

2010-01-01

# A Variational Approach To Non-Newtonian Flow In Angular Pores: An Application To Enhanced Oil Recovery

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**A VARIATIONAL APPROACH TO NON-NEWTONIAN FLOW IN  
ANGULAR PORES: AN APPLICATION TO ENHANCED OIL  
RECOVERY**

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by

Nithin Kavoori

2010

A VARIATIONAL APPROACH TO NON-NEWTONIAN FLOW IN ANGULAR  
PORES: AN APPLICATION TO ENHANCED OIL RECOVERY

by

NITHIN KAVOORI, B.S.

THESIS

Presented to the Faculty of the Graduate School of  
The University of Texas at El Paso  
in Partial Fulfillment  
of the Requirements  
for the Degree of  
MASTER OF SCIENCE

Department of Mechanical Engineering  
THE UNIVERSITY OF TEXAS AT EL PASO

December 2010

## **Acknowledgements**

I would like to thank Dr. Vinod Kumar, director of the Multiphysics Multiscale Computational modeling lab, for giving me the opportunity to perform this research and for the assistance he provided throughout my graduate studies. Dr. Kumar was always available to provide insight and advice for this project. He has been there for me as a good friend who was with me most of the time while I was working on the project. He has taken the effort to understand my problems and support me, and to bring the best in me. I would also like to thank my other committee members, Dr. Ramana chintalapalle and Dr. Leticia Velazquez for their assistance during the writing of this thesis.

I extend my gratitude to Dr. Chris Harris, MA, DPHIL (Oxon) the participating member of the project. Any amount of gratitude expressed to him will remain insufficient.

Several other people in the department deserve recognition. I would like to thank Fan Chen and Kiran Kumar, my fellow co-workers at the laboratory for their invaluable assistance throughout the length of the project.

Finally, I would like to thank my family for their support during my graduate studies, especially my parents, who have made my education a high priority from the beginning. Without them, I would not be where I am today.

This thesis was submitted to the supervising committee on December 2010.

## **Abstract**

With an alarming rise in carbon dioxide ( $\text{CO}_2$ ) emission from anthropogenic sources,  $\text{CO}_2$  sequestration has become an attractive choice to mitigate the emission. Some popular storage media for  $\text{CO}_2$  are oil reservoirs, deep coal-bed, deep oceanic-beds. These have been used for the long term  $\text{CO}_2$  storage. Due to special lowering viscosity and surface tension property of  $\text{CO}_2$ , it has been widely used for enhanced oil recovery. The sites for  $\text{CO}_2$  sequestration or enhanced oil recovery mostly consist of porous rocks. In this thesis work, I focus on understanding the flow through porous at pore-level using variational approach.

Variational approach is a method to approximate analytical expressions for computing flow conductance through various cross section pores. Variational method approach is a skillful technique enabling us to account for the physical processes developed at the pore scale. Here, I focus on triangular and circular cross section pores because theoretical expressions for these two geometries are possible. The variational approach allows an extension at the fluid to fluid interface concerning simple free-slip or no-slip boundary conditions that can minimize the computational efforts. The approach also allows us to study non-Newtonian fluid flows.

In this thesis, I developed a single-phase flow conductance model for the triangular and circular cross-section of a pore and validated variational results against theoretical and empirical formulations for both Newtonian and non-Newtonian flows. I observe that variational formulations gives very accurate results, provides an alternative to, if available, theoretical solutions and hence can be extended to study real life applications.

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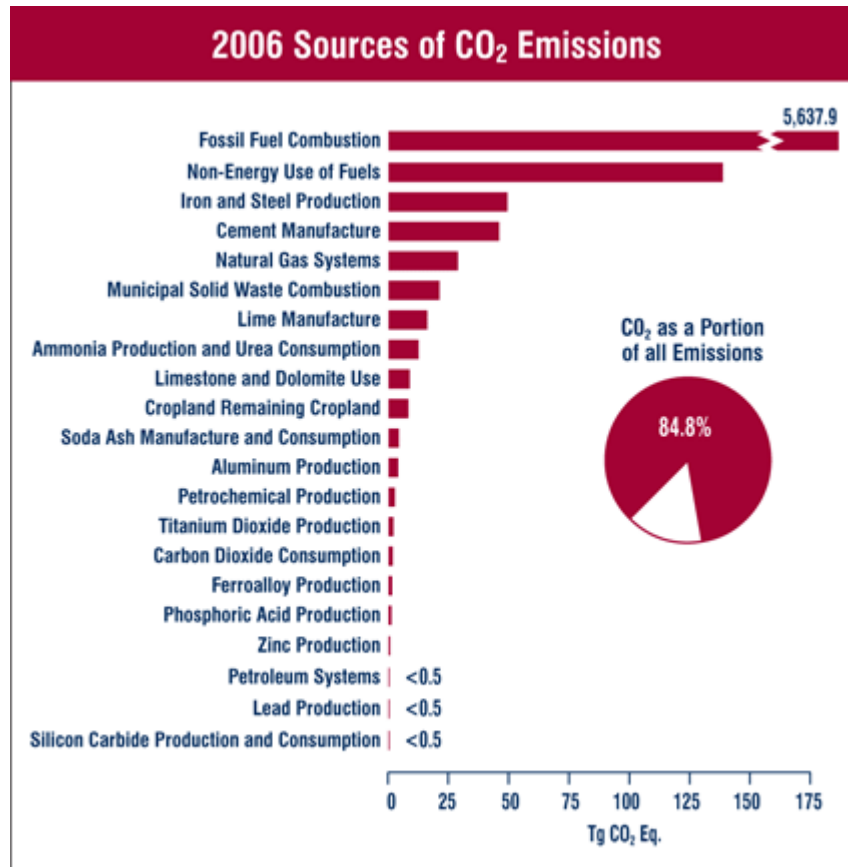
## **Chapter 1: Introduction**

Global warming is a well identified phenomenon for the rise in the average temperature of the planet. Greenhouse gases are the main contributors to the increase in the average temperature. Amongst all the greenhouse gases carbon dioxide (CO<sub>2</sub>) is the most common and principal agent of causing the global warming effect. CO<sub>2</sub> is one of the critical greenhouse gases and hence one of main source for global warming (Keeling & Whorf, 1998; Metz, Davidson, Coninck, Loos, & Meyer, 2005). Its enormous emission into the atmosphere results in a series of global problems such as warming of the climate. The state of Texas emits more CO<sub>2</sub> than any other state in the U.S (Brenstein, 2008). A large fraction of emissions are from industrial usage such as transportations and power-plants. A large CO<sub>2</sub> presence in atmosphere as a result of excessive coal-burning for example can cause acid rain and hence deforestation (Metz, Davidson, Coninck, Loos, & Meyer, 2005). It is believed that the unprecedented amount of human CO<sub>2</sub> emission is directly responsible for the alarming increase in ice-cap melting, dangerous hurricanes, and unpredictable changes in climatic patterns, resulting in drought and flooding. The state of Texas has vast coal resources which constitute one of the largest sources of generating power in the Gulf coastal region. The U.S. also has a large reserve of coal which would help the nation to reducing its dependence on foreign fossil fuel (Petroleum, june 2007).

CO<sub>2</sub> emissions have been on an upward trend in the early years of the 21<sup>st</sup> century. Fossil fuels are the dominant form of energy utilized in the world (86%) and account for about 75% of

current anthropogenic CO<sub>2</sub> emissions (houghton, et al., 2001c). Keeping in account of the recent trends in CO<sub>2</sub> emissions, it is absolutely necessary in control CO<sub>2</sub> emissions to the atmosphere.

The figure below shows the breakdown of sources of CO<sub>2</sub> emissions in the U.S. in 2006.



**Figure 1.1** Breakdown of sources of CO<sub>2</sub> emissions in the U.S. in 2006.

Source: epa.gov

The International Panel for Climate Change (IPCC) has made an effort to identify future GHG emission pathways. Using several assumptions, the IPCC built a set of scenarios of what might happen to emissions up to the year 2100. Six groups of scenarios were published (IPCC, 2000a): the ‘SRES scenarios’. SRES is nothing but Special Report on Emissions scenario. None of these assume any specific climate policy initiatives; in other words, they are base cases which

can be used for considering the effects of mitigation options. An illustrative scenario was chosen for each of the groups. The six groups were organized into four “families” covering a wide range of key “future” characteristics such as demographic change, economic development, and technological change (IPCC, 2000a). However, “The possibility that any single emissions path will occur as described in scenarios is highly uncertain” (IPCC, 2000a).

Given the role played by fossil fuels in supplying energy to modern society, and the long periods of time involved in changing energy systems (Marchetti and Nakicenovic, 1979), the continued use of fossil fuels is arguably a good base-case scenario. Most of these scenarios yield future emissions which are significantly higher than today’s levels. In 2100, these scenarios show, on average, between 50% and 250% as much annual CO<sub>2</sub> emissions as current rates. Adding together all of the CO<sub>2</sub> emissions projected for the 21st century, the cumulative totals lie in the range of 3,480 to 8,050 GtCO<sub>2</sub> (950 to 2,200 GtCO<sub>2</sub>) depending on the selected scenario (IPCC, 2001e). Furthermore, let’s look into the options we have to mitigate the climate change.

- Improve energy efficiency: Reduction in fossil fuel consumption can be achieved by improving the efficiency of energy conversion, transport and end-use, including enhancing less energy-intensive economic activities. Energy conversion efficiencies need to be increased in the production of electricity.
- Switch to less carbon intensive fossil fuels: Switching from high-carbon to low-carbon fuels can be cost effective today where suitable supplies of natural gas are available. With the introduction of the combined production of heat, cooling and electric power, the reduction in emissions would be even greater. This would make a substantial contribution to emissions

reduction from a particular plant but is restricted to plant where supplies of lower carbon fuels are available.

