Development of a ‘Quad Porosity’ Numerical Flow Model for Shale Gas Reservoirs

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Development of a ‘Quad Porosity’ Numerical Flow Model for Shale Gas Reservoirs

by

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A THESIS
SUBMITTED TO THE FACULTY OF GRADUATE STUDIES
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ABSTRACT

Shale gas production modeled with conventional simulators/models is often lower than actually observed field data, even when the effect of hydraulic fractures is taken into account. This is currently being explained by the development of secondary fracturing (the stimulated reservoir volume). While such geomechanical effects are often dominant, it is likely that other factors also contribute to the observed productivity, and these need to be quantified in order to understand the relative importance of all mechanisms. This work addresses one of these factors, namely the complexity of fluid flow physics in nanopore-size porous media. Traditionally, it has been perceived that in shale gas reservoirs gas is stored only in pore space (matrix pores and natural fractures) and adsorbed on pore surfaces. But with recent development in the visualization and measurement techniques, additional gas has been found dissolved in organic matter. In this work, a numerical model for complex ‘quad porosity’ system in shale reservoirs is proposed while also accounting for non-Darcy flow in shale nanopores. We begin with a theoretical model for gas flow inside one shale nanopore and upscale it to laboratory sample scale. Consequently, this model can be incorporated in a commercial reservoir simulator to simulate the flow behavior of shale gas reservoirs with higher confidence. This will help to improve reservoir modeling for shales and correctly predicting the gas in place and recovery.
Preface

This is a manuscript based masters’ thesis and the text of the papers has been adapted to suit thesis requirements. Chapters 2 and 3 are based on SPE papers I have presented during the course of my graduate studies. Chapter 4 has been selected for presentation at an SPE conference. Complete citation for all the chapters is provided below:

Chapter 2: Swami V., Clarkson C.R. and Settari A. “Non-Darcy Flow in Shale Nanopores: Do We Have a Final Answer?” SPE 162665-MS, presented at 2012 Canadian Unconventional Resources Conference held in Calgary. doi: 10.2118/162665-MS


Although the co-authors of these papers contributed by reviewing the works and providing direction as necessary, I am intellectually responsible for conceptualization and implementing all of these works. I am thankful to the co-authors for their guidance and support. In particular I would like to acknowledge Dr. Chris Clarkson who provided basic simulation files which were used in developing Chapter 2. Though SPE holds copyright in all of these works, we as authors still hold intellectual rights and I being the primary author can reproduce them in my thesis according to copyright agreement with SPE. Anyone using any material from the papers must follow SPE’s copyright laws detailed on their website and at http://www.spe.org/authors/docs/permissions_faq.pdf. I am thankful to SPE for permitting me to reproduce the papers in my thesis.
ACKNOWLEDGEMENTS

Though a thesis is student’s individual work, many people directly or indirectly contribute in it. I am thankful to many individuals who acted as mentors and friends and helped to make this work possible. First and foremost, I am grateful to my M.Sc. supervisor Prof. Antonin Settari for all his mentorship and support during my entire graduate studies, more so for always believing in me and for letting me develop and pursue my ideas independently but always being available for guidance whenever required. Having him a supervisor is an honour in itself and the way he has inspired me to be a better technical professional and even more to be a better human being is unparalleled. Dr. Farzam Javadpour at University of Texas at Austin deserves special thanks for seeding in very critical ideas which helped tremendously shape this work. I would like to thank Profs. Chris Clarkson and Roberto Aguilera for the direction and guidance provided at time; Dr. Stephen Larter for being on the examination committee and providing his comments on the work; Prof. Mehran Pooladi-Darvish whose course Advanced Reservoir Engineering taught me greatly the ‘approach’ to tackle problems; my friends and colleagues in university and town—Catalina, Nikhil, Akhil, Arshad, Somayeh, Meheran, Mohammad and Majid for the long discussions (incidentally which were non-technical most of the times) making these two years very enjoyable and unforgettable; Taurus personnel—Dale, Bob and Vikram for providing the industry ‘criticism’ whenever I got extremely theoretical; Cairn India, PennWest (for PennWest Exploration Graduate Scholarship) and Consortium for Shale Gas Modeling (which includes Taurus Reservoir Solutions, ENI, Statoil, Apache and Shell) for funding my research; Schlumberger for donating ECLIPSE® reservoir simulator to the university.

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Last but definitely not the least, all-out thanks to my family and the almighty for this beautiful life.
Mom and Dad—I dedicate this work to you

Thank you for everything
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CHAPTER ONE: INTRODUCTION

With rising population and energy consumption throughout the world, there is a tremendous pressure on fossil fuels. The International Energy Agency (IEA) which keeps a record of world energy supply and demand predicts that the total demand in energy will increase by one third from 2010 to 2035; with India and China accounting for 50% of the growth. Due to environmental concerns with oil and risks posed due to geopolitical reasons, most of the countries bank upon natural gas as the energy solution of future, it being the cleanest energy resource so far (IEA, 2012). With recent technological development, unconventional gas resources—Coal Bed Methane (CBM), shale and gas hydrates are slowly being touted as the ‘new conventional’. In fact, United States saw a decrease in gas import in 2007 for the first time since 1970s, all thanks for the production surge brought in by shale gas exploitation; and the trend continues (Energy Information Administration, 2012). With that, many energy hungry but resource deprived countries are lining up to replicate the shale success story; most notably China, Australia, Europe, India and Latin America (IEA, 2012).

The first gas production from shale reservoirs was from Appalachian Devonian shale in New York state, US in 1821 (Lancaster et al., 1996). By early 90s, thousands of vertical wells were drilled in the Appalachian Devonian shale (Gatens et al., 1980). However, the production surged massively only by late 1990s with development in horizontal wells drilling technology, hydraulic fracturing and also rapid increase in natural gas prices which fueled the interest and gas production from the Barnett Shale With Barnett being the flag bearer, other shale plays have also been developed after Barnett’s success story, most notable among them being Antrim, Bakken, Marcellus, Fayetteville, Eagle Ford and Haynesville (Kell, 2009). For the last 20 years or so, there have been thousands of wells drilled throughout US and Canada to tap this unconventional but abundant resource yielding one of the cleanest fossil fuel, natural gas. Owing to its abundance, being environment friendly and technically recoverable; shale gas has attracted attention throughout the world and is perceived as the energy solution for decades to come.

Despite drilling so many wells and analysing data from so many shale wells, the exact transport mechanism for gas in shales is still not very clear. It has been observed over the years that shale gas production modeled with conventional simulators/models by using the measured
matrix permeability and an estimate of stimulated reservoir volume (commonly called SRV, calculated as a function of fracturing fluid volume injected) and its permeability is typically lower than actually observed field data. The problem is further complicated by the fact that the matrix permeability can be orders of magnitude different based on the laboratory standards and method used (Tinni et al., 2012). There is also uncertainty in the determination of the size of the SRV and it is not uncommon to find hugely different estimates of SRV based on fracturing fluid volume injected and micro-seismic measurements (Jayakumar & Rai, 2012). Although attempts to estimate the permeability enhancement in the SRV from micro-seismic data are now being made, this technology is in its infancy. Generally reservoir and/or stimulated reservoir volume (SRV) parameters are modified (without much physical support) to match the production data (Javadpour, 2009; Shabro et al., 2012). The correct ‘effective’ permeability of the unstimulated formation is particularly important for long term predictions and economic forecasting. Instead of modifying the reservoir parameters arbitrarily, shale as a formation was investigated closely in this research work and it was analyzed to see if any vital part of the flow physics was missing.

Shale gas reservoirs differ significantly from conventional reservoirs in many aspects. First, shale has pores in nanometers range as opposed to micrometers in conventional reservoirs. Second, shale has a significant organic content also known as kerogen, but conventional reservoirs do not have any significant organic matter. This thesis aims to capture the resultant transport physics arising from above mentioned differences between shale and conventional reservoirs.

1.1 Research Objectives

Because of extremely small size of shale matrix pores compared to conventional reservoirs, additional transport mechanisms come into play and Darcy’s law alone is not sufficient to explain the flow behavior. Traditionally, it has been perceived that in shale gas reservoirs gas is stored only in pore space (matrix pores and natural fractures) and adsorbed on pore surfaces (Boyer et al., 2006). But with recent development in the visualization and measurement techniques, additional gas has been found dissolved in organic matter also. The
objective of this work was to incorporate the transport physics as described above. To capture the
same, following research objectives were defined:

1. To assess the impact of extremely small size of shale matrix pores on transport
mechanism inside the pores and validate various formulations available in the literature
on both theory and against experimental results.

2. To develop a theoretical model for gas flow in one nanopore while capturing the non-
Darcy flow mechanisms inside the pore, gas desorption from the pore surface and gas
diffusion from kerogen bulk.

3. To upscale the pore scale model to laboratory scale numerical model for ‘quad porosity’
system including the gas stored inside the natural fractures, matrix pores, adsorbed and
dissolved in kerogen bulk. This numerical model should be in a form to be readily
incorporated inside a reservoir simulator.

It should be noted that the term ‘nanopore’ is a generic term to signify the nanometer
scale pores. According to International Union of Pure and Applied Chemistry (IUPAC)
classification, micropores are <2 nm in diameter, mesopores are between 2 and 50 nm and
macropores are > 50 nm (Ross & Bustin, 2009). Accordingly, the term ‘nanopore’ in this work
essentially refers to the range given by IUPAC’s micropores and mesopores. Also, ‘quad
porosity’ in this work refers to four storage mechanisms; free gas in natural fractures, free gas in
matrix nanopores, adsorbed gas and gas dissolved in kerogen. It is analogous to the use of the
term ‘triple porosity’ in coal bed methane reservoirs which refers to three storage mechanism;
free gas in natural fractures, free gas in matrix pores and adsorbed gas.

1.2 Thesis Organization

This is a manuscript-based thesis and all the manuscripts (which are SPE papers) were
written in active voice. Correspondingly, the entire text (including introduction and conclusion
sections) is in active voice instead of more traditional passive voice which we believe may lead
to convoluted sentences. All the chapters (the SPE papers) have their own reference and
nomenclature section, so these are not repeated in the thesis. Bibliography at the end includes the only references which were cited in introduction and conclusion chapters.

Chapter one provides an introduction to thesis and its organization. Chapter two discusses the existence of non-Darcy flow mechanisms in shale nanopores. We evaluate various correlations for non-Darcy flow inside shale nanopores based on their theoretical approach and validate them against laboratory data from Mesaverde formation in Western U.S. We also conducted a few reservoir simulation runs to see the effect of these non-Darcy transport mechanisms on long term reservoir productivity (Objective 1). In chapter three, we postulate a pore scale flow model for shale gas reservoirs in which the results from chapter one are used for non-Darcy transport mechanisms inside shale pore. Additionally, we also take into account desorption from pore surface and diffusion from kerogen surrounding the pore (Objective 2). In chapter four, we upscale the pore scale model (described in chapter two) to a laboratory scale model. In this model, we include four gas storage mechanisms and three coupled transport mechanisms. This numerical model is then validated against laboratory observed dataset from a Canadian shale gas reservoir (Objective 3). Chapter five summarizes the conclusions of this work and provides direction for future research.
CHAPTER TWO: NON-DARCY FLOW IN SHALE NANOPORES: DO WE HAVE A FINAL ANSWER?\(^1\)

2.1 ABSTRACT

Many shale gas and ultra-low permeability tight gas reservoirs can have matrix permeability values in the range of tens to hundreds of nano-Darcies. The ultra-fine pore structure of these rocks can cause violation of the basic assumptions behind usage of Darcy’s law. Depending on a combination of P-T conditions, pore structure and gas properties, non-Darcy flow mechanisms such as Knudsen diffusion and/or gas slippage effects could be important. Quantifying these effects is critical for correcting laboratory permeability measurements to obtain true (intrinsic) matrix permeability; several authors have also noted that corrections for these effects may also be important when analyzing field data. In order to make corrections for non-Darcy flow, numerous authors have quantified these effects as an apparent permeability that changes as a function of Knudsen number or gas pressure. There are now many correlations available for quantifying apparent permeability changes, but it is not known which ones are applicable to the entire range of permeability/pressure of practical interest and how much impact they really have on the long term production performance of shale gas wells.

In this work, we summarize the various methods for quantifying non-Darcy flow in unconventional gas reservoirs, and compare the apparent permeability and slippage factor predictions for all the models we have compiled. We also evaluate predictions made by various models against actual data observed in Mesaverde formation. For determining the impact of the models’ predictions on well performance, we incorporate the apparent permeability predictions of each model into a numerical simulator, and compare rate-time and cumulative gas-time forecasts for each scenario. The importance of dual porosity (which is usually assumed necessary for shale gas) is also examined. The results of this work are important in several aspects. First, the differences between various formulations of the apparent matrix permeability in shales are illustrated. Secondly, the impact of non-Darcy effects on history matching and recovery

\(^1\) Complete citation of this work: Swami V., Clarkson C.R. and Settari A. “Non-Darcy Flow in Shale Nanopores: Do We Have a Final Answer?” SPE 162665-MS, presented at 2012 Canadian Unconventional Resources Conference held in Calgary. doi: 10.2118/162665-MS. This article has been reproduced with permission from SPE.
forecasting is demonstrated. Finally, it is shown that there may not be a need for dual porosity modeling in certain cases.

