2.1 represent the same things except there is a larger time space in the Graph 2 series. The larger time spacing shows that it does provide more points of data collection and can numerically analyze the data more fully. Graphs 1.1 and 2.1 are a 3D graph of the conctration in the fiber. As you approach the inside of the fiber the conctration is going to be less then the portion that is the very outer most layer. Graphs 1.2 and 2.2 are a portion section of the previous graphs which are a little bit easier to see then the 3D graphs because it is removing time from the element. As the radius distance increases the conctration at that particular point deacreases. Since the distance x=0 is the very most outer layer would be the highest level of concentration while the inside would have little to no conentration levels. Comparing the two graphs the more time steps that are used the smoother the curves appear

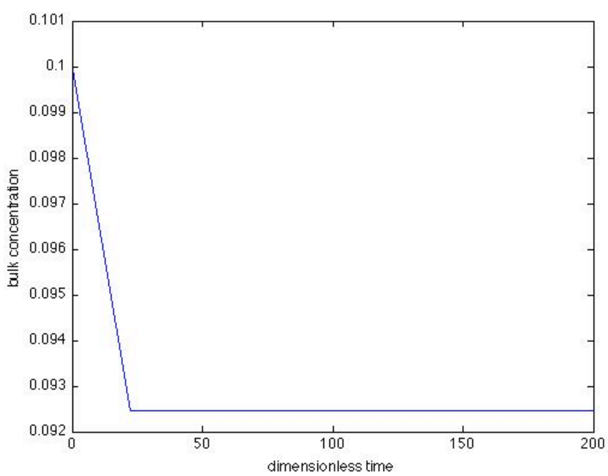
Graph 3.1



Graph 3.2



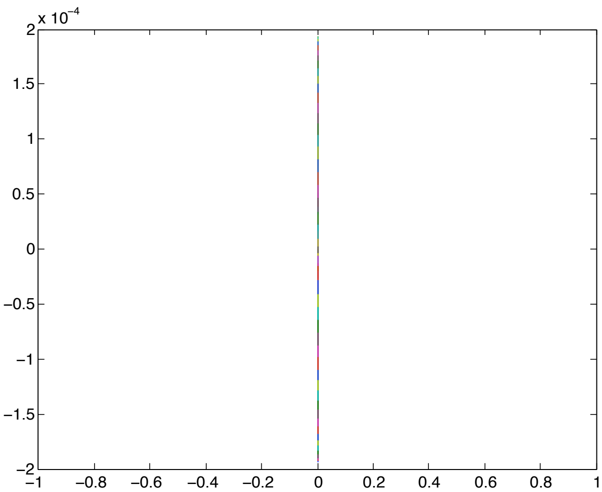
Graph 3.3



Graph 3.1-3.3 show the bulk concentration in the water vs. time. The water initially has a contration of the contaminate once the fibers are placed into the water the contaminate instantly begins to be absorbed. Graph 3.1 uses 25 time

steps, Graph 3.2 uses 100 time steps and Graph 3.3 uses 500 time steps. With each increase of the time step the time to complete the process increaded which was very expected. I would expect as each time step was incraesed the curve would continue smoothing out. Instead when 500 time steps was conducted a very sharp graph was obtained. It seams to level out at about 0.0935 where as for 100 time steps it levels out at about 0.09.

Graph 4



Graph 4 shows the error plot when comparing the ODE 45 to the ODE 113. As you can see the line is very straight with little to no variation from the x=0. The would indicate that ODE 45 would be a very sufficient method for this specific method. When I was comparing the two methods I plotted both methods then subtracted one from the other and ploted the result.

5 Conclusion and Future Work

5.1 Future Work

This project has a lot of similarities to the finite element work that I had been working on the past few semesters. There are a lot of practical applications of this method which are all ready being used. Tea bags filled with these nanofibers are being used in undeveloped countries to be able to filter out water available. This water that is filtered is not perfectly clean but it a huge improvement to what is currently available. The future work of this project would be to further investigate the different conditions that optimize the system. This is my third semester in CSUMS and will be graduating this May. I have really enjoyed working on this project and feel like it is exactly what I would like to do once I graduate. Working with the sustainability of water is something we talk about in class and we go over water treatment methods but I do not exactly get to see the computational side of it. I hope I will be able to use my skills I have learned in this program and apply it to a future project that I will work on. I have learned a lot of skills that I would not have normally learned. My Matlab skills and LaTeX skills have improved greatly over the three semesters. Personally I have taken a lot out of this project adn think it will help me expand my way of thinking of methods.

6 Appendix

Refer to additional documents for MatLab codes.

7 Acknoledgements

I would like to thank my advisor Dr. Sengupta, Sukalyan for assisting me with the code provide to me and learning about the topic. I would also like to thanks all the CSUMS staff for giving me such a wonderful opportunity to be a part of regardless of what I ended up pursuing as a career I know I will be able to accomplish anything. I have gone through such a hard time these past year and I never thought I would meet people that would be so supportive and genuinely caring to me.