- Increased use of low- and near zero- carbon energy sources: Deep reductions in emissions from stationary sources could be achieved by widespread switching to renewable energy or nuclear power (IPCC, 2001a). Cost, safety, long-term storage of nuclear wastes, proliferation and terrorism play a key role to which nuclear power could be applied. There is a wide variety of renewable supplies potentially available: commercial ones include wind, solar, biomass, hydro, geothermal and tidal power, depending on geographic location. Many of them could make significant contributions to electricity generation, as well as to vehicle fuelling and space heating or cooling, thereby displacing fossil fuels (IPCC, 2001a). Many of the renewable sources face constraints related to cost, intermittency of supply, land use and other environmental impacts. Liquid fuel derived from biomass is also considerable and is attracting the attention of several countries. Geothermal energy used for electricity is also growing in both developed and developing countries. There are therefore many options which could make deep reductions by substituting for fossil fuels, although the cost is significant for some and the potential varies from place to place (IPCC, 2001a).
- Sequester CO<sub>2</sub> through the enhancement of natural, biological sinks: Natural sinks for CO<sub>2</sub> already play a significant role in determining the concentration of CO<sub>2</sub> in the atmosphere. They may be enhanced to take up carbon from the atmosphere. Examples of natural sinks that might be used for this purpose include forests and soils (IPCC, 2000b). Enhancing these sinks through agricultural and forestry practices could significantly improve their storage capacity but this may be limited by land use practice, and social or environmental factors.

Carbon stored biologically already includes large quantities of emitted CO<sub>2</sub> but storage may not be permanent.

The Third Assessment Report by IPCC found that the option for reducing emissions with most potential in the short term (up to 2020) was energy efficiency improvement while the near-term potential for CO<sub>2</sub> capture and storage was considered modest. Nevertheless, faced with the longer-term climate challenge and in view of the growing interest in this option, it has become important to analyze the potential of this technology in more depth.

As a result of the 2002 IPCC workshop on CO<sub>2</sub> capture and storage (IPCC, 2002), it is now recognized that the amount of CO<sub>2</sub> emissions which could potentially be captured and stored may be higher than the value given in the Third Assessment Report. Indeed, the emissions reduction may be very significant compared with the values quoted above for the period after 2020. Global climate change has been an important concern due to the buildup of CO<sub>2</sub> (up to two-thirds of the total effect on climate change) and other greenhouse gases into the Earth's atmosphere. There are two main channels through which CO<sub>2</sub> can be removed from the atmosphere.

1. Direct sequestration and
2. Indirect sequestration.

Direct capture and sequestration involves capturing CO<sub>2</sub> at a source before it can be emitted to the atmosphere and sequestering it. An example is the capture of CO<sub>2</sub> from power plants and storing it in the underground reservoirs or in the deep ocean. The ocean already contains an estimated 40,000 GtC (billion tonnes of carbon) compared with 750 GtC in the atmosphere and 2,200 GtC in the terrestrial biosphere (Herzog, Caldeira, & Adams, 2005). The

most efficient concept would use specialized equipment to capture  $\text{CO}_2$  at large stationary sources like factories or power plants and then inject the  $\text{CO}_2$  into secure storage zones deep underground (geologic sequestration) or into the deep ocean.

Indirect sequestration, also known as terrestrial sequestration, does not require the  $\text{CO}_2$  to be concentrated into a stream prior to removing it from the atmosphere. With indirect sequestration practices,  $\text{CO}_2$  can be sequestered “indirectly” by transferring it to the marine or terrestrial biosphere. The practices uses land management practices that boost the ability of natural  $\text{CO}_2$  sinks like plants and soils to remove carbon as  $\text{CO}_2$  from the atmosphere, regardless of its source. Opportunities for indirect sequestration can be found in forests, grasslands, wetlands, and croplands. Indirect sequestration techniques are expected to provide less permanent carbon storage than when compared to direct sequestration, in the order of decades or at most centuries. This is because of the relatively rapid turnover time of the systems.

The subsequent material of this thesis is divided into the following chapters.

In chapter 2, we provide a literature review on what is carbon capture and storage,  $\text{CO}_2$  sequestration, the current status of the technology and what are the various types of sequestration technologies available now?, like geological sequestration,  $\text{CO}_2$  storage in oil and gas reservoirs, sequestration in saline formations and underground coal gasification.

In chapter 3, we talk about what pore and porous media is. We discuss about the flow through the porous media given by the Darcy’s equation. We explain the differences and difficulties encountered when modeling flow through a porous media when the fluid is Non-Newtonian. We then explain the methodology starting with the Navier-Stokes equation, the laws

of conservation of mass and continuity, the conditions assumed and the variational method used in our work.

In chapter 4, we put forward the results with single phase flow in a straight triangular duct and a single phase flow in circular duct and single phase flow in a circular duct when the fluid is a Non-Newtonian fluid. We calculate the empirical flow conductance and the flow conductance when variational method is used and validate the results with each other in every case. The velocity profiles for each of the cases are also given.

In chapter 5, we discuss the summary, conclusions of our thesis and the future recommendations and direction of the research.



## **Chapter 2: Literature review**

Fossil fuels such as petroleum, natural gas, and coal, supply most of the energy around the globe. They currently account to over 85% of the world's energy needs and will remain in abundant supply well into the 21<sup>st</sup> century (Herzog H. J., 1999). The high standards of living and the luxuries currently enjoyed by the industrialized world are due to the role played by fossil fuels. In spite all the goodies from fossil fuels, their future is not safe because of the economic and environmental threat they possess towards climate change. From those energy sources, coal is a compact stratified mass of metamorphosed plant that has, in part, undergone arrested decay to different extents of completeness. It originates from the arrested decay of the remains of trees, bushes, ferns, mosses, vines, and other forms of plant life that flourished in huge swamps and bogs millions of years ago during prolonged periods of humid, tropical climate, and abundant rainfall (Hendricks & al, 1945, 1984). It is the most abundant, cheaper, and the largest source of energy for the generation of electricity worldwide, however it is as well as one of the largest worldwide anthropogenic sources of CO<sub>2</sub> emissions. The emissions of NO<sub>x</sub>, SO<sub>2</sub>, unburned hydrocarbons, and particulates have been controlled by extracting energy from fossil fuels in an environmentally friendly way. Efforts to mitigate the greenhouse gas problem have traditionally focused on avoiding the production of CO<sub>2</sub> by reducing fossil fuel use (typically referred to as "CO<sub>2</sub> abatement") (Nordhaus, 1992). One alternative to CO<sub>2</sub> abatement would be to capture CO<sub>2</sub> emissions and sequester them in carbon reservoirs such as deep aquifers, deep oceans, or minerals (Lackner, Wendt, Butt, Joyce, & Sharp, 1995) (Herzog & Drake, 1996) (Hoffert, 2002). To sequester the CO<sub>2</sub> is to prevent it from entering to the atmosphere. CO<sub>2</sub> Sequestration

proposes to stabilize the CO<sub>2</sub> concentration emitted to the atmosphere by relocating it by some special techniques.

One of the ways to reduce CO<sub>2</sub> emission to atmosphere is to sequester CO<sub>2</sub> and inject it underground in coal-bed enhancing the residual methane production (White, Straeisar, Granite, Hoffman, & Pennline, 2003; Liu & Smirnov, 2007; Dooley, Dahowski, Davidson, Bachu, Gupta, & Gale, 2004). CO<sub>2</sub> capture and storage involves capturing the CO<sub>2</sub> arising from the combustion of fossil fuels, as in power generation, or from the preparation of fossil fuels, as in natural-gas processing. It can also be applied to the combustion of biomass-based fuels and in certain industrial processes, such as the production of hydrogen, ammonia, iron and steel, or cement. Capturing CO<sub>2</sub> involves separating the CO<sub>2</sub> from some other gases. The CO<sub>2</sub> must then be transported to a storage site where it will be stored away from the atmosphere for a very long time (Metz, Davidson, Swart, & Pan, 2001a). In order to have a significant effect on atmospheric concentrations of CO<sub>2</sub>, storage reservoirs would have to be large relative to annual emissions. Carbon capture and storage as a whole can be explained as follows

- Sources of CO<sub>2</sub> and technologies for capturing CO<sub>2</sub>;
- Transport of CO<sub>2</sub> from capture to storage;
- CO<sub>2</sub> storage options;
- Geographical potential of the technology;
- Possibility of re-using captured CO<sub>2</sub> in industrial applications;
- Costs and energy efficiency of capturing and storing CO<sub>2</sub> in comparison with other large-scale mitigation options;

- Implications of large-scale introduction, the environmental impact, as well as risks and risk management during capture, transport and storage;
- Permanence and safety of CO<sub>2</sub> storage, including methods of monitoring CO<sub>2</sub> storage;
- Barriers to the implementation of storage, and the modeling of CO<sub>2</sub> capture and storage in energy and climate models;
- Implications for national and international emission inventories, legal aspects and technology transfer.

Large scale industries and power plants are the primary sources for capture and separation. CO<sub>2</sub> capture is necessary in order to produce a stream of high pressure CO<sub>2</sub> which is readily transported to a storage site. Even low concentrated CO<sub>2</sub> streams can be transported, with costs and other economic reasons in mind, a high concentrated CO<sub>2</sub> at high pressure is desired. Hence, it is important to produce a nearly pure CO<sub>2</sub> stream for transport and storage. There are quite a few applications that separate CO<sub>2</sub> in large industrial plants including natural gas treatment plants and ammonia production facilities which are already in operation today. One of the current technologies includes the removal of CO<sub>2</sub> to purify other industrial gas streams. Typically the separated CO<sub>2</sub> is emitted to the atmosphere. Depending on the power plant application or the process involved there are three main technologies employed to capture CO<sub>2</sub> generated from the burning of fossil fuels which include coal, oil, natural gas, biomass, or mixture of any of these fuels.

Geological storage of CO<sub>2</sub> has as an objective to remove the CO<sub>2</sub> from the combustion by-products and accumulate it at a stable geological reservoir other than the atmosphere. In this

type of sequestration, CO<sub>2</sub> may be transformed into other compounds that are more stable, such transformation is due to the interaction of CO<sub>2</sub> with other minerals found in the geologic reservoir. However, geologically sequestered CO<sub>2</sub> may leak from the underground reservoir but, as long as the leakage rate is minimized, large amounts of CO<sub>2</sub> can be sequestered without representing a potential threat to the ecosystem surrounding the reservoir.

To remove the CO<sub>2</sub>, the processes taking place rely on two types of separation:

- Absorption is a process by which the compound whose removal is desired is incorporated to the mass of the absorbing agent. It is the process in which atoms, molecules, or ions enter some bulk phase- can be gas, liquid or solid material.
- Adsorption is a process by which the compound is only attached to the surface of the solid or liquid agent. It is the process in which there is an attraction of atoms or molecules from an adjacent gas or liquid to an exposed solid surface.