The results of this study will be important to professionals involved in laboratory measurement of matrix permeability in unconventional gas reservoirs, modeling well performance and forecasting shale gas recovery.

2.2 INTRODUCTION

Shale gas is a prolific energy resource that is currently being developed in North America and prospected for globally. A current area of research is the impact of shale pore structure on transport mechanisms and ultimate gas recovery. Whereas conventional sandstone and carbonate reservoirs have pore sizes in the range of 1 to 100 micrometers, shale reservoirs have pore throat radii in the range 5 to 1000 nanometers (Wang & Reed, 2009) or even smaller, 5 to 50 nm (Behar & Vandenbroucke, 1987; Bowker, 2003). In the nanometer scale pores in shales, in addition to conventional viscous flow (which is modeled with Darcy’s equation), other transport mechanisms may occur. Under certain conditions of pore size, pressure, temperature and gas properties, flow at the nanoscale may be greater than that predicted from Darcy’s equation. There have been numerous attempts to derive representative fluid flow equations for tight gas/shale pores. We summarize some of them in this work.

Jones & Owens (1980) conducted experiments on U.S. tight gas plays and derived an empirical static gas-slippage factor; they compared it with Klinkenberg’s (1941) slippage factor. Sampath & Keighin (1982) and Florence et al. (2007) also developed empirical relations for gas-slippage factor for tight gas reservoirs which are very similar to Jones & Owens’ relation. Ertekin et al. (1986) took it further and introduced a dynamic slippage factor using the Knudsen diffusion coefficient (based on Jones & Owens empirical equation) to make it a function of pressure. Michel et al. (2011) also used the Knudsen diffusion coefficient and developed their own dynamic slippage factor based on Beskok & Karniadakis’ work (1999). Civan (2010) and Sakhaee-Pour & Bryant (2012) determined slippage factor using Knudsen number criterion and also derived an apparent permeability that is a function of Knudsen number. Javadpour et al.
(2007) and Javadpour (2009) incorporated both Knudsen diffusion and slippage and derived an apparent permeability that is a function of pressure, temperature and gas properties.

There have been few studies that have investigated the impact of non-Darcy flow on shale gas well performance and gas recovery. Clarkson et al. (2012) used Ertekin et al.’s (1986) dynamic-slippage approach, coupled with conventional reservoir simulation, to investigate the impact of dynamic-slippage on gas production forecasts for a limited range of reservoir parameters, and incorporated the effect into rate-transient analysis. Ozkan et al. (2010) incorporated dynamic-slippage into their analytical trilinear flow solution and performed sensitivities. In this work, we will first discuss and compare each of the analytical models for predicting apparent permeability as a function of pressure and pore radius, then evaluate them against permeability measurements available in literature for the nano-Darcy range. Finally, we illustrate the impact of the models on shale gas production forecasts using a numerical simulator. To our knowledge, this is the first time all of the non-Darcy flow models have been compared quantitatively.

2.3 THEORY

Consider fluid flow through a pore of porous medium, as depicted in Figure 2.1. In classical fluid flow mechanics where continuum theory holds, fluid velocity is assumed to be zero at the pore wall. This is shown schematically in Figure 2.1a. For conventional reservoirs having pore radii in the range of 1 to 100 micrometer, this is a valid assumption because fluid acts as a continuous medium. Correspondingly, Darcy’s equation which models pressure-driven viscous flow has been working fine for such reservoirs. It is important to point out that Darcy’s equation consists of Darcy’s permeability. Darcy permeability is purely a function of pore geometry and shape only (Eqs. 4.12 and 4.13). It does not take into account for any effects of pressure, temperature or gas physical properties on flow. Consequently, it predicts the same flow rate for any fluid (liquid/gas) flowing through the porous medium.

Now, consider a contrasting situation where fluid flows in a shale pore (1 to 200 nm), depicted in Figure 2.1b. At this scale, a gas (methane) molecule size (i.e. 0.4 nm, Heidemann et al. 2010) is quite comparable to flow diameter. At the molecular level, fluid continuum theory
breaks down and gas molecules follow a somewhat random path while still maintaining a general flow direction dictated by pressure gradient. Many molecules strike against the pore walls and tend to slip at pore walls instead of having zero velocity there. Though it can be modeled accurately using molecular physics, this technique is not practical for modeling flow through shale on reservoirs scale because we are dealing with enormous number of these interconnected nanopores and gas molecules at the reservoir scale. To make simulation feasible, it is desirable to integrate (simplified) molecular flow behavior with the standard Darcy’s equation so that these mechanisms can be captured (approximately) with conventional reservoir simulators.

Klinkenberg (1941) was the first person in the petroleum industry to identify gas slippage in porous media. He studied gas flow through porous media and observed that at very low pressure, the actual gas flow was more than that predicted with Darcy’s equation. He attributed this higher flow to gas-slippage along the pore walls. He then proposed the following equation to predict apparent gas permeability as a function of pressure:

$$k_a = k_\infty \left(1 + \frac{b_k}{\bar{P}}\right)$$  \hspace{1cm} (2.1)

Where $k_a$ is apparent/effective gas permeability (mD), $k_\infty$ is the reference/liquid permeability (mD), $\bar{P}$ is average pressure (psi) at which the experiments were carried out and $b_k$ is the slippage factor. From Eq. 2.1, we see that at high pressures, the apparent gas permeability approaches the equivalent liquid permeability. The slippage factor, $b_k$ (psi), depends upon mean free path and pore radius as given by Eq. 2.2:

$$b_k = \frac{4c\lambda \bar{P}}{r}$$  \hspace{1cm} (2.2)

Where $\lambda$ is the mean free path of gas molecules at a given pressure and temperature conditions, $r$ is the pore radius and $c \approx 1$. The mean free path is the average distance a gas molecule travels before colliding with another molecule (Eq. 2.3). Klinkenberg’s approach is very practical in nature, but it was studied for rarified gas flowing at very low pressures. Theoretically, slippage becomes significant when the tube diameter (through which gas is flowing) becomes comparable to the mean free path of gas molecules at given pressure and temperature conditions (Amyx, Bass & Whiting, 1960). Recently, Fathi et al (2012) modified
Klinkenberg’s expression to include a double slip phenomenon. They try to capture the kinetic velocity of the molecules which have bounced back after colliding with the pore walls. This component was reportedly missed by Klinkenberg. We will discuss this important point later in the paper.

2.4 Knudsen Number and Gas Flow Regimes

A very important parameter which determines the flow regime (viscous flow, slip flow, transition and free molecular / Knudsen diffusion) is Knudsen number ($K_n$). It can be expressed mathematically as shown below (Civan et al., 2011):

$$K_n = \frac{\lambda}{r}$$  \hspace{1cm} (2.3)

The mean free path is given by (Civan et al., 2011):

$$\lambda = \frac{\mu}{P} \sqrt{\frac{\pi RT}{2M}}$$  \hspace{1cm} (2.4)

One the basis of Knudsen number, various flow regimes can be identified as shown in Table 2.1 (Schaaf & Chambre, 1961). Note that various researchers have different limits for the viscous flow region. While generally the researchers agree for Knudsen number’s limit to be 0.001 (Schaff & Chambre, 1961; Beskok & Karniadakis, 1999, Roy et al. 2003, Javadpour et. al 2007; Civan 2010, Sakhaee-Pour & Bryant, 2012) for viscous flow, some texts (Karniadakis et al., 2005; Ziarani & Aguilera, 2012a) limit it to 0.01. These limits are based on flow geometry and are empirical in nature. Hence, the limits might shift in reality based on actual flow geometry. We use the 0.001 limit in this work. The Navier Stokes’ equation, from which Darcy’s law is derived theoretically (Hubbert, 1956), works for the continuum flow regime which includes the viscous and slip flow regions (with some modifications). This approach breaks down in the transition region and for free molecular flow region. In this work, we assume pore size is 6.5 nm, so as pressure varies from 200 to 7000 psi, the correspondingly mean free path ($\lambda$) varies from 0.6 nm to 8 nm and Knudsen number ($K_n$) varies from 0.01 to 1.28 (using Eqs. 2.3,
2.4 and 2.5). The data therefore lies in the slip and transition flow regimes. We discuss each of the flow regimes further below:

2.4.1 Viscous flow

This is the region where $K_n$ has small values; $K_n \leq 0.001$. For conventional reservoirs, because pore radius is in micrometers, Knudsen number is very low ($K_n < 0.001$). In other words, the mean free path is negligible compared to pore throat size. For this range of Knudsen number, the intermolecular collisions are important and molecular collisions with pore walls are negligible. Correspondingly, the viscous flow regime prevails and Darcy’s equation works well. Darcy’s equation is therefore applicable under certain conditions: very low flow velocity; viscous forces only (inertial forces are not dominant); and flow velocity at the pore walls is zero.

2.4.2 Slip flow

This flow regime is valid for $0.001 \leq K_n \leq 0.1$. In this flow regime, the flow velocity at the pore boundary is not zero and viscous flow theory has to be modified to accommodate the slip boundary condition. Molecular collisions with pore walls start to become important compared to the intermolecular collisions because mean free path of gas molecules becomes significant compared to pore throat size. Depending upon pressure conditions, many tight gas plays fall in this region and Klinkenberg’s slippage theory generally works well. Correspondingly, most of the experimental studies measure the permeability as function of pressure and modify the Klinkenberg’s slippage factor to suit their experiments (Jones & Owens, 1980; Sampath & Keighin, 1982; Florence et al. 2007). Some of researchers try to capture the additional ‘slippage’ flux by including another physical phenomenon - Knudsen diffusion (Ertekin et al. 1986; Michel et al. 2011). We discuss all the correlations later in the paper.

2.4.3 Transition flow region

This flow regime is valid for the Knudsen number range $0.1 \leq K_n \leq 10$. This is the most difficult region for modeling but is of very high interest because most of the shales and many tight gas reservoirs fall in this region, depending on pressure conditions. For these tight reservoirs, the pore radius is much smaller (nanometer scale). Comparatively, fewer studies have
captured the flow behavior in this region - most notable amongst them is Beskok & Karniadakis’ (1999) work which forms the basis of the work of Civan (2010) and Florence et al. (2007).

2.4.4 Free molecular regime

This is the region where Knudsen number is large $K_n \geq 10$. This regime is not very frequently encountered in shales and tight gas plays, according to the experimental data study by Ziarani & Aguilera (2012a). It can be modeled using Knudsen diffusion (Sakhaee-Pour & Bryant, 2012; Ziarani & Aguilera, 2012a) or DSMC (Direct Simulation Monte Carlo) and Lattice Boltzmann simulation (Agarwal et al. 2001).

2.5 Present Approaches

Most of the studies found in literature can be grouped into 5 categories on the basis of their approach:

1. Permeability measurement in tight gas reservoirs and slippage factor determination
2. Slippage factor determination corresponding to Knudsen diffusion flux
3. Apparent permeability as a function of Knudsen number
4. Equivalent permeability including Knudsen diffusion and slippage
5. Correction to Klinkenberg’s theory

2.5.1 Permeability measurement and slippage factor determination

May authors have tried to measure the apparent or effective permeability and relate it to Klinkenberg’s slippage factor, $b_k$.

Jones & Owens (1980) studied more than 100 samples from various tight gas plays from United States and proposed the following empirical relation between slippage factor and reference permeability:

$$b_k = 12.639(k_{oo})^{-0.33} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots 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Sampath & Keighin (1982) studied 10 samples from a tight gas sand in Uinta County, Utah with nitrogen and gave an equivalent expression for slippage factor as below:
\[ b_k = 13.581 \left( \frac{k_\infty}{\phi} \right)^{-0.53} \]  \hspace{1cm} (2.6)

Florence et al. (2007) proposed a theoretical correlation for nitrogen flow in porous media by equating Klinkenberg’s slippage term with the theoretical expressions for mean free path and Knudsen number. It is expressed in terms of permeability and porosity as:

\[ b_k = 43.345 \left( \frac{k_\infty}{\phi} \right)^{-0.5} \]  \hspace{1cm} (2.7)

In the above equations, \( b_k \) is in psi and \( k_\infty \) is in mD. Note that since these expressions are independent of pressure, real gas consideration does not have any effect on the slippage factor and apparent permeability calculations. Although Sampath & Keighin and Florence et al. developed their respective correlations using nitrogen, we apply them for methane, which is an approximation.

### 2.5.2 Slippage factor on the basis of Knudsen diffusion

Ertekin et al. (1986) assumed that Knudsen diffusion causes greater than expected (compared to when only Darcy’s permeability is considered) flow. They then equated Knudsen diffusion flux to slippage postulated by Jones & Owens’ empirical relation (Eq. 2.5) and derived an expression for Knudsen diffusion coefficient as shown below:

\[ D_k = \frac{31.54}{\sqrt{M}} (k_\infty)^{0.67} \]  \hspace{1cm} (2.8)

They also expressed slippage factor as a function of Knudsen diffusion coefficient for a real gas as:

\[ b_k = \frac{\bar{p}D_k\mu c_g}{\alpha_1 k_\infty} \]  \hspace{1cm} (2.9)

In the above equations, \( D_k \) is in sq ft/D, \( M \) is gas molecular mass in kg/kmol, \( k_\infty \) is in mD, \( \bar{p} \) is average pressure in psi, \( \mu \) is gas viscosity in cP, \( c_g \) is gas compressibility in 1/psi and \( \alpha_1 \) is unit conversion factor and is equal to \( 6.328 \times 10^{-3} \text{ ft}^2\text{-cP/psi-mD-D} \). It can be seen from the above equation that \( b_k \) does not remain constant but changes with pressure. Although \( b_k \) increases with pressure, the apparent permeability decreases as pressure increases since it has a
term of $b_k/P$. Sakhaee-Pour & Bryant (2012) offer the same expression as an alternate for slippage factor in the slip flow regime.

Michel et al. (2011) used the Beskok & Karniadakis’ (1999) approach (described later) and modeled the apparent permeability with an approximation of Beskok & Karniadakis’ work. While relating the expressions for Knudsen diffusion, mean free path and average pressure, they found an equivalent expression for the slippage factor as below:

$$b_k = \frac{3\pi D_k \mu}{2r^2}$$ \hspace{1cm} (2.10)

In the above expression, $D_k$ denotes Knudsen diffusion and is given by the following equation (Igwe, 1987):

$$D_k = \frac{2r}{3 \left( \frac{8RT}{\pi M \mu} \right)^{0.5}}$$ \hspace{1cm} (2.11)

Further, Michel et al. assumed Darcy permeability to be in accordance with Hagen-Poiseuille’s equation for circular pores:

$$k_D \text{ or } k_\infty = \frac{r^2}{8}$$ \hspace{1cm} (2.12)

The above expression is valid for one pore, but porous media contain a network of pores. Taking into account matrix porosity ($\phi_m$) and tortuosity ($\tau$) gives an equivalent matrix permeability (Bear, 1972):

$$k_m = \frac{\phi_m}{\tau} k_D$$ \hspace{1cm} (2.13)

Similarly, Knudsen diffusion coefficient can also be scaled for porous media including porosity and tortuosity. Effective diffusion coefficient in the matrix can then be expressed as shown below (Grathwohl, 1998):

$$D_m = \frac{\phi_m}{\tau} D_k$$ \hspace{1cm} (2.14)

We can combine Eqs. 2.10, 2.12, 2.13 and 2.14 to find an equivalent slippage coefficient for porous media as below:
\[ b_k = \frac{3\pi D_m \mu}{16 k_m} \] \hspace{1cm} \text{(2.15)}

Michel et al. proposed the relation (Eq. 2.11) in SI units and therefore \( b_k \) is in Pa. Correspondingly, when it is applied in Eq. 2.1, average pressure (\( \overline{P} \)) should be used in Pa as well.

Note that we do not scale the Knudsen diffusion term in Ertekin’s formulation (Eq. 2.9) since their equation has a term for \( k_\infty \) which inherently has porosity and tortuosity in it.

2.5.3 Apparent permeability as a function of Knudsen number based on Beskok & Karniadakis’ work (1999)

Sakhaee-Pour & Bryant (2012) studied the different flow regimes on the basis of Knudsen number and derived flow expressions for each of them using Beskok & Karniadakis’ (1999) approach. They postulated that in the transition flow regime, the following relation holds between apparent and reference permeability:

\[ k_a = k_\infty (0.8453 + 5.4576 K_n + 0.1633 K_n^2) \] \hspace{1cm} \text{(2.16)}

This expression is valid for Knudsen number’s range: \( 0.1 \leq K_n \leq 0.8 \)

Civan (2010) studied gas flow through shale pores using Beskok & Karniadakis’ (1999) approach. He postulated an apparent permeability term based on Knudsen number as follows:

\[ k_a = k_\infty f(K_n) \] \hspace{1cm} \text{(2.17)}

\( f(K_n) \) is a function of the Knudsen number, rarefaction coefficient (\( \alpha_2 \)) and slip coefficient (b) and is given by:

\[ f(K_n) = (1 + \alpha_2 K_n) \left(1 + \frac{4K_n}{1 - bK_n}\right) \] \hspace{1cm} \text{(2.18)}

The dimensionless rarefaction coefficient (\( \alpha_2 \)) is given by:

\[ \alpha_2 = \alpha_o \left( \frac{K_n^B}{A + K_n^B} \right) \] \hspace{1cm} \text{(2.19)}

In the above expression, the lower limit for \( \alpha_2 \) is 0, which corresponds to slip flow regime. On the upper end, \( \alpha_o \) is the asymptotic limit for \( \alpha_2 \) as \( K_n \to \infty \), i.e. for free molecular flow, and A and B are curve fitting parameters. Civan (2010) determined the values to be \( \alpha_o = \)}
1.358, A = 0.178 and B = 0.4348 for a specific set of flow data in transition region for tight sands. The slip coefficient (b) was given as -1 by Beskok & Karniadakis. Knudsen number (\( K_n \)) can be determined using Eqs. 2.3 and 2.5. We refer to this correlation as Civan A (2010).

Civan (2010) also proposed an approximation to the above relation using Florence et al.’s (2007) results. For \( K_n \ll 1 \), he derived a dynamic slippage factor (function of viscosity which in turn is a function of pressure) as follows:

\[
b_k = \frac{2790 \mu}{\sqrt{M}} \left( \frac{k_{\infty}}{\phi} \right)^{-0.5}
\]

We refer to this correlation as Civan B (2010). The above equation is valid only when \( K_n \ll 1 \), but for our set of parameters, \( K_n \) becomes significantly less than one only when pressure is above 10 MPa. For such a high pressure value, however, the apparent permeability becomes negligible due to \( 1/P \) term (refer to Eq. 2.1). Hence, we do not plot the results for this prediction.

### 2.5.4 Equivalent permeability including Knudsen diffusion and slippage

Javadpour et al. (2007) and Javadpour (2009) studied flow in shale nanopores taking into account both the concentration driven flow (Knudsen diffusion) and slippage. They put forward an expression for apparent permeability as:

\[
k_a = \frac{D_k \mu M}{RT \rho} + F k_D
\]

In the above expression, \( D_k \) is Knudsen diffusion coefficient (same as used by Michel et al.), \( \mu \) is the gas viscosity, \( M \) is molecular mass, \( R \) is universal gas constant, \( T \) is temperature, \( \rho \) is average gas density, \( F \) is slippage factor (explained below) and \( k_D \) is Darcy’s permeability. The slippage factor (F) is given by (Brown et al., 1946):

\[
F = 1 + \left( \frac{8 \pi RT}{M} \right)^{0.5} \frac{\mu}{\bar{P} r} \left( \frac{2}{f} - 1 \right)
\]

In the above expression, \( \bar{P} \) is average pressure, \( r \) is nanopore radius and \( f \) is the fraction of molecules diffusely scattered on colliding with the pore wall. We infer that Javadpour developed
the ‘slippage’ term from molecular physics whereas most of the other analysts incorporated the other flow mechanisms dominant at shale nanoscale into the slippage term.

The apparent permeability term given by Javadpour can be modified for a real gas (Swami & Settari, 2012) as below:

\[ k_a = c_g D_k \mu + F_k D \] … … … … … … … … … … … … … … … … … … … … … … … … … … … … … … (2.23)

After including the effects of porosity and tortuosity in diffusion coefficient and permeability (using Eqs. 2.13 and 2.14), the apparent permeability can be expressed as:

\[ k_a = k_m \left( \frac{c_g D_m \mu}{k_m} + F \right) \] … … … … … … … … … … … … … … … … … … … … … … … … … … … … … … (2.24)

2.5.5 Theoretical correction to Klinkenberg’s theory

While many of the correlations mentioned earlier change Klinkenberg’s slippage factor to suit their experimental data, they do not cite any theoretical basis for their modification. Recently Fathi et al. (2012) modified Klinkenberg’s equation and introduced a new effective slippage factor. They claim that Klinkenberg took into account only the slippage caused by molecules which have collided elastically at the pore walls and he missed the molecules which have had inelastic collision. According to them, these molecules might make up the bulk of total molecules available and hence they introduce a new slippage term which captures double slippage. They then provide a new equation for apparent permeability as:

\[ k_a = k_{\infty} \left[ 1 + \left( \frac{b_k}{P} \right)^2 \left( \frac{L_{KE}}{\lambda} \right) \right] \] … … … … … … … … … … … … … … … … … … … … … … … … … … … … … … (2.25)

In above equation, all the terms remain the same as Klinkenberg’s original equation (Eq. 2.1 in this work), while \( L_{KE} \) is the length scale associated with the kinetic energy of molecules which bounce back after colliding with the pore walls. For the pore size considered in this work (6.5 nm), \( L_{KE}/\lambda \) is approximately 2.05 using Lattice Boltzmann simulations.
2.6 Reservoir Simulation and Well Performance Modeling

From previous work, it is shown that Knudsen number provides a reliable parameter to identify the flow regimes. Further correlations as a function of Knudsen number (Beskok & Karniadakis, 1999) can be used to estimate permeability change with pressure and/or pore size. For practical reservoir simulation, however, we would like to have a correlation relating permeability directly with pressure, which can then be readily incorporated in a reservoir simulator. Therefore, to investigate the impact of non-Darcy flow model choice on well production forecasts, we incorporate the models described above using tables of transmissibility multipliers as a function of pressure, analogous to the way Clarkson et al. (2012) incorporated dynamic-slippage. We used Schlumberger’s ECLIPSE® black oil simulator for this purpose. We built a shale reservoir model to investigate the effect of different formulations on reservoir performance. Reservoir dimensions are 500×5000×100 ft³ which is divided into 1×371×1 blocks in the X, Y and Z directions respectively. It is a dual porosity model with cubic matrix blocks of size varying from 100 ft to 10 ft. A horizontal well with a single hydraulic fracture was placed inside the reservoir with the horizontal leg penetrating along the Y axis and the hydraulic fracture parallel to X axis. The well is assumed to be perforated only at the hydraulic fracture location with no production from any other part in the horizontal section. To simulate the hydraulic fracture, we used a local grid refinement around the fracture and assigned a very high permeability to the fracture zone. Figure 2.2 shows the reservoir schematic. We did not include adsorption because we wanted to study the effect of pressure-dependent matrix permeability only. All the relevant data is tabulated in Table 2.2.

2.7 Results and Discussion

2.7.1 Apparent permeability prediction by different approaches

Using the non-Darcy expressions given above from various researchers, we investigated permeability variation with pressure and pore radius. All the calculations are for methane, which is the primary component of natural gas. We used the Benedict, Webb and Rubin (BWR) correlation as detailed by Matter et al. (1975) for calculating gas compressibility ($c_g$) and compressibility factor ($z$). Also, to calculate the gas viscosity ($\mu$), we used Carr, Kobayashi, and
Burrows correlation as detailed by Dempsey (1965). Figure 2.3 relates the pore throat radius with permeability and porosity in shale gas reservoirs. From Figure 2.3, we can see that corresponding to a pore throat radius of 6.5 nm and 15 % porosity, matrix permeability is approximately 12.5 nD. We then used Eq. 2.12 and Eq. 2.13 which relate pore radius and matrix permeability while accounting for matrix porosity and tortuosity. Using the above equations gives tortuosity value as 65. It should be emphasized that this value of tortuosity is back calculated from the ideal relations (Eq. 2.13 and 2.14), and hence may not be very representative of actual values, typically in the order of 1-5 (Ziarani & Aguilera, 2012b). But even with this consideration, it should not impact the results since it will affect all the correlations with similar magnitude. All the values assumed for analyzing the models are tabulated in Table 2.1. We can also use the empirical equation (Aguilera, 2002; Ziarani & Aguilera, 2012a):

\[
r = 2.665 \left( \frac{k_m}{100 \phi_m} \right)^{0.45}
\]

Eq. 2.26 is based on experiments on tight gas and shale gas reservoirs. Using the above equation, matrix permeability of 12.5 nD and a porosity of 0.15 yields nanopore size of 6.9 nm which is quite comparable to general equation used earlier (Eq. 2.12 and 2.13).

Figure 2.4 shows how the ratio of apparent permeability to matrix Darcy permeability varies with pressure using the various approaches. As can be seen, models given by Klinkenberg and Jones & Owens predict the lowest permeability change with pressure. Their models assume a static slippage factor (based on study of tight gas samples), which might not hold very well for shale where matrix pore size is much smaller than tight gas reservoirs. Michel et al. took Knudsen diffusion into account, and the results fall in between those by Jones & Owens and Ertekin et al. Ertekin et al. who included a dynamic slippage factor which changes with pressure, predicts a greater change in apparent permeability with pressure as compared to static slippage models. Their results are very close to Michel et al.’s work. The results of the Sakhaee-Pour & Bryant approach (using a relationship between apparent permeability and Knudsen number) almost overlaps with the results of the Civan A (2010) model. Javadpour’s model predicts much more permeability change than other models since it considers both Knudsen diffusion and slippage. The prediction using the Florence et al. theoretical model falls above those from other
models—we believe the reason is the multiplying factor 43.345 which amplifies the effect. Also notable is Fathi et al.’s prediction, which cuts across the other models. As can be seen, it predicts a higher change at low pressures and comparatively lower change at higher pressures. The practical implication of these predictions is that for the assumed pore size, the ratio of apparent permeability to Darcy permeability is small at high pressure, which is typical of reservoir pressure for many shale reservoirs, but is high at low pressure. Because flowing pressures of shale gas wells can approach the lower pressure values, however, non-Darcy flow effects could be important near the wellbore and close to the fracture face.