Geological storage of CO<sub>2</sub> includes oil and gas reservoirs, un-mineable coal seams, and deep saline reservoirs. These are structures that have stored crude oil, natural gas, brine and CO<sub>2</sub> over millions of years. Many power plants and other large emitters of CO<sub>2</sub> are located near geologic formations that are amenable to CO<sub>2</sub> storage. Further, in many cases, injection of CO<sub>2</sub> into a geologic formation can enhance the recovery of hydrocarbons, providing value-added byproducts that can offset the cost of CO<sub>2</sub> capture and sequestration. For the purpose of research, the geological processes attractive to study are the Oil and Gas Reservoirs, Saline Formations and Underground Coal Gasification. In some cases, production from an oil or natural gas reservoir can be enhanced by pumping CO<sub>2</sub> gas into the reservoir to push out the product. This is called enhanced oil recovery. The United States is the world leader in enhanced

oil recovery technology, using about 32 million tons of CO<sub>2</sub> per year for this purpose (U.S. Department of Energy). In an enhanced oil recovery application, the integrity of the CO<sub>2</sub> that remains in the reservoir is well-understood and very high, as long as the original pressure of the reservoir is not exceeded.

Sequestration of CO<sub>2</sub> in deep saline formations does not produce value-added by-products, but it has other advantages. First, the estimated carbon storage capacity of saline formations in the United States is large, making them a viable long-term solution. It has been estimated that deep saline formations in the United States could potentially store up to 500 billion tons of CO<sub>2</sub> (U.S. Department of Energy). Second, most existing large CO<sub>2</sub> point sources are within easy access to a saline formation injection point and, therefore, sequestration in saline formations is compatible with a strategy of transforming large portions of the existing U.S. energy and industrial assets to near-zero carbon emissions via low-cost carbon sequestration retrofits. Assuring the environmental acceptability and safety of CO<sub>2</sub> storage in saline formations is a key component of this program element. Determining that CO<sub>2</sub> will not escape from formations and either migrate up to the earth's surface or contaminate drinking water supplies is a key aspect of sequestration research. Although much work is needed to better understand and characterize sequestration of CO<sub>2</sub> in deep saline formations, a significant baseline of information and experience exists. For example, as part of enhanced oil recovery operations, the oil industry routinely injects brines from the recovered oil into saline reservoirs, and the U.S. Environmental Protection Agency (EPA) has permitted some hazardous waste disposal sites that inject liquid wastes into deep saline formations.

Underground Coal Gasification is a process in which the coal is gasified in the un-mined coal seams by drilling deep underground wells and executing the combustion and gasification reactions in there. By doing that, the quantities of commercial gas produced could be utilized as a source of power generation and as chemical feedstock. The UCG system is a more environment-friendly process, meaning that the emissions of sulfur, nitrous oxides, and mercury are more controlled than in the regular system. In addition, this method can represent an increase of the coal resources, due to the fact that deep coal seams that were not mineable before can now be exploited. Moreover, by using this technique, once a cavity is formed, CO<sub>2</sub> could be pumped back which would represent an innovative idea for CO<sub>2</sub> storage.

UCG basically consists of various parts. First, a well has to be drilled into the coal seam. Once the seam is reached, air or oxygen is injected. On the other side, another well is drilled to position a pipe through which the gases produced in the process are to be extracted. The coal then is burned from the first well. The reaction between coal, oxygen, and water generates CO<sub>2</sub>, CH<sub>4</sub>, CO, H<sub>2</sub>, N<sub>2</sub>, and other gases. Once the coal is totally consumed, they restart the whole process again. By doing this process over and over, cavities are formed underground, which could represent a good site to test the CO<sub>2</sub> sequestration process. According to the data presented in the articles, the UCG technique has been tested in different countries since the 1930s when it was recognized as a viable method of coal power-generation. Different trials have been run in China, U.S, Russia (and former Soviet Union), Australia, and Europe. Nowadays, China has the biggest UCG program running with 16 trials developed since the late 1980's. However, Australia, with the Chinchilla Project, has run the largest UCG project. In regards to the coal composition, it must consist of a total ash content of less than 60% and the seam has to

be continuous with minimum discontinuities. From the environmental perspective, it is recommended that aquifers are not located nearby to avoid any type of water contamination. As seen the UCG is a well-researched process and has been around for some decades, but it has not been commercialized in large scale. However, the CO<sub>2</sub> sequestration from this process is relatively new and in the process of developing. At the present moment, a set of protocols have not been developed yet and, the ones that have been developed, have not received a widespread acceptance due to the doubtful arguments such protocols generate.

Talking about the general process of CO<sub>2</sub> sequestration, there are some basic steps to follow in order to achieve the CO<sub>2</sub> storage. First, CO<sub>2</sub> would have to be separated from the other gases, with a minimum of 95% CO<sub>2</sub> purity. This could be achieved by using the Selexol or Rectisol processes. It is important to point out that if oxygen is used to separate the CO<sub>2</sub>, separation is easy, but oxygen is expensive. Once it is separated, the CO<sub>2</sub> can be stored, and storing it requires more advanced techniques that, nowadays, are still in development. According to the articles mentioned, in order to understand the operational concerns of the CO<sub>2</sub> storage more technical knowledge is needed which is why an accelerated research program is needed to provide new innovative ways of storing CO<sub>2</sub> with a high rate of success. Of course, there are many constraints about the “how” of the CO<sub>2</sub> sequestration process. Some of them are: Temperature and Pressure constraints, Geo-mechanical response, Ground –water displacement risk, Geochemical Response, and CO<sub>2</sub> fate.

Some key points about Underground Coal Gasification are as follows:

- To avoid leakage volume flow, the CO<sub>2</sub> sealing pressure of the cap rock should be considered as a basic constraint in designing and implementing CO<sub>2</sub> storage injection such that the cap rock will never be broken through by the injected CO<sub>2</sub>.
- The leakage of CO<sub>2</sub> through cap rock by molecular diffusion is negligible during the short-term injection stage.
- Investigations should focus on the cap rock property changes due to the mineralogical reactions caused by the diffused CO<sub>2</sub> in the long-term containment.
- According to studies, the storage capacity for a given reservoir shows that once the reservoir pressure reaches a certain high level, a continuous increase in pressure alone is not effective in enhancing the storage capacity

The Underground Coal Gasification process represents an effective way of coal power-generation. This process eliminates conventional coal mining. By doing so, the operating costs, surface damage, and mine safety concerns are greatly improved. Also, it increases the coal resources of the country due to the increase of minable deep seams with this process. It is an environment friendly process if done it correctly because no coal is transported to the surface, the ash stays underground, some of the gas contaminants are not produced, more energy for mining is saved, and it could lead to the generation of a well develop protocol for CO<sub>2</sub> sequestration. CO<sub>2</sub> sequestration is crucial for making fossil fuel use sustainable over the long term. It represents a realistic method of preventing CO<sub>2</sub> to be emitted to the atmosphere.

Geological sequestration in saline aquifers may develop to enlarge the volume of CO<sub>2</sub> being stored. It is important to mention again, that the CO<sub>2</sub> sequestration process following the UCG technique is relatively new and more research and information needs to be performed in



order to attain a well-founded base to develop a standard protocol satisfying all the constraints and requirements previously presented.

For all sequestration techniques, there is no accurate method to measure how much CO<sub>2</sub> can be stored and what consequences it will bring in the long run. Once sequestration is put into action, research is needed to help determine which methods are the most secure and effective techniques to prevent the CO<sub>2</sub> to reach the atmosphere. The three technologies will be discussed in the following section.

There are different types of CO<sub>2</sub> capture systems: post combustion, pre-combustion and oxyfuel combustion. The important factors that decide on selecting the capture system are:

- The concentration of CO<sub>2</sub> in the gas stream
- The pressure of the gas stream
- The fuel type (solid or gas).

Post-combustion capture of CO<sub>2</sub> in power plants is economically feasible under specific conditions. This means that the technology is well understood and is applied in selected commercial applications. In this system, CO<sub>2</sub> is separated from the flue gases produced by the combustion of the primary fuel in air. The percentage of CO<sub>2</sub> captured is typically 3 to 15 percent by volume. They use a liquid solvent to capture the CO<sub>2</sub>. Monoethanolamine (MEA) is the typically employed organic solvent in today's coal power plant or a natural gas combined cycle (NGCC) power plant.

Pre-combustion capture is widely applied in fertilizer manufacturing and in hydrogen production. Although the initial fuel conversion steps of pre-combustion are more elaborate and costly, the higher concentrations of CO<sub>2</sub> in the gas stream and the higher pressure make the

separation easier. These systems process the primary fuel in a reactor with steam and air or oxygen to produce a mixture consisting mainly of carbon monoxide and hydrogen (synthesis gas). A second reactor known as a shift reactor is employed to react with the carbon monoxide with steam to produce hydrogen along with  $\text{CO}_2$ . The resulting mixture is then separated to produce different streams of hydrogen and  $\text{CO}_2$ . Once the  $\text{CO}_2$  is stored, the hydrogen is a carbon free energy carrier that can be combusted to generate power and/or heat. The  $\text{CO}_2$  produced in the shift reactor is typically of the order 15 to 60 percent by volume. Thus this process is more feasible even though the initial fuel conversion methods are more elaborate and more expensive than in a post combustion process. This process is used in power plants that employ integrated gasification combined cycle (IGCC) technology.

Oxyfuel combustion systems use oxygen instead of air for the combustion of the primary fuel in order to produce a flue gas which is mainly water vapor and  $\text{CO}_2$ . The result is a flue gas with high concentrations of  $\text{CO}_2$ . The amount of  $\text{CO}_2$  is typically greater than 80% by volume. The gas stream is then cooled and compressed to remove the water vapor. This results in high  $\text{CO}_2$  concentrations in the gas streams and therefore, in easier separation of  $\text{CO}_2$  and in increased energy requirements in the separation of oxygen from air. Oxy fuel combustion is still in the demonstration phase.