Figure 2.5 shows the variation in the ratio of apparent permeability to matrix Darcy permeability with respect to pore radius. As can be seen, the predictions follow generally the same order as in Figure 2.4 but there are some subtle differences. Predictions by Sampath & Keighin, Sakhaee-Pour & Bryant and Sampath & Keighin almost overlap. Also, prediction by Javadpour et al is even greater than Florence et al. for this case. In Figure 2.6, we show all the predictions again for the pore radius in a more practical range (for shale), 1 nm to 1000 nm. It can be deduced that apparent permeability effect is more prominent as pore radius decreases.

In Figure 2.7, we show the variation of slippage factor $b_k$ with pressure as predicted by the different approaches. Static slippage predicted by Klinkenberg, Jones & Owens, Sampath & Keighin and Florence et al. remains constant with pressure (hence static), Ertekin et al. slippage factor first increases and then decreases with pressure. Michel et al. considered Knudsen diffusion and the resulting slippage factor increases continuously with pressure. We see also that Klinkenberg’s slippage factor increases as a linear function of pressure. It should be noted that although slippage factor increases with pressure, apparent permeability is an inverse function of pressure (refer to Eq. 2.1), hence the net effect is that apparent permeability approaches Darcy permeability at high pressure values. In Figure 2.8, we show the variation of slippage factor as pore radius decreases. Because the slippage factor given by all the approaches has an inverse term of pore radius ($r$) or matrix permeability (refer to Eqs. 2.12 and 2.13 which relate matrix permeability with pore radius), they predict an increasing slippage factor as the pore radius decreases.
2.7.2 Case Study

Data from the Mesaverde Formation from the United States (Byrnes et al., 2009) is used for comparison of various models. Samples were obtained from the Green River, Piceance, Powder River, Sand Wash, Uinta, Washakie and Wind River basins. Nearly 2030 measurements on 776 core samples were performed including capillary pressures, permeability, porosity, and water saturation. Permeabilities of the samples were measured at 600 psi confining stress and extrapolated to 4000 psi net confining stress (above pore pressure) to simulate the reservoir conditions. Nitrogen was used as the measurement fluid with 20 to 400 psi upstream pressure and atmospheric pressure at the downstream. Further, Klinkenberg gas permeability (which we refer to as matrix absolute Darcy permeability, $k_m$) was determined by extrapolating the measured in-situ gas permeability (which we call apparent permeability, $k_a$) to infinite pressure corresponding to liquid permeability. Absolute permeability ranged from 1 nD to 200 mD which covers a wide range of shale and tight gas formations. Whereas most (52%) of the samples had permeabilities in the range 0.0001-0.01 mD (which corresponds to tight gas), a significant fraction (18%) had permeabilities less than 100 nD (which can be assumed representative of shales). Average porosity was found to be 7% with over 75% of all the samples exhibiting porosities within 10% of the mean porosity. For the Mesaverde Formation, the typical range for reservoir pressure and temperature is 2500-13000 psi and 32.2-126.7 °C, respectively.

Figure 2.9 provides a comparison of the measured apparent vs. absolute Darcy permeability values. In Figure 2.10 we plot the ratio of measured apparent to absolute Darcy permeability ($k_a/k_m$) variation with matrix absolute permeability ($k_m$). As can be seen in the figures, apparent permeability can be up to 1000 times of absolute Darcy permeability values towards the lower end, when absolute permeability goes to 1 nD. Based on their measurements, Byrnes et al. (2009) developed a correlation for Klinkenberg’s slippage factor as follows:

$$b_k = 12.3395(k_\infty)^{-0.341}$$

In the above equation, $b_k$ is in psi and $k_\infty$ is in mD. Byrnes et al. provided a range of pressure values at which the permeability measurements were carried out (20 to 400 psi). We calculated back the pressure values using their reported values for $k_a$, $k_\infty$ and $b_k$ and Eq. 2.1. Their relation for $b_k$ (Eq. 2.27) gives a reasonable match with the observed data but does not
provide a general relation which can be used later for other cases. We checked how the existing
correlations compare against the observed data. Figure 2.11 shows the ratio of apparent and
absolute permeability as predicted by various correlations against the data observed by Byrnes et
al. It shows a scattered dataset because of huge variation in measured values of apparent
permeability for same absolute permeability. This scatter is due to usage of different pressure
values to measure the apparent permeability for same absolute permeability. Additionally,
porosity is also different for different samples making the scatter even worse. To reduce the huge
scatter, we plotted the predictions by various correlations vs. Knudsen number in Figure 2.12.
Knudsen number is related to pressure, pore radius with the Eqs. 2.3, 2.4, 2.12 and 2.13. As can
be seen, incorporating porosity and pressure into Knudsen number readily reduces the scatter.
While calculating Knudsen number, the dependence of porosity on confining pressure (stress)
was also taken into account. Byrnes et al. gave the porosity dependence on confining pressure
with following relation:

\[ \phi_{in} = 0.943 \times \phi_a - 0.23 \]

In Eq. 2.28, \( \phi_{in} \) is the matrix porosity at \( in situ \) stress conditions (4000 psi confining
stress) and \( \phi_a \) is the porosity measured at ambient conditions.

As can be seen from Figure 2.12, Fathi et al.’s and Michel et al.’s correlations fail to give
good match with the observed data. Correlations given by Sakaee-Pour & Bryant, Civan A,
Klinkenberg’s and Florence et al.’s (overlapped by Klinkenberg’s prediction) correlations give
good results for comparatively low values of Knudsen number (0.01 – 1). As Knudsen number
becomes bigger than 1, these correlations over predict the increase the apparent permeability and
do not give a very good match with the observed dataset. We get a very good match with the
observed dataset using correlations given by Javadpour et al., Sampath & Keighin, Jones &
Owens, Ertekin et al. and Byrnes et al.’s own correlation. Out of these, the correlations given by
Byrnes et al. and Sampath & Keighin are empirical in nature so they do provide any information
about the physical processes which are important. Further, Ertekin et al.’s correlation is based on
Jones & Owen’s equation which itself is an empirical relation. Javadpour et al.’s relation on the
other hand is theoretical in nature and matches with the experimentally observed data – this leads
us to the conclusion that both Knudsen diffusion and slippage are important.
2.7.3 Results from Reservoir Simulation

We ran our simulation model for 30 years, while incorporating the various permeability predictions. We first discuss the results for a matrix size of 100 ft. Figure 2.13 shows the gas production rate vs. time corresponding to Darcy permeability only, as well as all the apparent permeability correlations. Figure 2.14 shows cumulative production vs. time corresponding to Darcy permeability only, as well as all the apparent permeability correlations. As can be seen, the apparent permeability correlation may increase the cumulative production significantly. In particular, with Javadpour et al.’s (2007) correlation, the cumulative production can be up to 40% higher than predicted by the Darcy’s permeability. For comparison, we also show the prediction made by the single porosity model. The single porosity model’s porosity is the sum of matrix and fracture porosities whereas the permeability is sum of matrix and fracture permeabilities respectively. Now, for our system, fracture porosity is negligible as compared to matrix porosity whereas matrix permeability is insignificant compared to fracture permeability. With this setup, the single porosity model takes the permeability of fractures and porosity of matrix from the dual porosity model. As can be seen, single porosity model gives a significantly higher prediction in this case. Note that the average reservoir pressure decreased to approx. 1500 psi at the end of the simulation run.

Next, let’s consider the case for matrix size of 10 ft. Figure 2.15 shows the gas production rate vs. time corresponding to Darcy permeability and Javadpour et al.’s correlation (which gave a very good match with the actually observed data) for apparent permeability. Figure 2.16 shows the cumulative production vs. time for the same correlations. We also show the single porosity model prediction in both the figures. Again, single porosity model’s permeability is approximated by fracture permeability and porosity by matrix porosity respectively. As can be seen, all the models give almost identical results. We can infer from this exercise that for a matrix size 10 ft, a single porosity model is adequate for production prediction. A single porosity model requires fewer parameters and is faster to run; hence it is preferred over a dual porosity model. The lack of sensitivity to the matrix permeability (which is the only variable affected by the different correlations) is explained by a rapid mass transfer between matrix and fracture due to small size of matrix blocks. For the same reason, the dual porosity and the equivalent single porosity model are almost identical.
2.8 Conclusions

Gas flow in shale nanopores can be approximated by including molecular physics in Darcy’s equation. Various approaches in the literature investigate the reasons for higher flow rates associated with non-Darcy flow and try to develop mathematical models to predict the flow. We analyzed some of the models and determined their predictions for the same set of base parameters. Though all of them predict apparent permeability change with both reservoir pressure and radii, their predictions vary quite significantly. Most of the flow in shale reservoirs occurs in slip or transition region, but it can reach free molecular flow regime as well in certain instances. We can summarize the conclusions as follows:

1. As the pressure falls from initial reservoir pressure (assumed 5000 psi in this case) to abandonment pressure (taken as 200 psi) the apparent permeability can change significantly. At 5000 psi, all the approaches predict the ratio of apparent permeability to matrix Darcy permeability to be almost 1. But at 200 psi, the ratio is predicted to be between 5 and 25 as predicted by different approaches. The practical implication is that non-Darcy effects may be important near the wellbore (or fracture face), depending on flowing pressure, but not at initial pressure in most shale plays.

2. Apparent permeability is also dependent upon pore radius. As pore radius changes from 1000 nm to 1 nm, apparent permeability can change considerably. At a pore radius of 1000 nm, the ratio of apparent permeability to matrix Darcy permeability is one, but as pore radius decreases to 1 nm, the ratio is predicted to be in the range of 3 to 45 by different approaches.

3. Knudsen number combines the effects of pressure, temperature, porosity and pore radius and hence is a better scale to compare data against. In particular it is a better parameter for evaluating effect of pressure and/or pore radius on apparent permeability in laboratory where different basins having different absolute permeability and porosity values may be studied.

4. Sakhaee-Pour & Bryant and Civan (Civan A) developed an apparent permeability model as a function of Knudsen number based on Beskok and Karniadakis’ work. The Sakhaee-Pour & Bryant, Civan A, Klinkenberg’s and Florence et al.’s correlations give a good
match with Mesaverde formation for comparatively low values of Knudsen number (0.01 to 1) and but should be used with caution for $K_n \geq 1$

5. Though the correlations postulated by Jones & Owens and Sampath & Keighin and Florence et al. were based on experiments for tight gas reservoirs, the results of predictions for shale reservoirs are reasonable. However, it should be noted that these relations are empirical in nature and do not provide any information about physical processes in play.

6. Ertekin et al. and Michel et al. introduced a dynamic slippage factor which changes with pressure. This dynamic slippage represents extra flux due to Knudsen diffusion. Though this approach takes into account the Knudsen diffusion, it does not account for actual ‘slippage’. Also, Ertekin et al.’s correlation is based on Jones & Owen’s correlation which itself is an empirical relation. Michel et al.’s prediction does not give a very good match with the Mesaverde formation data and hence it should be used with caution.

7. Javadpour et al. developed an expression for apparent permeability considering both diffusive flow (Knudsen diffusion) and slippage taking into account the molecular physics. This seems to be a more reasonable approach on a theoretical basis and also provides a reasonable match to real field data.

8. Fathi et al.’s approach investigates a new phenomenon which gives quite contrasting results compared with the other correlations. Its theoretical credibility needs to be investigated more.

9. Apparent permeability casts significant effect on cumulative production prediction. For a 100ft matrix block, we observed that taking into account the apparent permeability predicted the cumulative production to be 40 % higher than the case when it was not taken into account.

The Knudsen number is in the range of $10^{-3}$ to 1 for most of the shale reservoirs (verified from experimental data by Sakhaee-Pour & Bryant and Ziarani & Aguilera) but it can be bigger than 1 as seen with Byrnes et al.’s data set (at relatively low pressures). Nevertheless, contrary to conventional belief that non-Darcy effects affect the flow behavior at low pressures only, we
observed that it does impact the production prediction quite significantly particularly for a large matrix block, smaller pore throat radius and for low flowing bottom hole pressures. This will help us determine which of the approaches can be used for history matching and making predictions for a real reservoir. It is important to deduce here that a common practice employed in reservoir simulation, which is to arbitrarily increase matrix permeability to match the production data, might not be entirely correct. Instead the higher permeability may be a function of reservoir pressure, and therefore due to non-Darcy flow, as we demonstrated in this work. Further, matrix size was seen to have a profound effect on the production predictions.