There has been a lot of research going on this topic. There are several projects undergoing to enhance methane production by sequestering  $\text{CO}_2$  underground. Bromhal and his group at NETL studied the various issues associated with the  $\text{CO}_2$  sequestration such as effects of sorption in coal-beds, cross-over from capillary fingering, spatial avalanches, and transient analysis for measure permeability (Ferer, Bromhal, & Smith, 2004) (Bromhal, Sams, Jikich,

Ertekin, & Smith, 2005) (Ferer, Bromhal, & Smith, 2002) (Ferer, Bromhal, & Smith, 2003). Melnichenko et al. and his group at ORNL used small angle neutron scattering (SANS) to understand the pore-size specific details into the mechanisms of CO<sub>2</sub> sorption in coals and to characterize the density and volume of the sorbed CO<sub>2</sub>, factors that are key to determining the efficacy of potential sequestration reservoirs (Melnichenko, Radlinski, Mastalerz, Cheng, & Rupp, 2009; Melnichenko, Wignall, D.R., & Frielinghaus, 2006; Melnichenko, Wignall, D.R., & Frielinghaus, 2004; Radlinski, et al., 2009). A feasibility of CO<sub>2</sub> sequestration in deep unminerable coalseams is presented in the report by Advanced Resources International (ARI), a Department of Energy contractor, by performing detailed reservoir studies of two enhanced coalbed methane recovery field projects in the San Juan basin (Dooley, Dahowski, Davidson, Bachu, Gupta, & Gale, 2004; Smith & Reeves, 2002; Reeves, 2003). Pore network modeling of a variety of transport processes in porous media originally cast great insight into the dynamics of supercritical CO<sub>2</sub> fluid or gaseous form, oil and water in reservoir pore spaces (Fatt, 1996; Ferer, Bromhal, & Smith, 2003; Pan, Dalla, Franzosi, & Miller, 2007; Oleinikova & Brovchenko, 2008) and have seen resurgence in recent years. Examples of such processes for which the details of the pore structure have a key impact are two-phase (Patzek, 2001; Knackstedt, Sheppard, & Sahimi, 2001; Bravo, Araujo, & Lago, 2007; Stevenson, Bromhal, Ferer, Wilder, & Smith, 2004) and three-phase (Piri & Blunt, 2005) flows, leading to relative permeability relationships for input into reservoir simulators, non-Newtonian displacement processes (Lopez, Valvatne, & Blunt, 2003; Stevenson, Ferer, Bromhal, Gump, Wilder, & Smith, 2006), such as in polymer floods, and reactive transport (Dadvar & Sahimi, 2003; Thullner & Baveye, 2008), in which chemical reactions occur at fluid-fluid and/or fluid-solid interfaces. An example of such

reactive transport is the conversion of sequestered carbon dioxide into carbonate (Li, Peters, & Celia, 2006).

SRI International is an independent nonprofit research and development institute has been awarded a \$4.5M Department of Energy (DoE) project to evaluate the technical and economic viability of carbon dioxide capture using an ammonium carbonate-ammonium bicarbonate (AC-ABC) process at gasification plants, including integrated gasification combined cycle (IGCC) power plants. This new project is one of several projects at SRI aimed at finding cost-effective ways to recover carbon dioxide from power plants so it can be sequestered. Qatar shell, collaborating with the department of earth science and engineering, Imperial College, London have been widely involved in the various aspects of capturing and sequestering CO<sub>2</sub>. A few of their research papers have been reviewed. The Energy Technologies Institute (ETI) has launched a review of potential sites for storing carbon dioxide offshore. The United Kingdom CO<sub>2</sub> Storage Appraisal Project (UKSAP), costing more than £3.5 million, will help answer the question of exactly how much storage capacity the UK has, enabling a better evaluation of the extent and roll out of the country's carbon capture and storage (CCS) market. As we now understand, carbon capture is a time consuming procedure. Energy efficiency and an increased use of renewable energy sources still remain the best solutions for a short term. At the current moment, the various elements of carbon capture and storage of CO<sub>2</sub> have been well demonstrated but bringing down the costs still remains a challenge. According to the European commission, "CCS will only be deployed if the cost per tonne of CO<sub>2</sub> avoided is lower than the carbon price".

In our work, we develop a single phase flow conductance model for various shapes which include generalized triangular and circular geometries. We develop the model for a Newtonian fluid and Non-Newtonian fluid. The differences between a Newtonian and a Non-Newtonian fluid are explained in the following section. We then validate the results against analytical and the empirical solutions. Using the variational method we consider two test functions to approximate the velocity. The flow considered is continuous inside the pore geometry that satisfies the no-slip boundary conditions. We work on deriving the formula for conductance model for the triangular and the circular cross section pore duct in Non-Newtonian flows. The derivation process has been described in chapter 3 which gives a detailed explanation on the methodology and procedure used.

## **Chapter 3: Methodology and Procedure**

### **3.1 INTRODUCTION**

Fluid flow in circular and non-circular pipes is a common phenomenon. For example the water flow in pipes is very common at homes. Examples of fluid flow are flow of river, flow of air over an airplane etc. In the case of CO<sub>2</sub> sequestration, the CO<sub>2</sub> to be stored is in supercritical state which is a liquid. The liquefied CO<sub>2</sub> is injected into the oil fields. Here the CO<sub>2</sub> flows through the porous rock and is stored for the long term usage. Description about a pore and porous media is discussed in the later section. Navier-Stokes equations are the generalized equations that describe the motion of a fluid. The derivation of the Navier-Stokes equations is discussed in the following section. We also explain why these equations are insufficient for describing the motion of flow in our case. We then explain the variational method and its advantages and how it is employed in our case.

### **3.2 NAVIER- STOKES EQUATIONS**

The Navier-stokes equations describe the motion of a fluid. These equations are derived from the Newton's second law of fluid motion assuming that the fluid stresses are the sum of the viscous stresses and the pressure. A solution to the Navier-stokes equation gives us the velocity of the fluid at a given point in space and time. The equations such as mass continuity are derived from the laws of conservation of mass, momentum and energy.

The flow of fluid is governed by the conservation principles of mass, energy and linear and angular momentum. These equations describe how the mass, energy and momentum of a fluid change with respect to time and position. The continuity equation is a differential equation

which describes the transport of some kind of conserved quantity. This can be done using the Reynolds transport theorem; an integral relation stating sum of changes of an intensive property(L) over a control volume should be equal to what is lost or gained on the boundaries of the volume and also what is created by sources inside the control volume. This is defined by the following integral equation:

$$\frac{d}{dt} \int_{\Omega} L dV = - \int_{\partial\Omega} L \mathbf{v} \cdot \mathbf{n} dA - \int_{\Omega} Q dV \quad (3.1)$$

Here

$\mathbf{v}$  = flow velocity

L= intensive property

Q = sources in the fluid

$\Omega$  = control volume

$\partial\Omega$  = bounding surface

When divergence theorem is applied on the above surface integral it changes to a volume integral

$$\frac{d}{dt} \int_{\Omega} L dV = - \int_{\Omega} \nabla \cdot (L \mathbf{v}) dV - \int_{\Omega} Q dV \quad (3.2)$$

Now upon applying Leibniz's rule to the integral, we obtain

$$\int_{\Omega} \left( \frac{\partial L}{\partial t} + \nabla \cdot (L \mathbf{v}) + Q \right) dV = 0 \quad (3.3)$$

The integral should be zero for any control volume if and only if

$$\frac{\partial L}{\partial t} + \nabla \cdot (L\mathbf{v}) + Q = 0 \quad (3.4)$$

### Mass Continuity Equation

The general form of the mass continuity equation can be obtained from the above equation taking  $L$  as density and putting  $Q$  as zero since there are no sources of mass. The mass continuity equation can thus be defined as follows

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (3.5)$$

Where  $\rho$  = density of the fluid

$\mathbf{v}$  = flow velocity

In an incompressible fluid, since  $\rho$  is constant.

$$(\nabla \cdot \mathbf{v}) = 0 \quad (3.6)$$

### Momentum Equation

The Navier-stokes momentum equation can be described as

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla P + \mu \nabla^2 \mathbf{v} \quad (3.7)$$

Here, substitute equation (3.6) into equation (3.7),

We get,

$$\nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla P + \mu \nabla^2 \mathbf{v} \quad (3.8)$$

Where  $P$  is pressure.

Since density is constant, using eqn (3.6), we get

$$\rho(\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla P + \mu \nabla^2 \mathbf{v} \quad (3.9)$$



The equation (3.9) can be expanded in X, Y, Z directions as:

X- Component:

$$\rho \left( u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \right) u = - \frac{\partial P}{\partial x} + \mu \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) u \quad (3.10)$$

Y- Component:

$$\rho \left( u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \right) v = - \frac{\partial P}{\partial y} + \mu \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) v \quad (3.11)$$

Z- Component:

$$\rho \left( u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} \right) w = - \frac{\partial P}{\partial z} + \mu \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) w \quad (3.12)$$

Where

$u$  = flow velocity in X direction

$v$  = flow velocity in Y direction

$w$  = flow velocity in Z direction

The flow is assumed to be fully developed and only in Z direction which gives us the following conditions:

$$u = 0, v = 0, w = w(x, y) \text{ i.e. } \frac{\partial}{\partial z} w = 0, \frac{\partial^2}{\partial z^2} w = 0 \quad (3.13)$$

Applying these conditions in equation (3.12), we arrive at

$$\rho \left( w \frac{\partial}{\partial z} \right) w = - \frac{\partial P}{\partial z} + \mu \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) w \quad (3.14)$$

$$0 = -\frac{\partial P}{\partial z} + \mu \left( \frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} \right) \quad (3.15)$$

Defining pressure drop per unit length,  $-\frac{\partial P}{\partial z} = G$

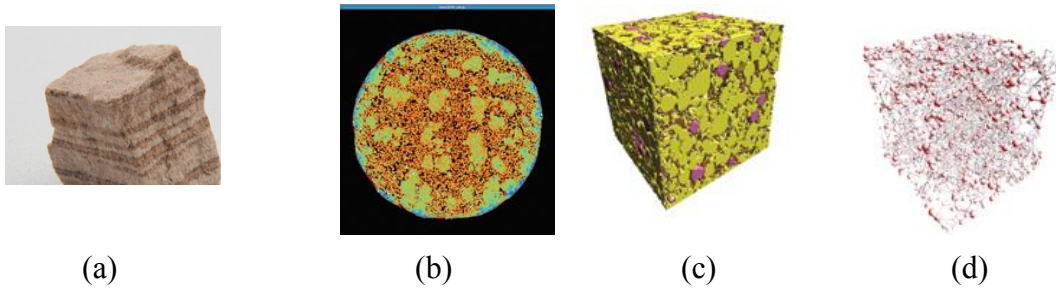
We get

$$0 = G + \mu \nabla^2 w$$

$$-\frac{G}{\mu} = \nabla^2 w \quad (3.16)$$

### 3.3 FLOW THROUGH POROUS MEDIA

A pore or pore space is a microscopic narrow tube where fluid can pass. Figure 3.1 describes pore spaces. A combination of a large number of pores and throats gives us a porous medium. For example soil, sand stone, carbonate etc. are good examples of a porous media. Fluid flow through a porous media is similar to pouring a cup of water over soil and letting the water seep through. Given below is an example how a porous rock material is modeled to generate a pore network starting from a Micro-CT image to a pore network construction.