2.9 NOMENCLATURE

A = Constant used by Civan (2010), 0.178 in this work
b = Slip coefficient used by Civan, considered equal to -1 in this work
\( b_k \) = Klinkenberg’s slippage factor, Pa (or psi when specified)
B = Constant used by Civan, 0.4348 in this work
\( c_g \) = Gas compressibility Pa\(^{-1}\) (or psi\(^{-1}\) when specified)
\( D_k \) = Knudsen diffusion constant, m\(^2\)/s (or sq ft/D when specified)
\( D_m \) = Effective Knudsen diffusion constant for the matrix taking into account porosity and tortuosity, m\(^2\)/s
\( f \) = Fraction of molecules striking pore wall which are diffusely reflected, used as 0.8 (Javadpour, 2009)
\( F \) = Gas slippage factor, dimensionless
\( k_a \) = Apparent / effective permeability, m\(^2\) (or mD when specified)
\( k_D \) = Darcy permeability, m\(^2\) (or mD when specified)
\( k_m \) or \( k_\infty \) = Matrix/Absolute liquid permeability taking into account porosity and tortuosity, m\(^2\) (or mD when specified)
\( K_n \) = Knudsen number
\( M \) = Molecular mass, kg/mol (or kg/kmol when specified)
\( P \) = Average reservoir pressure, Pa (or psi when specified)
r = Pore radius, m
\( R \) = Universal Gas constant, 8.314 J/K/mole  
\( T \) = Temperature, K  
\( u \) = Gas velocity, m/s  
\( z \) = Gas compressibility factor

**GREEK LETTERS**  
\( \alpha_1 \) = Unit conversion constant used by Ertekin et al., equal to 6.328×10^{-3} \text{ sq ft-cP/psi-mD-D} 
\( \alpha_2 \) = Dimensionless rarefaction coefficient used by Civan to define the permeability function  
\( \mu \) = Gas viscosity, Pa.s (or cP when specified)  
\( \rho \) = Gas density, kg/m³  
\( \tau \) = Tortuosity, dimensionless  
\( \phi_m \) = Matrix porosity, fraction  
\( \phi_{in} \) = Matrix porosity at \textit{in situ} stress conditions, fraction  
\( \phi_a \) = Matrix porosity at ambient conditions, fraction  
\( \lambda \) = Mean free path of gas molecules at given pressure and temperature conditions, m  
\( \lambda_1 \) = Constant used by Sakhaee-Pour & Bryant

2.10 ACKNOWLEDGEMENT

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2.11 REFERENCES


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2.12 Figures

Figure 2.1: Gas flow in (a) micropores with zero flow velocity at pore walls and (b) nanopores where gas molecules slip at pore boundary (Javadpour et al., 2007)

Figure 2.2: Reservoir schematic showing matrix pressure distribution at the end of 30 years. Also visible is the hydraulic fracture at the centre of reservoir.
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Figure 2.6: Ratio of apparent to absolute permeability ($k_a/k_m$) as a function of pore radius (1 to 1000 nm) at an average pressure 1000 psi
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Figure 2.8: Slippage factor $b_k$ as a function of pore radius (0.1 to 1000 nm) at an average pressure 1000 psi
Figure 2.9: Apparent permeability vs. absolute permeability in Mesaverde formation at 4000 psi confining pressure

Figure 2.10: Ratio of apparent to absolute permeability ($k_a/k_m$) vs. absolute permeability observed in Mesaverde formation at 4000 psi confining pressure
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Figure 2.12: Ratio of apparent to absolute permeability ($k_a/k_m$) vs. Knudsen number as predicted by various correlations compared with observed data in Mesaverde formation at 4000 psi confining pressure.
Figure 2.13: Production Rate vs. Time corresponding to different apparent permeability correlations for matrix block size 100 ft. Single Porosity Model gives the highest rate in the beginning and gradually depletes.

Figure 2.14: Cumulative Production corresponding to different apparent permeability correlations for matrix block size 100 ft. Single porosity model predicts highest production whereas Darcy permeability predicts lowest production.
Figure 2.15: Production Rate vs. Time corresponding to different apparent permeability correlations for matrix block size 10 ft. All the correlations predict almost identical production rates.

Figure 2.16: Cumulative Production corresponding to different apparent permeability correlations for matrix block size 10 ft. All the correlations predict almost identical cumulative production.
### 2.13 TABLES

**Table 2.1:** Flow Regime Based On Knudsen Number

<table>
<thead>
<tr>
<th>Knudsen number (Kn) range</th>
<th>Flow regime</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \leq 0.001 )</td>
<td>Viscous flow</td>
</tr>
<tr>
<td>( 0.001 &lt; \text{Kn} &lt; 0.1 )</td>
<td>Slip flow</td>
</tr>
<tr>
<td>( 0.1 &lt; \text{Kn} &lt; 10 )</td>
<td>Transition flow</td>
</tr>
<tr>
<td>( \text{Kn} \geq 10 )</td>
<td>Knudsen’s (free molecular) flow</td>
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**Table 2.2:** Values of Variables Used In This Paper

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
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</thead>
<tbody>
<tr>
<td>Reservoir temperature, ( T )</td>
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<td>K</td>
</tr>
<tr>
<td>Gas Molecular mass, ( M )</td>
<td>0.016</td>
<td>kg/mol</td>
</tr>
<tr>
<td>Matrix pore size</td>
<td>6.5</td>
<td>nm</td>
</tr>
<tr>
<td>Matrix Porosity, ( \phi_m )</td>
<td>0.15</td>
<td>Fraction</td>
</tr>
<tr>
<td>Tortuosity, ( \tau )</td>
<td>65</td>
<td>Dimensionless</td>
</tr>
<tr>
<td>Matrix Darcy permeability, ( k_m )</td>
<td>12.5</td>
<td>nD</td>
</tr>
<tr>
<td>Fracture Porosity, ( \phi_f )</td>
<td>0.001</td>
<td>Fraction</td>
</tr>
<tr>
<td>Fracture permeability, ( k_f )</td>
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<td>mD</td>
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<tr>
<td>Hydraulic fracture permeability</td>
<td>100000</td>
<td>mD</td>
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<tr>
<td>Matrix block size</td>
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<td>Initial reservoir pressure</td>
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<td>psi</td>
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<tr>
<td>Wellbore pressure</td>
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<td>psi</td>
</tr>
<tr>
<td>Single Porosity Model porosity</td>
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<td>Fraction</td>
</tr>
<tr>
<td>Single Porosity Model permeability</td>
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<td>mD</td>
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</table>
CHAPTER THREE: A PORE SCALE GAS FLOW MODEL FOR SHALE GAS RESERVOIR

3.1 ABSTRACT

It has been observed that the shale gas production modeled with conventional simulators/models is much lower than actually observed field data. Generally reservoir and/or stimulated reservoir volume (SRV) parameters are modified (without much physical support) to match production data. One of the important parameters controlling flow is the effective permeability of the intact shale. In this project we aim to model flow in shale nano pores by capturing the physics behind the actual process. For the flow dynamics, in addition to Darcy flow, the effects of slippage at the boundary of pores and Knudsen diffusion have been included. For the gas source, the compressed gas stored in pore spaces, gas adsorbed at pore walls and gas dissolved in kerogen bulk have been considered. To imitate the actual scenario, real gas has been considered to model the flow. Partial differential equations were derived capturing the physics and finite difference method was used to solve the coupled differential equations numerically. The contribution of Knudsen diffusion and gas slippage, gas desorption and gas diffusion from kerogen bulk to total production was studied in detail. It was seen that including the additional physics causes significant differences in pressure gradients and increases cumulative production. We conclude that the above effects should be considered while modeling and making production forecasts for shale gas reservoirs.

3.2 INTRODUCTION

A very high proportion of shale gas research has been focused towards understanding and improving the hydraulic fracturing in shales and comparatively less work has been done towards understanding the flow mechanism in the shale matrix. As a matter of fact, permeability of hydraulic fractures is higher than that of the shale matrix by orders of magnitude and it is the gas flow in the matrix which is limiting the long-term production rate. Based on our understanding of

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2 Complete citation of this work: Swami V. and Settari A. "A Pore Scale Gas Flow Model for Shale Gas Reservoirs". SPE 155756-MS, presented at 2012 SPE Americas Unconventional Resources Conference held in Pittsburgh, USA. doi: 10.2118/155756-MS. This article has been reproduced with permission from SPE.
the shale systems at present, production predicted with models developed for conventional reservoirs do not match the real data and are mostly pessimistic (Javadpour, 2009). To match the production data, the core derived matrix permeability and/or the stimulated reservoir volume (SRV) are often increased artificially. Shale gas reservoirs invariably have extremely low permeability. Pore size is usually in the range of nano meters, 5 to 1000 nm (Wang & Reed, 2009) or even smaller, 5 to 50 nm (Behar & Vandenbroucke, 1987; Bowker, 2003) and hence the permeability is in the range of nano Darcy (Cipolla et al., 2009). The equations and mathematical models developed for conventional sandstone and carbonate hydrocarbon reservoirs (pore size range 1 to 100 micron) are not applicable for shales with pores at nanoscale. More realistic treatment may be therefore able to explain part of the discrepancy between field and theory, and also assess the potential contribution of the kerogen bulk to reserves.

Generation and migration of hydrocarbons in conventional reservoirs is explained using oil migration theory. Organic matter gets deposited in the source rock and is converted into oil and gas over geologic period of time. The hydrocarbon formed then migrates until it finds a structural or stratigraphic trap which stops its further movement. The rock which finally stores the hydrocarbons is termed the reservoir rock. The cap rock is very frequently shale which has an extremely low permeability and hence does not allow any more hydrocarbon migration. In the case of shale gas reservoirs, gas forms in the source rock (which is shale) but does not migrate because of source rock’s extremely low permeability. Hence, the source rock is the same as the reservoir rock or (as sometimes called) self-sourcing rock where organic matter is still stored. This explains the presence of organic material within shale gas reservoirs (Boyer et al., 2006). This organic material or kerogen can occupy as high as 40% (v/v) of the reservoir bulk in some of the organic rich shales (Passey et al., 2010).

Several studies have proposed flow models capturing pore scale flow mechanism in shale reservoirs. Almost all the studies modify the Darcy’s equation incorporating the physics at molecular level to account for higher equivalent permeability. Most of the authors (Ertekin et al., 1986; Science Applications Inc., 1980) incorporated Klinkenberg’s slippage effect (Klinkenberg, 1941) to account for the higher than predicted value of production in tight/shale reservoirs. Clarkson et al. (2011) also modified the Darcy’s permeability with Ertekin’s dynamic slippage concept and looked for its applicability in the rate transient analysis. Ozkan et al. (2010) states
that in addition to Darcy flow, there will be concentration driven diffusion term as well. In all the above analyses, the authors used Jones & Owens’ (1980) experimental data. Jones & Owens’ conducted their experiments at 24 °C and 500 psi using air and found an expression for diffusivity constant. This concentration driven diffusion term is then modeled as an additional permeability term (slippage). Though Jones & Owens’ data can be used as a good start, it might not hold for all temperature and pressure values. Further, it is to note that Knudsen diffusion is a concentration driven flux which is different from slippage. Javadpour (2009) stated that both slippage and Knudsen diffusion become important at the shale nano pore scale. He derived the expressions based on theoretical parameters. Javadpour’s work offers good theoretical basis for a broad pressure and temperature range.

Further, lot of research has been devoted towards the study of gas adsorbed on the pore walls. While it is largely attributed to as a surface phenomenon, some authors (Chalmers & Bustin, 2007; Ross & Bustin, 2009; Clarkson & Bustin, 2011) include both; gas dissolved in organic matter and adsorbed gas into the ‘sorbed’ gas and in fact show that the dissolved gas in not insignificant in some Coal Bed Methane (CBM) reservoirs. The solution gas is normally ignored and most of the authors model the adsorption phenomenon in CBM and shale using Langmuir or Brunauer-Emmet-Teller (BET) monolayer isotherms. Note that both Langmuir and BET models assume adsorption only. We will follow Langmuir’s isotherm for the scope of this paper.

The first aim of this project is to improve the understanding on flow aspect of the shale gas reservoirs. The second aim of this project is to evaluate kerogen bulk as a gas source. We have included Knudsen diffusion and slippage both to model flow in shale nanopores. As the gas source, we have included gas adsorbed at the pore walls and gas diffusing out from kerogen bulk.

3.3 Theory

With the current knowledge and scientific advancements, we have been able to look at the shales at nano scale. Figure 3.1 (Ambrose et al., 2010) and Figure 3.2 (Loucks et al., 2009) show Scanning Electron Microscope (SEM) images of different shale samples. As can be seen from the sections in red circles, the reservoir matrix is composed primarily of clay/silica (light
grey material), organic matter/kerogen (dark grey) and some minerals like feldspar (white). Note that almost all the pores are exclusively located inside the kerogen.

Figure 3.3 shows a simplified view of shale gas reservoirs at different scales. At the nano and molecular scale, we can see gas present as free (compressed) gas in the pore space, adsorbed at the pore walls and also gas diffusing out from kerogen bulk.

Conventional belief is that the amount of gas dissolved in kerogen bulk is negligible and further to that, even if there is any gas at all, the rate of diffusion is extremely low making this quantity even more insignificant. In our best knowledge, only two papers (Javadpour et al., 2007 and Javadpour, 2009) talk about an appreciable quantity of gas diffusing out from kerogen bulk in shales. They showed statistically that a significant amount of gas diffuses out from kerogen bulk.

A classic example of continuous accumulation, shale is a self-sourcing rock. Over the geologic period of time, the organic matter gets converted into gas and builds up pressure in the system. Over time, this gas is liberated into the nanopores and it is stored as free/compressed gas and also adsorbed on the pore walls. The basic premise of our work is that kerogen bulk has to be saturated with gas at a particular pressure before it can liberate gas into the pores. In the laboratory, it may be practically impossible to determine gas solubility in kerogen bulk at a particular pressure (and temperature). We are therefore using the corresponding values for bitumen. Bitumen is a product of kerogen diagenesis. Chemically kerogen is very similar to bitumen but physically there is a major difference between them. Whereas kerogen is found to consist of a large network of interconnected pores at nano scale, bitumen is devoid of them (Tissot & Welte, 1984). However, kerogen bulk (not containing pore space) can be considered very similar to bitumen. Therefore, for this paper, we have used the saturation value corresponding to bitumen due to lack of data.

3.4 METHODOLOGY

To emulate gas flow, we represent a nanopore by a cylindrical tube. Figure 3.4 shows the physical model. Model has a single nanopore surrounded by kerogen bulk. The figure shows gas
in nano pores (free/compressed gas), gas adsorbed at the pore walls and gas dissolved in the kerogen bulk. The entire system is at initial reservoir pressure in the beginning. Left boundary of the pore is open to a constant pressure (wellbore or fracture) and the right boundary is a no flow boundary. Gas concentration at the pore boundary is related to pore pressure with Henry’s law by assuming a thermodynamic equilibrium (Sheikha et al., 2005, Felder & Rousseau, 1986). Also, the outer boundary of the kerogen bulk is assumed to be a no flow boundary.

As we open the well to flow, at first the free gas flows out. As pressure drops down, gas desorbs from the pore walls and finally gas starts diffusing from the kerogen bulk. We formulated the differential equation taking into account Knudsen diffusion, slippage, gas desorption and gas diffusing from kerogen bulk for a real gas. The complete derivation is shown in Appendix A. We referred to Javadpour’s previous works (Javadpour et al., 2007 and Javadpour, 2009) for the derivation of basic equations for non-Darcy flow mechanisms. The final equation for gas flow in the nano pore takes on the following form:

\[
\frac{M}{RT} \frac{\partial}{\partial x} \left( \frac{k_{app} \partial p_n^2}{z \mu} \right) - \frac{\rho_{ntp} \rho_{bi} G_L}{SV} \frac{b}{r_n (1 + b p_n)^2} \frac{\partial p_n}{\partial t} + \frac{4}{r_n} D_k \frac{\partial C}{\partial r} \bigg|_{(r=r_n)} = \frac{M}{RT z c_g} \frac{\partial p_n^2}{\partial t} \ldots \ldots (3.1)
\]

Here the first term shows apparent permeability taking into account Knudsen diffusion and slippage, second term accounts for gas desorption and third term shows gas diffusion flux from kerogen bulk. All the symbols are explained in the nomenclature.

### 3.5 Results and Discussion

Before using the numerical model, we did a very simple gas in place and time magnitude analyses to compare the free gas, adsorbed gas and gas dissolved in kerogen bulk. For a pore radius of 2 nm and length of 1 cm, we calculated free gas as $1.4 \times 10^{-17}$ m³, adsorbed gas as $2.5 \times 10^{-17}$ m³ and gas dissolved in kerogen bulk as $2.25 \times 10^{-16}$ m³ at Normal Temperature and Pressure (NTP) condition. This shows that the quantities of gas stored as free gas, adsorbed gas and dissolved in kerogen bulk have similar order of magnitudes and are comparable. Details of the calculations are shown in Appendix B. We also tried to check the time scales of gas flow in nano pore and rate of diffusion from kerogen bulk. We observed that the two time scales are
quite comparable using the values tabulated in Table 3.1. Details of the calculations can be found in Appendix C.

Next, we solve the Eq. 3.1 numerically. We formed an implicit model to imitate the gas flow in nano pore while kerogen bulk feeds the pore. Nanopore was discretized along its length and kerogen bulk both radially and along the length of nanopore. The nanopore length has been found to be in the range of 100 nm (Ambrose et al., 2010) and matrix size after hydraulic fracturing is in sub-meter range. To study the behavior, we took various length scales for the pore; 100 nm to 1 m to see the effects over a wide range of pore lengths. Also, we took the kerogen bulk diffusion coefficient in the range of $2 \times 10^{-12}$ to $2 \times 10^{-10}$ m$^2$/s which correspond to typical value for bitumen (Svrcek & Mehrotra, 1982; Sheikha et al., 2005) and kerogen (Stainforth & Reinders, 1990; Thomas & Clouse, 1990).

We will discuss the results for two extremes of pore length; 100 nm and 1 m. Figure 3.5 shows pressure profile in 100 nm long pore along its length after a time of 5 ns. Pressure profile corresponding to Darcy permeability is shown by line with crosses (purple). If we take Knudsen diffusion and slippage into account, the effective permeability increases, and correspondingly pressure drops faster in the pore. This is shown by the line with solid squares (red). If we take desorption into account, it acts as an extra source of gas and helps in maintaining the pressure. Correspondingly the pressure profiles shifts up, as shown by the line with tiles (blue). Now, if we take gas diffusion from kerogen bulk into account, it acts as another gas source and increases the pressure further along the pore, as shown by the line with triangles (green). It can be noted that diffusion from kerogen bulk does bump up the pressure profile inside nanopore but not very considerably. This is due to the very small time frame we have considered, over which gas diffusion from kerogen bulk does not contribute significantly to nanopore pressure. Figure 3.6 shows the cumulative production at different times. As can be seen, all the additional effects increase the production when compared with the case when only the Darcy permeability was considered. Again, consideration of diffusion from kerogen bulk does increase the production but not very significantly.

Figure 3.7 and Figure 3.8 show pressure and production profiles respectively along nanopore length for 1 m long nanopore after 100 hr. As can been seen in the figures, here the
above mentioned effects are much more prominent as compared to the pore length of 100 nm. Gas diffusion from kerogen bulk helps to maintain the pressure and increases the total production very significantly.

Table 3.2 shows the net increment in production values after considering additional physics. For a 100 nm long pore, production increases by 108% when considering Knudsen diffusion and slippage, by further 26% when taking desorption into account and by approximately another 7% by accounting for gas diffusion from kerogen bulk. The corresponding values for 1 m long pore are 128%, 22% and 430% respectively.

Having presented the above results, we now discuss the limitations of this model. First, the methane gas solubility for kerogen bulk might not be the same as bitumen. But as stated earlier, it’s almost impossible to separate nanopores from the kerogen and determine the solubility for kerogen bulk and hence bitumen is the closest approximation at this stage. Further, methane content of a particular kerogen will also depend upon its type and maturity (Ross & Bustin, 2009). Second, kerogen bulk radius assigned to the simulated pore may not be ten times of the pore radius. A given kerogen bulk volume is feeding many pores which it is in contact with, and the correct volume to be assigned to a single pore will depend on the number density of nanopores. Third, the length of the nanopore is uncertain as it can be visualized as the total length of short pores that are connected together. Finally, the inorganic matter (clay, silica and other minerals) present along with kerogen bulk will also impact the final permeability and productivity calculations.

The results raise the old debate: is organic matter good for gas production or not? Fracturing operations prefer brittle rocks, which would shatter the rock in small fragments on fracturing. On the other hand, organic matter may account for most of the gas in place, but it makes the rocks less brittle and hence lessens their propensity to be fractured.

Another point we wish to bring out is the comparison with Coal Bed Methane (CBM). Coal in CBM reservoirs has similar kerogen content and hence gas is dissolved in CBM kerogen bulk too. There are similarities between the “Triple Porosity” model in CBM and the formulation proposed here. However, whereas reservoir pressure in coal is usually low—typically (less than 200 psi to over 1500 psi, depending on the seam depth), for shale gas reservoirs the initial
pressure is much higher (less than 5000 psi to over 10,000 psi). Because of this high pressure, amount of gas dissolved in shale kerogen bulk may be very significant. Ultimately more research is needed to ascertain the controlling parameters for kerogen bulk more confidently and to be able to predict production with more certainty. We can then upscale this model for the porous media and actual reservoir.

Last but not least, the consideration of kerogen bulk will have an impact on the way canister tests are interpreted and modeled for shale reservoirs. Canister test has been widely used in the industry to assess the amount of adsorbed gas in CBM reservoirs and has now been extended to shales as well. This is done owing to the presence of similar organic matter (kerogen) in coal and shale. This organic matter keeps the gas adsorbed; hence gas is primarily stored in adsorbed state only. Therefore, when a canister test is performed in coal, only the desorbed gas in coal is measured. Shale differs from coal in many aspects. The major differences are higher reservoir pressure, pore size (Jenkins & Boyer, 2008) and size and density of natural fractures. In shale gases coming from matrix pores, desorption and diffusion from kerogen bulk have similar order of magnitude. Hence, gas obtained during a canister test is not only the desorbing gas. Mengal & Wattenbarger (2011) concluded that total evolved (perceived as adsorbed gas only) gas can account for up to 30% of the OGIP for a Barnett shale sample. We believe that this gas may be a combination of free (in nanopores and natural fractures), adsorbed and kerogen bulk dissolved gas. Work is ongoing in this direction to be able to separate the gas obtained during canister test into the gas stored in nanopores, gas adsorbed on the pore walls and gas dissolved in kerogen bulk.

3.6 CONCLUSIONS

Instead of answering all the questions about the flow mechanisms for shale nanopores, we actually raise further questions and show potential for further research. What we get at the surface is a certain quantity of gas and our aim is to assign this gas to proper sources, and proper modeling of the flow including all the related physics. Our results for Knudsen diffusion, slippage and desorption are in agreement with the results available in literature, concluding that these effects should be included in the production modeling. Additionally, the above results
show that gas diffusion from kerogen bulk is quite significant for shale gas reservoirs and should not be ignored. We draw final conclusions as below:

1. Gas dissolved in kerogen bulk is significant. The simulation was based on the methane solubility data for bitumen and further research is needed to make a conclusive statement. However, on the basis of the above study we can say that one should consider the gas dissolved in kerogen bulk while calculating the Original Gas in Place.

2. Rate of gas diffusion from kerogen bulk is substantial and should not be ignored while modeling the shale reservoirs.

3. Canister tests used to determine the desorbed gas in shale need to be reinterpreted and modeled in order to distinguish desorbed gas from the kerogen bulk dissolved gas.

4. More research is required to upscale the physics to macro-scale which can be used in numerical models.

5. Similarities with CBM can be employed to develop field-scale modeling techniques for shale reservoirs which would incorporate diffusion from kerogen bulk.

### 3.7 Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>Cross sectional area, m$^2$</td>
</tr>
<tr>
<td>AFM</td>
<td>Atomic Force Microscope</td>
</tr>
<tr>
<td>$b$</td>
<td>Langmuir’s constant, Pa$^{-1}$</td>
</tr>
<tr>
<td>$c_g$</td>
<td>Gas compressibility Pa$^{-1}$</td>
</tr>
<tr>
<td>$c_f$</td>
<td>Formation compressibility, Pa$^{-1}$</td>
</tr>
<tr>
<td>$c_t$</td>
<td>Total compressibility, Pa$^{-1}$. $c_t = c_g + c_f$, since we consider only one pore here whose porosity remains constant, $c_f = 0$ and hence $c_t = c_g$</td>
</tr>
<tr>
<td>$C$</td>
<td>Gas concentration in kerogen bulk, kg/m$^3$</td>
</tr>
<tr>
<td>$C_i$</td>
<td>Gas concentration in kerogen bulk at initial reservoir pressure and temperature, kg/m$^3$</td>
</tr>
<tr>
<td>$D$</td>
<td>Knudsen diffusion constant, m$^2$/s</td>
</tr>
</tbody>
</table>
\( D_k \) = Diffusion constant for gas diffusion through kerogen bulk, \( m^2/s \)

\( f \) = Fraction of molecules striking pore wall which are diffusely reflected

\( F \) = Gas slippage factor, dimensionless

\( G_L \) = Langmuir’s volume, NTP \( m^3 \) of gas/kg of shale sample

\( J_{des} \) = Desorption Mass Flux, \( kg/m^2-s \)

\( J_{diff} \) = Gas Mass Flux from kerogen bulk diffusion, \( kg/m^2-s \)

\( J_{ads} \) = Adsorption Mass Flux, \( kg/m^2-s \)

\( k_{app} \) = Apparent permeability, \( m^2 \)

\( k_D \) = Darcy permeability, \( m^2 \)

\( k_H \) = Henry’s constant, \( kg/Pa/m^3 \)

\( K_{des} \) = Equilibrium constant for desorption, \( kg/m^2-s \)

\( K_{ads} \) = Equilibrium constant for adsorption, \( kg/Pa-m^2-s \)

\( L \) = Length of the nanopore, \( m \)

\( M \) = Molecular mass, \( kg/mol \)

\( N \) = Avagadro’s number, \( 6.022 \times 10^{23} \)

\( NTP \) = Normal temperature and pressure conditions. Normal temperature is defined as 273 K and normal pressure as \( 1.01325 \times 10^5 \) Pa

\( p_n \) = Nanopore pressure, \( Pa \)

\( p_{avg} \) = Average pressure, \( Pa \)

\( Q \) = Production rate, \( m^3/s \)

\( r_n \) = Pore radius, \( m \)

\( R \) = Universal Gas constant, \( 8.314 \) J/K/mol

\( R_k \) = Kerogen bulk radius, \( m \)

\( S_o \) = Total number of surface sites (per unit area) available for adsorption

SEM = Scanning Electron Microscope

\( SV \) = Surface area to volume ratio, \( m^{-1} \)

\( T \) = Temperature, \( K \)

\( u \) = Gas velocity, \( m/s \)

\( z \) = Gas compressibility factor

Greek Letters

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\( \mu = \) Gas viscosity, Pa.s  
\( \rho = \) Gas density, kg/m³  
\( \rho_{bi} = \) Bulk density of shale at initial reservoir pressure, kg/m³  
\( \tau = \) Tortuosity, dimensionless  
\( \phi = \) Matrix porosity, fraction  
\( \theta = \) Fraction of total available surface sites occupied by molecules

3.8 Acknowledgement

We wish to thank Dr. Chris Clarkson, Arshad Islam and Catalina Sanchez at University of Calgary and Dr. Farzam Javadpour and Vahid Shabro at University of Texas (Austin) for their valuable comments and discussions. We also wish to acknowledge the financial aid from the consortium for Shale Gas Modeling at University of Calgary for supporting the research funding.