**Figure 3.1** (a) Porous rock sample (sandstone). (b) Micro-CT image of the cross section. (c) 3-D model to represent the rock model. (d) Pore network construction. (Images source: Numerical Rocks)

It is not easy to describe the flow in a porous media owing to the complexity of the medium. Even if we know the flow in a single tube which can be simple equations but still the combination of all the tubes makes it very hard to know the flow. The two important properties

describing the characteristics of a porous medium are porosity and the permeability. The porosity is defined as the ratio of pore volume over the matrix volume. Pore volume is the total volume of the pore spaces while the matrix volume is the total volume including the pore spaces. Very often the porosity of the medium is assumed constant for the whole medium. Permeability is the ability of the fluid to flow through the medium. Also often called absolute permeability, it only depends on the geometry of the medium. Another important quantity is the dynamic viscosity which characterizes the fluid flow in pore space. At microscopic level there is an interchange of momentum in collisions between the molecules which cause the friction forces. The viscosity of the fluid is nothing but the strength of the frictional forces.

The fluid flow in a porous medium is given by the Darcy equation.

$$U = -\frac{K}{\mu} \cdot (\nabla P - \rho g) \quad (3.17)$$

Where  $U$  = Flow rate,

$K$  = permeability,

$\mu$  = viscosity,

$\nabla P$  = pressure gradient,

$\rho$  = density of the fluid,

$g$  = acceleration due to the gravitational forces.

This equation has been very popular but it gets complicated and the number crunching becomes huge when applied to a network of pores of different shapes. The variational method presented in the following section provides a method of finding approximate solutions to the variables. When compared to the traditional slip/ no-slip methods, the formulational and computational efforts of variational approach would be much less. These variational techniques appear to provide powerful means of finding approximate solutions over domains of known

simple shapes with predetermined boundary conditions. This methodology will now be used for a variety of one and two dimensional problems.

### 3.5 VARIATIONAL METHOD

In a straight channel or for a weakly converging-diverging geometry by way of the lubrication approximation, the flow velocity  $w_i(x,y)$  at a point  $(x, y)$  in the cross section satisfies the equation 3.16.

For one phase flow:

A function  $I[f]$  is defined in eqn 3.18. Minimization of this function, which also corresponds to minimizing total energy, is used to find the parameter  $\alpha$ . Here,  $f$  is a test function that satisfies the boundary conditions and weakly approximate the solution to equation 3.16.

$$I[f] = \frac{1}{2} \int_R dx dy \{ \mu \nabla^2 f \nabla^2 f - 2G f \} \quad (3.18)$$

$$I[f] \geq -\frac{1}{2} G q \quad (3.19)$$

The flux ( $q$ ) and hydraulic conductance ( $g$ ) is given by

$$q_1 = \int_R dx dy w \quad ; \quad g = \frac{q}{G/\mu} \quad (3.20)$$

We use the test function,

$$f = \alpha(r - a)/(r_1 - a) \quad (3.21)$$

For two phase flow,

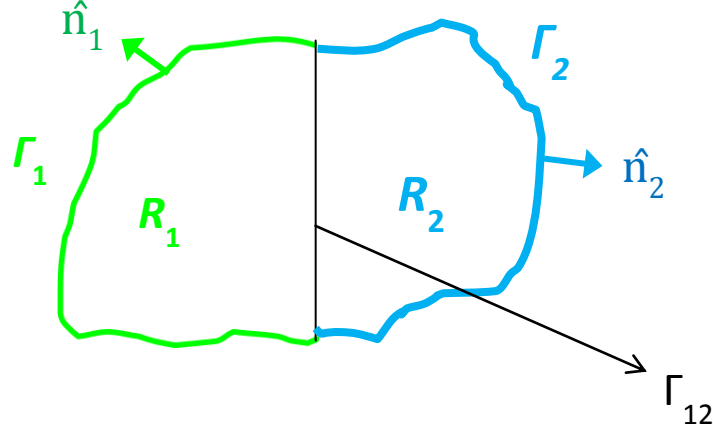
$$-\frac{G_i}{\mu_i} = \nabla^2 w_i \quad ; \quad i=1,2 \quad (3.22)$$

$G_i$  is the pressure drop per unit length in phase  $i$  and  $\mu$  is the phase viscosity.

The boundary conditions on the fluid- solid boundaries are no slip.

$$w_i(x, y) = 0 \quad (3.23)$$

For  $(x, y) \in \Gamma_i; i = 1, 2$



**Figure 3.2** Two phase description

With equal velocities and shear stresses at the fluid-fluid interface:

$$w_1(x, y) = w_2(x, y) \quad \text{for } (x, y) \in \Gamma_{12} \quad (3.24)$$

and

$$\begin{aligned} \mu_1 \hat{n}_{12} \nabla w_1(x, y) + \mu_2 \hat{n}_{21} \nabla w_2(x, y) &= 0 \\ \text{for } (x, y) \in \Gamma_{12} \end{aligned} \quad (3.25)$$

To address this problem in a variational context, the velocities  $w_1$  and  $w_2$  are replaced by test functions  $f_1$  and  $f_2$  containing free parameters that are chosen to minimize a functional, given in Eq. (3.26) below. The test functions need not satisfy the governing equations in Eqs. (3.16), nor the boundary condition in Eq. (3.25). They must, however, satisfy Eqs. (3.23) and (3.24). Under these conditions, and rather weak conditions on continuity, it can be shown that an optimal choice of the test parameters is the one that minimizes the functional

$$I[f_1, f_2] = \frac{1}{2} \int_{R_1} dx dy \{ \mu_1 \nabla f_1 \cdot \nabla f_1 - 2G_1 f_1 \} + \frac{1}{2} \int_{R_2} dx dy \{ \mu_2 \nabla f_2 \cdot \nabla f_2 - 2G_2 f_2 \} \quad (3.26)$$

The choice is optimal because it minimizes the viscous dissipation in the system within the constraints of the actual functional forms deployed for  $f_1$  and  $f_2$  : the absolute minimum in the dissipation is obtained when  $f_i = w_i$ . We have,

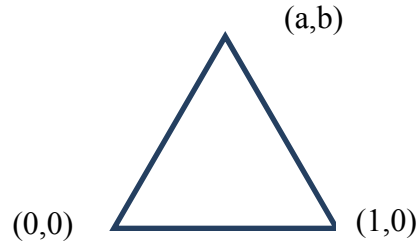
$$I[f_1, f_2] \geq -\frac{1}{2}G_1q_1 - \frac{1}{2}G_2q_2 \quad (3.27)$$

where the phase fluxes are given by

$$q_i = \int_{R_i} dx dy w_i \quad ; \quad i = 1, 2 \quad (3.28)$$

Equality in Eq. (3.27) holds if and only if  $f_i = w_i$ .

### 3.6 NEWTONIAN FLOW



$$\gamma = b/a, \gamma' = b/(1-a)$$

To apply the variational approach for an straight triangular duct for a Newtonian flow, we consider the one-parameter ( $\alpha$ ) test functions as

$$f_1 = \alpha (r - a)/(r_1 - a); \quad f_2 = \alpha (b - r)/(b - r_1) \quad (3.29)$$

Eqs. (3.29) do not satisfy Eqs. (3.16) or (3.25) but do satisfy Eqs. (3.23) and (3.24). The single parameter  $\alpha$  appearing in Eqs. (3.29) is determined by minimizing  $I(f_1, f_2)$  and the approximate fluxes are computed by replacing  $w_i$  by  $f_i$  in Eqs. (3.28).

To validate, we consider the simple test function,  $f$ . Test function is given in the equation 3.30 and satisfies the boundary condition in eqn 3.23 as

$$f = cy(y - \gamma x)(y - \gamma' x') \quad (3.30)$$

Where  $\gamma = b/a$ ,  $\gamma' = b/(1 - a)$ , and  $x' = (1 - x)$ .

We consider an isosceles triangle cross section as we know the empirical results for this geometry.

For an isosceles triangle, we get  $a=1/2$  and  $\gamma = \gamma'$ .

After performing variational analysis for this case, we compute the formula for the hydraulic conductance,  $g$ , which is given by

$$g = \frac{\gamma^3}{160(3 + \gamma^2)} \quad (3.31)$$

From the lubrication theory, the empirical formula for the hydraulic conductances given by

$$g_{emp} = 0.6 \frac{area^3}{perimeter^2} = \frac{3\gamma^3}{320(1 + \sqrt{1 + \gamma^2})^2} \quad (3.32)$$

To validate we have considered a simple test function for  $f$ . one parameter ( $\alpha$ ) test function, that satisfies the boundary condition in equation 3.23, is given in the eqn 3.33 as

$$f = \alpha(1 - r)(r - a) \quad (3.33)$$

And the two parameters ( $\alpha, \beta$ ) test function is given in eqn 3.34 as

$$f = (1 - r)[\alpha(r - a) + \beta(r - a)^2] \quad (3.34)$$

Where ,  $a < r < 1$ .

By solving the eqns 3.16 for circular cross-section , we calculated for the exact solution as

$$w = \frac{1}{4} \left[ (1 - r^2) - \frac{1 - a^2}{\ln(1/a)} \ln(1/r) \right] \quad (3.35)$$

### 3.7 NON- NEWTONIAN FLOW

In the following case, we apply the variational method for a Non-Newtonian fluid. A Non-Newtonian fluid is a fluid whose viscosity ( $\mu$ ) is not independent of shear rate or shear rate history. For example, surfactant addition in CO<sub>2</sub> flooding for enhanced oil recovery, polymer solutions, blood, shampoo, ketchup, paint etc. The relation between shear stress and shear rate is different and can be time dependent. Hence a constant coefficient of viscosity cannot be defined.

For a Non Newtonian fluid, the viscosity is not constant. To solve for this case we use the power law for modeling viscosity. Power law is simple and one of the widely used Non-Newtonian viscosity model that describes the flow for a Non-Newtonian fluid. For Non-Newtonian flow, the Stokes equations (eqn 3.16) can be written as  $-G = \nabla \cdot (\mu \nabla w)$

$$\mu = k \left( \left| \frac{dw}{dr} \right| \right)^{n-1} \quad (3.36)$$

$$\mu r \left( \frac{dw}{dr} \right) = -\frac{Gr^2}{2} + C, \text{ where } C \text{ is the integrating constant} \quad (3.37)$$

Substituting the eqn (3.36) in the eqn (3.37) and solving, we get

$$\frac{dw}{dr} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C}{r} \right) \right)^{\frac{1}{n}} \quad (3.38)$$

$\frac{dw}{dr}$  describes the velocity profile with  $w$  on the x- axis and the radius( $r$ ) on the y- axis. Here we have 2 cases.



**Case 1:**

If  $dw/dr < 0$ , we have

$$\left| \frac{dw}{dr} \right| = -\frac{dw}{dr} \quad (3.39)$$

Applying this condition and assuming the necessary constants, we have

$$\frac{dw}{dr} = -\alpha \left( r^2 + 2\beta_1 + \frac{\beta_1^2}{r^2} \right) \quad (3.40)$$

No-slip assumption at the wall (i.e.  $w_1(1) = 0$ ) results in

$$w_1 = \int dw = \int -\alpha \left( r^2 + 2\beta_1 + \frac{\beta_1^2}{r^2} \right) dr = -\alpha \left( \frac{r^3}{3} + 2\beta_1 r - \frac{\beta_1^2}{r} \right) + d_1 \quad (3.41)$$

$$w_1 = -\alpha \left( \frac{r^3}{3} + 2\beta_1 r - \frac{\beta_1^2}{r} \right) - \left( -\alpha \left( \frac{1}{3} + 2\beta_1 - \beta_1^2 \right) \right) \quad (3.42)$$

**Case 2:**

If  $\frac{dw}{dr} > 0$ ,

Taking  $n = 0.5$ ,

Substituting  $\frac{dw}{dr}$  in the power law we have,

$$\left| \frac{dw}{dr} \right| = \frac{dw}{dr} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_2}{r} \right) \right)^{\frac{1}{n}} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_2}{r} \right) \right)^2 \quad (3.43)$$

Assuming the necessary constants and solving, we have

$$k \left( \frac{dw}{dr} \right)^n = -\frac{Gr}{2} + \frac{C_2}{r} \quad (3.44)$$

For the exact solution,

$$\frac{dw}{dr} = \alpha \left( -r + \frac{\beta_2}{r} \right)^2 = \alpha \left( r^2 - 2\beta_2 + \frac{\beta_2^2}{r^2} \right) \quad (3.45)$$

$$w_2 = \int dw \quad (3.46)$$

At the boundary,

$$w_2(a) = 0 \Rightarrow$$

$$w_2 = \alpha \left( \frac{r^3}{3} + 2\beta_2 r - \frac{\beta_2^2}{r} \right) - \alpha \left( \frac{a^3}{3} + 2\beta_2 a - \frac{\beta_2^2}{a} \right) \quad (3.47)$$

At the interface the velocities are equal.

Applying this condition,

$$w_1(r_0) = w_2(r_0) \quad (3.48)$$

$$\begin{aligned} & -\alpha \left( \frac{r_0^3}{3} + 2(-r_0^2)r_0 - \frac{(-r_0^2)^2}{r_0} \right) - \left( -\alpha \left( \frac{1}{3} + 2(-r_0^2) - (-r_0^2)^2 \right) \right) \\ & = \alpha \left( \frac{r_0^3}{3} + 2r_0^2 r_0 - \frac{r_0^2}{r_0} \right) - \alpha \left( \frac{a^3}{3} + 2r_0^2 a - \frac{(r_0^2)^2}{a} \right) \end{aligned} \quad (3.49)$$

Assuming  $a = 0.1$ , and solving for  $r_0$ ,

We get  $r_0 = 0.419$

### Variational Approach for Non-Newtonian Flow:

We consider a simple one parameter test function,  $f$ :

$$\begin{aligned} f &= c(1-r)(r-a) = c(r-a-r^2-ra) \\ &= c((1-a)r - r^2 - a) \end{aligned} \quad (3.50)$$

Integrating,

$$f' = c((1 + a) - 2r) \quad (3.51)$$

We now have the power law as,

$$\mu = k \left| \frac{df}{dr} \right|^{n-1} = k|c((1 + a) - 2r)|^{n-1} \quad (3.52)$$

$$f' \geq 0 \Rightarrow c((1 + a) - 2r) \geq 0 \Rightarrow r \leq \frac{1 + a}{2}, r_0 = \frac{1 + a}{2} \quad (3.53)$$

$$\mu = \frac{k}{\sqrt{|f'|}} \quad (3.54)$$

$$I = \int (\mu \nabla f \nabla f - 2Gf) r dr = \int \left( \frac{k}{\sqrt{|f'|}} (f')^2 - Gf \right) r dr \quad (3.55)$$

Considering taking  $n=0.5$ , we solve for  $c$  by minimizing eqn 3.55,

$$c = \left[ \frac{5(1 - 2a + 2a^3 - a^4)}{18((1 - a)^{5/2} + (1 - a)^{5/2}a)} \right]^2 \quad \text{When } a=0.1, c= 0.07$$

When  $a/r_2 = 0.1$ ,  $c= 0.7$

We then plot the exact solution. The results are shown in the next chapter to follow.

### 3.9 SUMMARY

Experiments are being conducted to prevent the  $\text{CO}_2$  from entering the atmosphere. In the endless quest for coming up with solutions from preventing global warming,  $\text{CO}_2$  sequestration has been foreseen as a viable solution. The approach in our case is to understand the trapping mechanism of carbon dioxide in pore networks of permeable rocks. It has been determined that

such approach would be ideal due to the complexity of the physics, migration and chemical alterations of CO<sub>2</sub> trapping meaning that CO<sub>2</sub> sequestration would be feasible at a pore scale. In order to approximate analytical expressions for pore network multiphase hydraulic conductances with a complex variety of shapes for input into the pore network models, a variational approach method was utilized. Using the variational approach method is a skillful technique that enables us to account for the physical processes developed at the pore scale. It allows an extension at the fluid to fluid interface concerning simple free-slip or no-slip boundary conditions. Such extensions help us by minimizing the computational effort. Results from this work will provide mechanical engineers with important data to enhance the further studies on pore scale network modeling to sequester carbon dioxide.

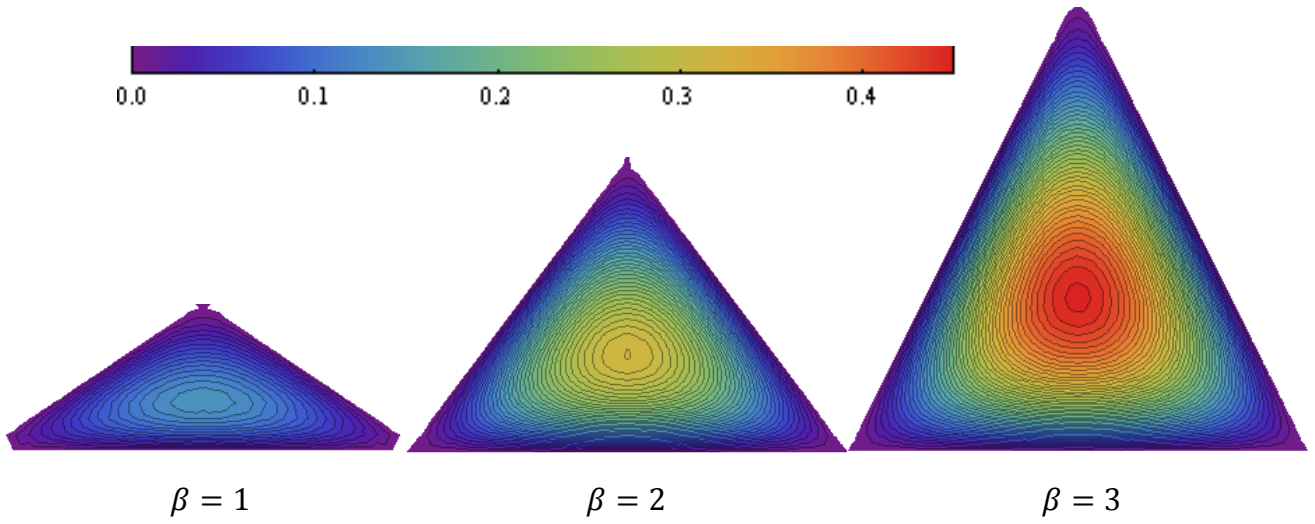
## **Chapter 4: Results and Discussions**

### **4.1 INTRODUCTION**

In the following section, the results generated by Variational method mentioned in the previous chapter are shown. The velocity profiles of different shapes i.e. triangular and circular shapes are shown for Newtonian fluids. Using different aspect ratios for triangular pores velocity profiles are produced. The ratio of computed and empirical hydraulic conductance is shown for an equilateral triangular pore. Error in flux is calculated using one and two parameters in the test function for a circular pore, using the computed and the empirical results the error is calculated. The velocity profile of Non-Newtonian flow through circular pore is shown in section 4.4 and also the error in flux are presented using Variational vs exact method.

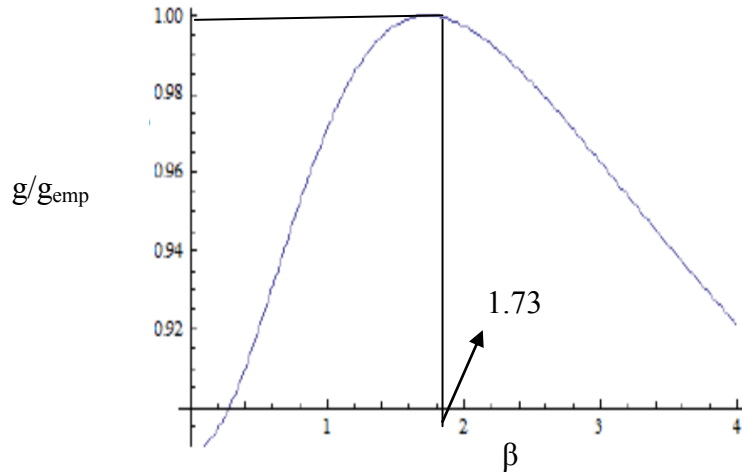
### **4.2 NEWTONIAN FLOW IN STRAIGHT TRIANGULAR DUCT**

The velocity profile for various aspect ratios is shown in the figure 4.1 and the ratio of computed and empirical hydraulic conductance is plotted in figure 4.2. For a range of shapes around an equilateral triangle, for which the two formulae coincide, the values are equal to the analytical result.