3.9 References


Ruthven, D. M. 1984 *Principles of Adsorption and Adsorption Processes*. John Wiley and Sons, USA


### 3.10 Appendix 3A

Referring to Figure 3.4, we see that gas is stored as free/compressed gas in the nano pores, as adsorbed gas on the pore walls and dissolved in kerogen bulk as well. Consider an element of length $\Delta x$ at a distance $x$ from left boundary as shown in Figure 3.9.

Taking into account the diffusive flow (attributed to Knudsen diffusion) and convective flow (owing to Darcy permeability), we can write the mass balance equation as:

\[
\left\{ \left( -D \frac{\partial \rho}{\partial x} A + uA\rho \right)_x - \left( -D \frac{\partial \rho}{\partial x} A + uA\rho \right)_{x+\Delta x} \right\} = \frac{\Delta(\rho A \Delta x)}{\Delta t} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (3.2)
\]

Where $D$ refers to Knudsen diffusion coefficient, $\rho$ is gas density, $A$ denotes the cross sectional area ($\pi r^2_n$) for the cylindrical tube and $u$ is convective (Darcy) velocity accounting for slippage. $k_D$ is the Darcy permeability and is given by Poiseuille equation for circular capillaries as:

\[
k_D = \frac{r_n^2}{8} \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (3.3)
\]
$p_n$ denotes pressure in nanopore at any time in the element $\Delta x$. Slippage factor $F$ (Brown et al., 1946; Javadpour et al., 2007) and Knudsen diffusion coefficient $D$ (Igwe, 1987; Javadpour et al., 2007) are defined as follows:

\[ F = 1 + \left( \frac{8\pi RT}{M} \right)^{0.5} \frac{\mu_g}{p_{avg}r_n} \left( \frac{2}{f} - 1 \right) \] ................................. (3.4)

\[ D = \frac{2r_n}{3} \left( \frac{8RT}{\pi M} \right)^{0.5} \] ................................. (3.5)

Ruthven (1984) also proposed an expression for Knudsen diffusion coefficient as follows. In this equation, pore radius is expressed in cm.

\[ D = 9700r_n \left( \frac{T}{M} \right)^{0.5} \] ................................. (3.6)

We found the above two expressions to be almost identical. Just as a quick note, the slippage we encounter in shale gas reservoirs is analogous to Klinkenberg’s slippage which was an experimentally observed behavior. Theoretically, slippage becomes significant when the tube diameter (through which gas is flowing) becomes comparable to the mean free path of gas molecules at given pressure and temperature conditions (Amyx, Bass & Whiting, 1960). Klinkenberg’s slippage becomes active for conventional reservoirs only at low pressure when the above condition is met. For shale gas reservoirs, even though the reservoir pressure is very high, slippage becomes important due to the extremely small size of pores.

For a porous matrix, Darcy’s permeability and Knudsen diffusion coefficient can be expressed using matrix porosity and tortuosity as follows. We have assumed $\phi$ and $\tau$ as one inside the pore for this paper.

\[ k_m = \frac{\phi}{\tau} k_D \] ................................. (3.7)

\[ D_m = \frac{\phi}{\tau} D \] ................................. (3.8)

If we assume that the adsorption-desorption follows Langmuir’s isotherm, desorption flux per unit area is given by:
\[ J_{des} = K_{des} \theta \] (3.9)

Where \( J_{des} \) denotes the desorption flux per unit area, \( K_{des} \) denotes the equilibrium constant for desorption and \( \theta \) denotes the fraction of surface sites occupied by gas molecules.

Adsorption flux per unit area can be given by:
\[ J_{ads} = K_{ads} (1 - \theta) p_n \] (3.10)

Where \( J_{ads} \) denotes the adsorption flux per unit area, \( K_{ads} \) denotes the equilibrium constant for adsorption. There will always be a dynamic equilibrium between adsorption and desorption. As the pressure drops in nanopore (due to gas flow), \( \theta \) will readjust to attain equilibrium corresponding to the lower pressure value. Hence, we get by equating the two fluxes:
\[ \theta = \frac{K_{ads} p_n}{K_{des} + K_{ads} p_n} \] (3.11)

Referring to Shabro et al. (2011), desorption flux per unit area can be written as:
\[ \left( \frac{S_o M}{N} \frac{\Delta \theta}{\Delta t} \right) \] (3.12)

Where \( S_o \) is the total number of surface sites available for adsorption per unit area (referred to at the initial reservoir temperature and pressure conditions), \( M \) is gas molecular mass and \( N \) is Avogadro’s number. Desorption flux for the elemental area will then be:
\[ \left( \frac{S_o M}{N} \frac{\Delta \theta}{\Delta t} \right) 2 \pi r_n \Delta x \] (3.13)

Adding this desorption flux will make the equation as:
\[ \left\{ \left( \frac{\partial \rho}{\partial x} A - u A \rho \right) \right\}_{x+\Delta x} - \left\{ \left( \frac{\partial \rho}{\partial x} A - u A \rho \right) \right\}_x - \left( \frac{S_o M \Delta \theta}{N} \frac{\Delta \rho}{\Delta t} \right) 2 \pi r_n \Delta x = \frac{\Delta (\rho A \Delta x)}{\Delta t} \] (3.14)

Note that desorption term has a negative sign since the fraction of sites covered with molecules (\( \theta \)) decreases with desorption as pressure falls in the nanopore due to gas flow. On dividing by the element’s volume (\( \pi r_n^2 \Delta x \)) and taking limit changes Eq. 3.14 into the partial differential equation:
\[
\frac{\partial}{\partial x} \left\{ \rho \left( c_gD + F \frac{k_D}{\mu} \right) \frac{\partial p_n}{\partial x} \right\} - \left( \frac{S_oM \partial \theta}{N \partial t} \right) \frac{2}{r_n} = \rho c_g \frac{\partial p_n}{\partial t} \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots (3.15)
\]

Gas compressibility \( c_g \) is simply:

\[
c_g = \frac{1}{\rho} \frac{\partial \rho}{\partial p} \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots . \quad (3.16)
\]

We can now introduce a term for apparent permeability,

\[
k_{app} = c_gD\mu + Fk_D \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots . \quad (3.17)
\]

We can write desorption term in a more recognizable form. Recalling the equation for fraction of surface sites occupied by gas molecules (Eq. 3.11):

\[
\theta = \frac{K_{ads}p_n}{K_{des} + K_{ads}p_n}
\]

Dividing numerator and denominator by \( K_{des} \) and replacing \( K_{ads}/K_{des} \) by more commonly known parameter \( b \) (Langmuir’s constant), we get,

\[
\theta = \frac{bp_n}{1 + bp_n} \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots . \quad (3.18)
\]

Implying:

\[
\frac{\partial \theta}{\partial t} = \frac{b}{(1 + bp_n)^2} \frac{\partial p_n}{\partial t} \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots . \quad (3.19)
\]

\( S_oM/N \) denotes total weight of gas molecules occupying the available surface sites per unit area. This can be expressed as:

\[
\frac{S_oM}{N} = \frac{\rho_{ntp}\rho_bG_L}{SV} \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots . \quad (3.20)
\]

Where \( \rho_{ntp} \) is gas density at normal temperature and pressure conditions, \( \rho_b \) is the bulk density of shale sample at initial reservoir pressure, \( G_L \) is the Langmuir’s volume and \( SV \) is surface area to volume ratio for the shale sample. We can then write the combined equation as:

\[
\frac{\partial}{\partial x} \left( \rho \frac{k_{app}}{\mu} \frac{\partial p_n}{\partial x} \right) - \frac{\rho_{ntp}\rho_bG_L}{SV} \frac{2}{r_n(1 + bp_n)^2} \frac{\partial p_n}{\partial t} = \rho c_g \frac{\partial p_n}{\partial t} \quad \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots \cdots . \quad (3.21)
\]
This can be rewritten as:

\[
\frac{M}{2RT} \frac{\partial}{\partial x} \left( k_{app} \frac{\partial p_n^2}{\partial x} \right) - \frac{\rho_{ntp} \rho_b G_L}{5V} \frac{b}{r_n (1 + b p_n)^2} \frac{\partial p_n}{\partial t} = \frac{M}{2RTz} c_g \frac{\partial p_n^2}{\partial t}
\] ………………………………… (3.22)

\( z \) is the gas compressibility factor. The initial and boundary conditions can be represented as:

**I.C.** \( \rightarrow p_n = p_i \); \( t = 0 \); \( 0 \leq x < L \) …………………………………………………………………………………………………………………… (3.23)

**B.C. 1 \( \rightarrow p_n = p_w \); \( x = 0 \), \( t > 0 \) ………………………………………………………………………………………………………………… (3.24)

**B.C. 2 \( \rightarrow \frac{\partial p_n}{\partial x} = 0 \); \( x = L \), \( t > 0 \) ………………………………………………………………………………………………………………… (3.25)

Where \( p_i \) is initial reservoir pressure, \( p_w \) is the constant well bore/fracture pressure at which well is produced. Right boundary is assumed to be a no flow boundary.

Now, let’s consider the diffusion from kerogen bulk. Refer to Figure 3.4 for the physical model. Kerogen bulk is assumed to surround the nanopore radially. It is of finite extent and known radius (assumed 10 times of the nanopore radius for this work). Let \( C \) denote the gas concentration in kerogen bulk \((\text{kg/m}^3)\) at any time; we can write the diffusivity equation in radial coordinates as below:

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( D_k \frac{\partial C}{\partial r} \right) = \frac{\partial C}{\partial t}
\] ………………………………………………………………………………………………………………………………………………….. (3.26)

Where \( D_k \) denotes diffusivity coefficient in kerogen bulk, \( r \) denotes kerogen bulk radius. The initial and boundary conditions can be written as:

**I.C.** \( \rightarrow C = C_i = k_H p_i \); \( t = 0 \); \( 0 \leq r \leq R_k \) ……………………………………………………………………………………………………………………………………… (3.27)

**B.C. 1 \( \rightarrow C = k_H p_n \); \( r = r_n \), \( t > 0 \) …………………………………………………………………………………………………………… (3.28)

**B.C. 2 \( \rightarrow \frac{\partial C}{\partial r} = 0 \); \( r = R_k \), \( t > 0 \) …………………………………………………………………………………………………………… (3.29)

\( C_i \) is the gas concentration at initial reservoir pressure and \( k_H \) is Henry’s constant (Sheikha et al., 2005, Felder & Rousseau, 1986). The nanopore and Kerogen bulk equations get coupled with the boundary condition 1 (Eq. 3.28). At outer boundary kerogen bulk is surrounded
by silica/clay/minerals and hence it can be assumed to be a no flow boundary. Diffusive gas flux per unit area \((\text{kg/m}^2)\) can then be represented as:

\[
J_{\text{diff}} = -D_k \frac{\partial C}{\partial r} \bigg|_{(r=r_n)}
\]  

(3.30)

Which can be combined with Eq. 3.22 to form the final equation having Knudsen diffusion, slippage, desorption and gas diffusion from kerogen bulk as:

\[
\frac{M}{RT} \frac{\partial}{\partial x} \left( \frac{k_{\text{app}} \rho_{\text{ntp}} G_L 4 b \frac{\partial p_n}{\partial t}}{z \mu SV r_n (1 + b p_n)^2} + \frac{4}{r_n} D_k \frac{\partial C}{\partial r} \right) \bigg|_{(r=r_n)} = \frac{M}{RT z c_g} \frac{\partial p_n^2}{\partial t} \]  

(3.1)

3.11 AppE3B

Consider the Figure 3.9 and nano pore of length 1 cm. Compressed/free gas in the pore at NTP can be given by:

\[
G_c = \frac{\pi r_n^2 L}{p_{\text{ntp}} T_{\text{ntp}}} \frac{p_{\text{ntp}} T_{\text{res}}}{p_{\text{ntp}} T_{\text{res}}} \]  

(3.31)

Using the values in Table 3.1: \(r_n = 2 \text{ nm}, L = 1 \text{ cm}, p_{\text{ntp}} = 1.72 \times 10^7 \text{ Pa}, T_{\text{ntp}} = 273 \text{ K}, p_{\text{ntp}} = 1.01325 \times 10^5 \text{ Pa}, T_{\text{res}} = 423 \text{ K};\) we can calculate the compressed gas as:

\[
G_c = 1.4 \times 10^{-17} \text{ m}^3 (\text{NTP})
\]  

(3.32)

Quantity of adsorbed gas can be calculated as shown below:

\[
G_{\text{ads}} = 2\pi r_n L \frac{G_L \rho_{\text{bi}}}{SV}
\]  