**Figure 4.1** Velocity profile through triangular duct (isosceles triangle) for various aspect ratios.

Following is the graph showing a ratio of  $g$  to  $g_{emp}$  for a range of values. We observe the variational solution is exact at  $\beta = \sqrt{3}$ .

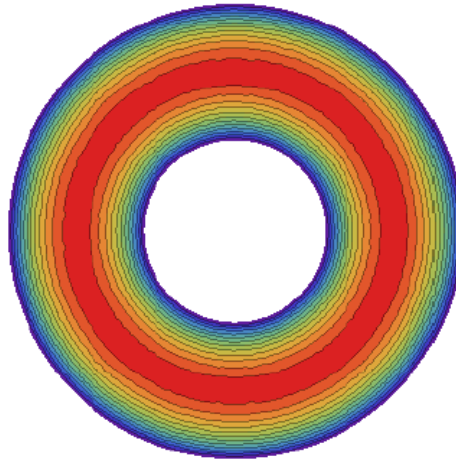


**Figure 4.2** Ratio of  $g$  to  $g_{emp}$  for a range of values of  $\beta$  around the equilateral triangle value  $\beta = \sqrt{3}$ .

### 4.3 NEWTONIAN FLOW IN CIRCULAR DUCT

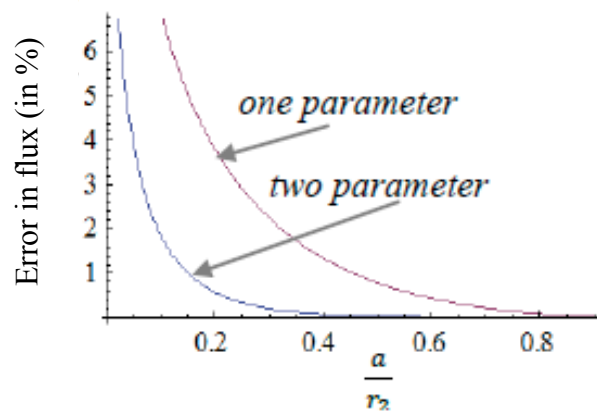
In this section. We present results from variational analysis for single phase Newtonian flow through circular ducts. Analytical solution is available for the circular ducts, so this case provides a reliable verification and validation test case for the variational approach.

Velocity profile through the annulus section as predicted by the variational formulation and relative error in flux is shown in the figure 4.3. It has been observed that even for the very thin core (e.g.  $a/r_2=0.2$ ), the variational approach with both the one parameter ( $<5\%$  error) and the two parameters ( $<2\%$  error) gives a very accurate prediction for the flux through the pore.



**Figure 4.3** Velocity profile through circular cross- section as computed from the variational principles.

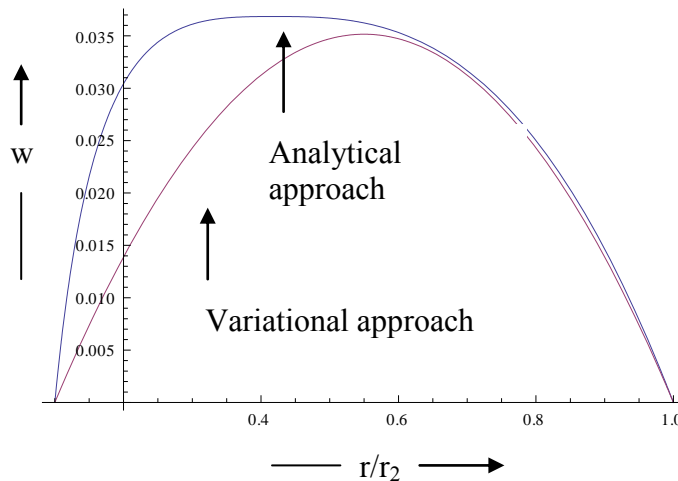
The figure 4.4 is the graph showing the comparison of error in flux (in %) with one parameter and two parameter, where  $a$  is the inner radius of the core and  $r_2$  is the outer radius.



**Figure 4.4** Comparison of error in flux (in %) with one parameter and two parameter, where  $a$  is the radius and  $r_2$  is the outer radius.

#### 4.4 NON-NEWTONIAN FLOW IN CIRCULAR DUCT

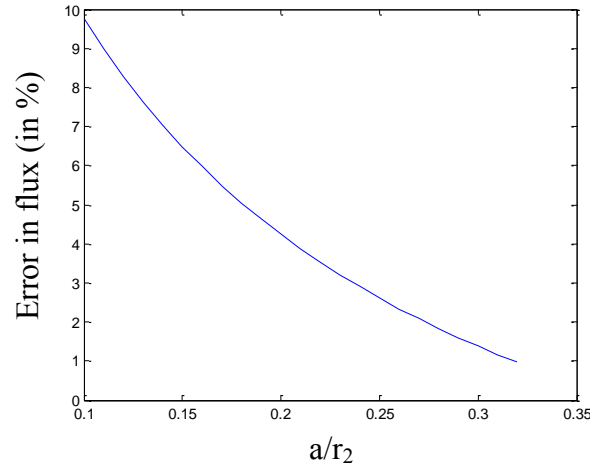
In the previous two cases, we assumed the viscosity to be constant. In other words, the fluid considered is a Newtonian fluid. In this case the fluid is considered to be Non-Newtonian fluid i.e. the viscosity is not a constant. In figure 4.5 is the plot showing the exact solution and the solution we get from the variational method for the velocity.



**Figure 4.5** Comparison of solutions from exact and variational method for a Non-Newtonian case in a circular duct. Here 'w' is non-dimensionalized with  $\frac{G^2 r^{2/3}}{K^2}$

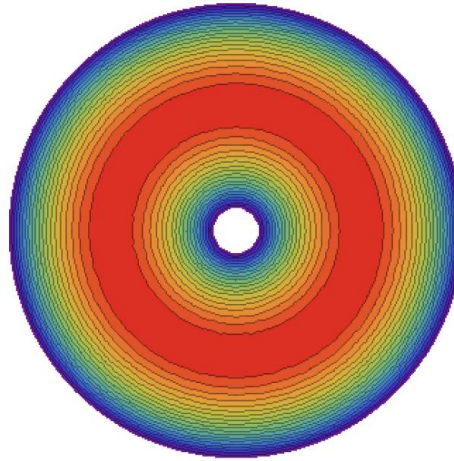


The blue curve represents the exact solution while the red curve represents the solution from variational method. In figure 4.6, we plot the relative error in flux (in percentage). The results are in good agreement for larger  $a/r_2$  ratio. We believe that better approximation for test functions (i.e., 2-parameter or 3- parameter test functions) can improve the results.



**Figure 4.6** Error in flux (in %) for Non-Newtonian flow in a circular duct.

The velocity profile through the circular cross-section as predicted by the variational formulation is shown in the figure 4.7.



**Figure 4.7** Velocity profile through circular cross- section as computed from the variational principles when  $\mu$  is not a constant (Non-Newtonian fluid).

## **Chapter 5: Conclusions and Future work**

In this chapter, we present the summary and conclusions of the research and recommendations for the future direction of the research. In this thesis, we have employed by developing a new methodology for fluid flow in pores. The variational method used give us very good results when approximating the analytic expressions for calculating the conductance of pore elements for input into pore network models.

### **5.1 CONCLUSIONS**

In this thesis, we have presented a new methodology based on variational method for studying the fluid flow through porous medium at pore scale. We found that variational method gives us very good results when approximating the analytic expressions for calculating the conductance of pore elements for input into pore network models. In conclusion, variational methods seem a promising way of obtaining approximate analytical expressions for hydraulic conductance of pore elements for input into pore network models. The methods promise better approximations for hydraulic conductance of pore throats partitioned among two or more phases than the traditional free-slip/no-slip approach. For very thin core (e.g.,  $a/r = 0.2$ ), variational approach with both one parameter ( $<5\%$  error) and two parameters ( $<2\%$  error) gives very accurate prediction for the flux through the pore. Additionally, variational method can be extended to irregular geometries and non-Newtonian flows.

### **5.2 FUTURE WORK**

Further analysis and validation of the variational technique for two-phase and three-phase fluid configurations in pore network models of porous media, including benchmarking against

numerical solutions, will be carried out as part of future project. This work needs to be extended in capabilities for providing input into the description of pore-scale processes necessary for upscaling to reservoir scale. The conductance model developed here shall be applied to a pore-scale representation that is obtained from thin section images, micro-CT scanning and simulations of depositional processes and is mapped onto a framework of links and nodes.

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## Appendix

Derivation for the exact and variational solution for a Non-Newtonian flow.

Power law:

$$\mu = k \left( \left| \frac{dw}{dr} \right| \right)^{n-1}$$

Stokes equation,

$$\mu r \left( \frac{dw}{dr} \right) = -\frac{Gr^2}{2} + C$$

Substituting power law in the stokes eqn,

We get

$$kr \left( \left| \frac{dw}{dr} \right| \right)^n = k \left( \left| \frac{dw}{dr} \right| \right)^{n-1} r \left( \frac{dw}{dr} \right) = -\frac{Gr^2}{2} + C$$

Upon solving,

$$\left( \left| \frac{dw}{dr} \right| \right)^n = -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C}{r} \right)$$

$$\frac{dw}{dr} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C}{r} \right) \right)^{\frac{1}{n}}$$

Defining  $n = 0.5$ ,

$$\frac{dw}{dr} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C}{r} \right) \right)^{\frac{1}{0.5}} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right) \right)^2$$

$$\mu = k \left( \left| \frac{dw}{dr} \right| \right)^{n-1} = k \left( \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right) \right)^2 \right)^{0.5-1} = k \left( \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right) \right)^2 \right)^{-0.5}$$

$\frac{dw}{dr}$  describes the velocity profile with  $w$  on the x- axis and the radius( $r$ )on the y- axis.

Here we have 3 cases.

Case 1:

If  $\frac{dw}{dr} < 0$ ,

$$\left| \frac{dw}{dr} \right| = -\frac{dw}{dr} = -\left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right) \right)^{\frac{1}{n}} = -\left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right) \right)^2$$

$$\mu = k \left( \left| \frac{dw}{dr} \right| \right)^{n-1} = k \left( -\frac{dw}{dr} \right)^{n-1}$$

$$\mu = k \left( -\left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right) \right)^2 \right)^{-0.5} = -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_1}{r} \right)^{-1}$$

$$\mu \left( \frac{dw}{dr} \right) = -\frac{Gr}{2} + \frac{C_1}{r}$$

$$-k \left( -\frac{dw}{dr} \right)^{n-1} \left( -\frac{dw}{dr} \right) = -\frac{Gr}{2} + \frac{C_1}{r}$$

$$-k \left( -\frac{dw}{dr} \right)^n = -\frac{Gr}{2} + \frac{C_1}{r}$$

Let k=1

$$-\left( -\frac{dw}{dr} \right)^n = -\frac{Gr}{2} + \frac{C_1}{r} = -\frac{G}{2} \left( r + \left( -\frac{\frac{2}{G}C_1}{r} \right) \right)$$

$$\left( -\frac{dw}{dr} \right)^n = \frac{G}{2} \left( r + \left( -\frac{\frac{2}{G}C_1}{r} \right) \right)$$

$$-\frac{dw}{dr} = \left( \frac{G}{2} \right)^{\frac{1}{n}} \left( r + \left( -\frac{\frac{2}{G}C_1}{r} \right) \right)^{\frac{1}{n}} = \alpha \left( r + \frac{\beta_1}{r} \right)^m$$

$$\text{where } \alpha = \left( \frac{G}{2} \right)^{\frac{1}{n}}, \beta_1 = -\frac{2}{G}C_1, m = \frac{1}{n}$$

n=0.5, m=2

$$-\frac{dw}{dr} = \alpha \left( r + \frac{\beta_1}{r} \right)^m = \alpha \left( r^2 + 2\beta_1 + \frac{\beta_1^2}{r^2} \right)$$

$$\frac{dw}{dr} = -\alpha \left( r^2 + 2\beta_1 + \frac{\beta_1^2}{r^2} \right)$$

$$w_1 = \int dw = \int -\alpha \left( r^2 + 2\beta_1 + \frac{\beta_1^2}{r^2} \right) dr = -\alpha \left( \frac{r^3}{3} + 2\beta_1 r - \frac{\beta_1^2}{r} \right) + d_1$$



Velocity at the boundary is 0, hence

$$w_1(1) = 0 \Rightarrow -\alpha \left( \frac{1^3}{3} + 2\beta_1(1) - \frac{\beta_1^2}{1} \right) + d_1 = 0 \Rightarrow d_1 = \alpha \left( \frac{1}{3} + 2\beta_1 - \beta_1^2 \right)$$

$$w_1 = -\alpha \left( \frac{r^3}{3} + 2\beta_1 r - \frac{\beta_1^2}{r} \right) - \left( -\alpha \left( \frac{1}{3} + 2\beta_1 - \beta_1^2 \right) \right)$$

Case 2:

If  $\frac{dw}{dr} > 0$ ,

Taking  $n = 0.5$ ,

$$\left| \frac{dw}{dr} \right| = \frac{dw}{dr} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_2}{r} \right) \right)^{\frac{1}{n}} = \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_2}{r} \right) \right)^2$$

$$\mu = k \left( \left| \frac{dw}{dr} \right| \right)^{n-1} = k \left( \frac{dw}{dr} \right)^{n-1}$$

$$\mu = k \left( \left( -\frac{1}{k} \left( \frac{Gr}{2} - \frac{C_2}{r} \right) \right)^2 \right)^{-0.5} = \frac{1}{k} \left( \frac{Gr}{2} - \frac{C_2}{r} \right)^{-1}$$

$$\mu \left( \frac{dw}{dr} \right) = -\frac{Gr}{2} + \frac{C_2}{r}$$

$$k \left( \frac{dw}{dr} \right)^{n-1} \left( \frac{dw}{dr} \right) = -\frac{Gr}{2} + \frac{C_2}{r}$$

$$k \left( \frac{dw}{dr} \right)^n = -\frac{Gr}{2} + \frac{C_2}{r}$$

Let  $k = 1$

$$\left( \frac{dw}{dr} \right)^n = -\frac{Gr}{2} + \frac{C_2}{r} = \frac{G}{2} \left( -r + \frac{\frac{2}{G}C_2}{r} \right)$$

$$\frac{dw}{dr} = \left( \frac{G}{2} \right)^{\frac{1}{n}} \left( -r + \frac{\frac{2}{G}C_2}{r} \right)^{\frac{1}{n}} = \alpha \left( -r + \frac{\beta_2}{r} \right)^m, \text{ where } \alpha = \left( \frac{G}{2} \right)^{\frac{1}{n}}, \beta_2 = \frac{2}{G}C_2, m = \frac{1}{n}$$

$n = 0.5, m = 2$

$$\frac{dw}{dr} = \alpha \left( -r + \frac{\beta_2}{r} \right)^2 = \alpha \left( r^2 - 2\beta_2 + \frac{\beta_2^2}{r^2} \right)$$

$$w_2 = \int dw = \int \alpha \left( r^2 - 2\beta_2 + \frac{\beta_2^2}{r^2} \right) dr = \alpha \left( \frac{r^3}{3} + 2\beta_2 r - \frac{\beta_2^2}{r} \right) + d_2$$

$$w_2(a) = 0 \Rightarrow \alpha \left( \frac{a^3}{3} + 2\beta_2 a - \frac{\beta_2^2}{a} \right) + d_2 = 0 \Rightarrow d_2 = -\alpha \left( \frac{a^3}{3} + 2\beta_2 a - \frac{\beta_2^2}{a} \right)$$

$$w_2 = \alpha \left( \frac{r^3}{3} + 2\beta_2 r - \frac{\beta_2^2}{r} \right) - \alpha \left( \frac{a^3}{3} + 2\beta_2 a - \frac{\beta_2^2}{a} \right)$$

At the interface the velocities are equal.

$$w_1(r_0) = w_2(r_0)$$

Applying this condition,

$$\begin{aligned} &\Rightarrow -\alpha \left( \frac{r_0^3}{3} + 2\beta_1 r_0 - \frac{\beta_1^2}{r_0} \right) - \left( -\alpha \left( \frac{1}{3} + 2\beta_1 - \beta_1^2 \right) \right) \\ &= \alpha \left( \frac{r_0^3}{3} + 2\beta_2 r_0 - \frac{\beta_2^2}{r_0} \right) - \alpha \left( \frac{a^3}{3} + 2\beta_2 a - \frac{\beta_2^2}{a} \right) \end{aligned}$$

$$r_0 + \frac{\beta_1}{r_0} = 0 \Rightarrow \beta_1 = -r_0^2$$

$$-r_0 + \frac{\beta_2}{r_0} = 0 \Rightarrow \beta_2 = r_0^2$$

Therefore,

$$\begin{aligned} &-\alpha \left( \frac{r_0^3}{3} + 2(-r_0^2)r_0 - \frac{(-r_0^2)^2}{r_0} \right) - \left( -\alpha \left( \frac{1}{3} + 2(-r_0^2) - (-r_0^2)^2 \right) \right) \\ &= \alpha \left( \frac{r_0^3}{3} + 2r_0^2 r_0 - \frac{r_0^2^2}{r_0} \right) - \alpha \left( \frac{a^3}{3} + 2r_0^2 a - \frac{(r_0^2)^2}{a} \right) \end{aligned}$$

Assuming  $a = 0.1$ ,  
And solving for  $r_0$ ,  
We get  $r_0 = 0.419$

Testing function, f:

$$f = c(1-r)(r-a) = c(r-a-r^2+ra) = c((1+a)r-r^2-a)$$

$$f' = c((1+a) - 2r)$$

$$\mu = k \left| \frac{df}{dr} \right|^{n-1} = k |c((1+a) - 2r)|^{n-1}$$

$$f' \geq 0 \Rightarrow c((1+a) - 2r) \geq 0 \Rightarrow r \leq \frac{1+a}{2}, r_0 = \frac{1+a}{2}$$

$$n=0.5$$

$$\mu = \frac{k}{\sqrt{|f'|}}$$

$$\begin{aligned} I &= \int (\mu \nabla f \nabla f - 2Gf) r dr = \int \left( \frac{k}{\sqrt{|f'|}} (f')^2 - Gf \right) r dr \\ &= \int_a^{r_0} \left( \frac{k}{\sqrt{f'}} (f')^2 - Gf \right) r dr + \int_{r_0}^1 \left( \frac{k}{\sqrt{-f'}} (f')^2 - Gf \right) r dr \\ &= \int_a^{r_0} \left( k(f')^{\frac{3}{2}} - Gf \right) r dr + \int_{r_0}^1 \left( k(-f')^{\frac{3}{2}} - Gf \right) r dr \\ &= \int_a^{\frac{1+a}{2}} \left( k \left( c((1+a) - 2r) \right)^{\frac{3}{2}} - G(c(1-r)(r-a)) \right) r dr \\ &\quad + \int_{\frac{1+a}{2}}^1 \left( k \left( - \left( c((1+a) - 2r) \right) \right)^{\frac{3}{2}} - G(c(1-r)(r-a)) \right) r dr \\ &= \frac{kc^{\frac{3}{2}}}{35} \left[ (1-3a)^{\frac{5}{2}}(1+4a) - (a-6)(1+a)^{\frac{5}{2}} \right] - \frac{Gc}{12} (1-2a+2a^2-a^4) \end{aligned}$$

$$\text{Use } \frac{\partial I}{\partial c} = 0 \text{ solve for } c.$$

$$c = \left[ \frac{5(1 - 2a + 2a^3 - a^4)}{18((1 - a)^{5/2} + (1 - a)^{5/2}a)} \right]^2$$

When  $a=.1$ ,  $c= 0.07$

## **Curriculum vita**

Nithin kavoori was born on April 5, 1985 in Hyderabad, India. He is the eldest child of Rajendra prasad kavoori and Jyothi kavoori. He came to the United States of America to attend University of Texas at El Paso for his Masters in 2009. He completed his high school education in Vignan Jr. College, Hyderabad, India in 2002 and was awarded a bachelor's of science (Mechanical engineering) by Magadh University in 2006. While at the master's program Nithin kavoori has worked as a graduate research assistant.

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