(3.33)

Using values from Table 3.1: \(G_L = 0.02 \text{ m}^3 (\text{NTP)/kg}, \rho_{\text{bi}} = 2500 \text{ kg/m}^3, SV = 2.5 \times 10^8 \text{ m}^{-1},\) we evaluate adsorbed gas as:

\[
G_{\text{ads}} = 2.5 \times 10^{-17} \text{ m}^3 (\text{NTP})
\]  

(3.34)

Finally, the amount of gas dissolved in kerogen bulk (using the solubility corresponding to bitumen) can be calculated from following relation:

\[
G_k = \text{sol}_i \times \pi (R_k - r_n^2) L
\]  

(3.35)
Using values from Table 3.1: \( \textit{sol} = 17.94 \text{ m}^3 \text{ (NTP)/m}^3 \), \( R_k = 20 \text{ nm} \), we can evaluate dissolved gas as:

\[
G_k = 2.25 \times 10^{-16} \text{ m}^3 \text{ (NTP)}
\] ……………………………………………………………………………………………………… (3.36)

3.12 APPENDIX 3C

We can compare two processes by having a comparison of their characteristic times. We define the characteristic time for flow through nanopore as:

\[
t_D1 = \frac{\Delta t \ast \eta}{L^2}
\] ……………………………………………………………………………………………………… (3.37)

And for gas diffusion from kerogen bulk:

\[
t_D2 = \frac{\Delta t \ast D_k}{R_k^2}
\] ……………………………………………………………………………………………………… (3.38)

Hydraulic diffusivity is normally defined as:

\[
\eta = \frac{k}{\phi \mu c_t}
\] ……………………………………………………………………………………………………… (3.39)

But for this case when we have an apparent permeability term, and using the values in Table 3.1:

\[
\eta = \frac{k_{app}}{\phi \mu c_t} = \frac{c_g D + F \frac{k_D}{\mu}}{\phi c_t} \approx 1 \times 10^{-5} \text{ m}^2 / \text{s} ……………………………………………………………………………………………………… (3.40)
\]

And using the diffusivity constant corresponding to methane diffusion in kerogen,

\[
D_k \approx 1 \times 10^{-12} \text{ m}^2 / \text{s} ………………………………………………………………………………………………… (3.41)
\]

We find the two characteristic times are quite comparable.
3.13 **Figures**

**Figure 3.1:** SEM image of shale gas reservoir (Ambrose et al., 2010)

**Figure 3.2:** SEM image of shale gas reservoir showing kerogen and location of pores (Loucks et al., 2009)
**Figure 3.3:** From macro to nano scale (modified from Javadpour et al., 2007)

**Figure 3.4:** Physical model to model the flow in nanopore
Figure 3.5: Pressure profiles in 100 nm long pore after 5 ns with $D_k = 2 \times 10^{-10}$ m$^2$/s

Figure 3.6: Production profiles in 100 nm long pore after 5 ns with $D_k = 2 \times 10^{-10}$ m$^2$/s
Figure 3.7: Pressure profiles in 1 m long pore after 100 hr with \( D_k = 2 \times 10^{-12} \text{ m}^2/\text{s} \)

Figure 3.8: Production profiles for 1 m long pore after 100 hr with \( D_k = 2 \times 10^{-12} \text{ m}^2/\text{s} \)
Figure 3.9: Gas flow in shale nanopore

3.14 Tables

Table 3.1: Values of parameters used in this paper

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f$</td>
<td>0.8</td>
<td>Dimensionless</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Reservoir temperature, $T$</td>
<td>423</td>
<td>K</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Viscosity, $\mu$</td>
<td>$1.75 \times 10^5$</td>
<td>Pa.s</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Nano pore radius, $r_n$</td>
<td>$2.00 \times 10^{-9}$</td>
<td>m</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Nano pore length, $L$</td>
<td>100 nm to 1 m</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Kerogen bulk diffusion coefficient, $D_k$</td>
<td>$2.00 \times 10^{-12}$ to $2.00 \times 10^{-10}$</td>
<td>m$^2$/s</td>
<td>Stainforth &amp; Reinders (1990) and Thomas &amp; Clouse (1990)</td>
</tr>
<tr>
<td>Knudsen diffusion coefficient, $D$</td>
<td>$9.98 \times 10^{-7}$</td>
<td>m$^2$/s</td>
<td>Calculated</td>
</tr>
<tr>
<td>Langmuir volume, $G_L$</td>
<td>0.02</td>
<td>m$^3$ (NTP)/kg</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Langmuir constant, $b$</td>
<td>$4.00 \times 10^{-7}$</td>
<td>l/Pa</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Initial reservoir pressure, $p_i$</td>
<td>$1.72 \times 10^7$</td>
<td>Pa</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Wellbore/fracture pressure, $p_w$</td>
<td>$8.60 \times 10^6$</td>
<td>Pa</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Initial bulk density, $p_{bi}$</td>
<td>2500</td>
<td>kg/m$^3$</td>
<td>Schamel (2005)</td>
</tr>
<tr>
<td>Surface to volume ratio, $SV$</td>
<td>$2.50 \times 10^8$</td>
<td>m$^{-1}$</td>
<td>Howard (1991)</td>
</tr>
<tr>
<td>CH$_4$ solubility</td>
<td>17.94</td>
<td>m$^3$ (NTP)/m$^3$</td>
<td>Svrcek &amp; Mehrotra (1982)</td>
</tr>
<tr>
<td>Kerogen bulk radius, $R_k$</td>
<td>$2.00 \times 10^{-8}$</td>
<td>m</td>
<td>Assumed 10 times of nanopore</td>
</tr>
<tr>
<td>Henry's constant, $k_H$</td>
<td>$7.45 \times 10^{-7}$</td>
<td>kg/Pa/m$^3$</td>
<td>Calculated</td>
</tr>
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</table>
**Table 3.2:** Incremental production values corresponding to additional physics considered

<table>
<thead>
<tr>
<th>Effect</th>
<th>Increase in production</th>
<th>Increase in production</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100 nm, $\Delta t = 5$ ns</td>
<td>1 m, $\Delta t = 100$ hr</td>
</tr>
<tr>
<td>Darcy permeability</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>+ Knudsen diffusion and slippage</td>
<td>108 %</td>
<td>128 %</td>
</tr>
<tr>
<td>+ Desorption</td>
<td>26 %</td>
<td>22 %</td>
</tr>
<tr>
<td>+ Diffusion from kerogen bulk</td>
<td>7 %</td>
<td>430 %</td>
</tr>
</tbody>
</table>
CHAPTER FOUR: A NUMERICAL MODEL FOR MULTI-MECHANISM FLOW IN SHALE GAS RESERVOIRS WITH APPLICATION TO LABORATORY SCALE TESTING

4.1 ABSTRACT

Shale is a complex unconventional reservoir having a variety of storage and flow mechanisms coupled together. Contrary to conventional reservoirs where gas is stored only in the pore space as free gas; current numerical simulators assume gas is stored as free and adsorbed phase in shale. Recent advancement of visualization and measurement techniques has enabled us to look at shale more closely. Shale has been found to contain a well-developed nanopore network in the organic matter or kerogen. Correspondingly we believe that gas is stored via four storage mechanisms: gas in natural fractures, free gas in pores, adsorbed gas and gas dissolved in kerogen bulk in the shales.

In this work we formulate a flow model for shale gas reservoirs including the physics at nano scale. The model incorporates the gas stored in micro-fractures, gas stored in nanopores, gas adsorbed on the pore walls and gas dissolved in kerogen bulk. This complex quad porosity system has coupled equations between three interconnected systems; between matrix and fracture set, between matrix and adsorbed gas and between matrix and kerogen bulk. Sets of governing equations were derived for the coupled systems and numerically solved to find gas production as a function of time. The model was validated against laboratory observed data for a shale canister test from a Canadian shale gas field. This laboratory scale model can be suitably up-scaled for field scale simulation of shale reservoirs.

4.2 INTRODUCTION

Shale reservoirs are quite different from conventional reservoirs with respect to deposition history, storage mechanisms and rock pore size. First—whereas in a conventional

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3 Complete citation of this work: Swami V., Settari A. and Javadpour F. In press “A Numerical Model for Multi-mechanism Flow in Shale Gas Reservoirs with Application to Laboratory Scale Testing”. SPE-164840-MS, to be presented at 2013 SPE EUROPEC in London, UK. doi: 10.2118/164840-MS. This article has been reproduced under copyright agreement with SPE.
reservoir the hydrocarbons migrate from source rock to reservoir rock, shale is both the source and reservoir rock in itself. The organic matter gets deposited and converted into gas but does not escape. This is a result of the extremely low permeability of shale pores and the absence of large pressure gradients. Second—in conventional reservoirs, hydrocarbon is stored only in the pore spaces but there are multiple storage mechanisms active in shale owing to its complex composition. Current belief is that the gas associated with shale gas reservoirs is stored as free gas (natural fractures and nanopores) and adsorbed only (Boyer et al., 2006). Shale is a complex mixture of organic matter (kerogen), inorganic matter (clay, silica) and interbedded minerals (feldspar etc.). The organic matter is found to contain a well-developed network of nanopores. As can be seen in Figure 4.1 (SEM image from a Barnett shale sample) almost all the nanopores are only located inside the kerogen. It can be deduced that almost entire porous space occurs inside kerogen only. Hashmy et al. (2011) claim that the porosity inside the kerogen can reach up to 40%. Kerogen can be further subdivided into two parts; porous structure (nanopores) and kerogen bulk (solid). Traditionally kerogen bulk has not been considered a very significant gas holder. Assuming kerogen bulk’s equivalence with bitumen, it would have appreciable gas solubility. Kerogen fraction can reach up to 40% v/v compared to total shale bulk volume (Passey et al., 2011). Therefore kerogen can store a significant amount of gas in the dissolved phase. Also, the rate of diffusion from kerogen bulk to shale pores has historically been considered negligible (Hashmy et al., 2011). In our previous work (Swami & Settari, 2012) we showed that it is very significant theoretically and in fact can affect the pressure transients and cumulative recovery behavior. The total gas in place should consist of free gas stored in the natural fractures (if present), the nanopores, adsorbed gas on the organic matter surface and gas dissolved inside the kerogen bulk.

Finally, the fluid continuum theory breaks down for shale pores where the size of pores which are typically 5-1000 nm (Wang & Reed, 2009) or even smaller, 5 to 50 nm (Behar & Vandenbroucke, 1987; Bowker, 2003) is comparable to the kinetic diameter of methane molecules, i.e., ~0.4 nm (Heidemann et al., 2010). At this scale, diffusive flow also becomes active in addition to conventional convective flow. Correspondingly Darcy’s equation, which accounts for the convective flow in conventional simulators, is not sufficient. Darcy’s equation is therefore modified to incorporate the diffusive flow and slippage at the pore boundaries. In our
previous work (Swami & Settari, 2012), we developed a model for gas flow through one nanopore in a shale gas reservoir. It was a theoretical model with many simplifying assumptions. We incorporated the effects of non-Darcy flow mechanisms on flow behavior and analyzed the contribution of kerogen bulk on pressure transients and cumulative recovery of gas. In this work, we extend it to a more practical laboratory scale model. Governing equations and parameters have been verified against laboratory obtained data. Akkutlu & Fathi (2011) developed a model to accommodate desorption and diffusion from kerogen into the shale gas reservoir modeling, but we believe that the model postulated in this paper is better for incorporation into a standard dual or Coal Bed Methane (CBM) ‘Triple Porosity’ model.

4.3 THEORY AND MODEL DEVELOPMENT

In this work, we develop a flow model for quad porosity system where gas is stored in natural fractures, pores, adsorbed and dissolved in kerogen bulk. Matrix feeds the fracture network and matrix is in turn fed by gas dissolved in kerogen bulk and adsorbed on kerogen surface exposed inside the nanopores. It is worth noting that matrix means kerogen and inorganic matter. But as seen in Figure 4.1, nanopores which store the free gas are located mostly inside kerogen only. Inorganic fraction does have pores, but they are generally much bigger and can be classified as micro-fractures. These micro-fractures may be disconnected and become active only with a stimulation job (hydraulic fracturing). Moreover, the micro-fractures store most of the in-situ water associated with shales and hence may not contain significant gas compared to nanopores inside kerogen. Consequently, matrix essentially implies the pore space inside kerogen. Correspondingly, matrix pressure means the pressure of free gas in the nanopores. A simplified physical model to depict the above formulation is shown in Figure 4.2. In actual shale reservoirs, kerogen is dispersed throughout the inorganic matter as can be seen in Figure 4.1. For ease of modeling, we assume it to be localized at one place as shown in Figure 4.2. It does not make any difference to total gas in place in kerogen bulk but makes the modeling convenient. Figure 4.2a shows a laboratory scale model in which the matrix block has a network of fractures. Figure 4.2b shows a zoomed-in view whereby natural fracture, nanopores and kerogen bulk can be seen. The circles represent the gas in the various media.
Our numerical model is based on a number of assumptions. Firstly, kerogen bulk and desorption feed the matrix (nanopores) only and do not contact the fractures directly. Kerogen bulk feeds gas to matrix and is assumed to reach pseudo steady state at each time step. Gas adsorbed onto the pore walls also desorbs into matrix only. The matrix then feeds gas to the fracture network and again is assumed to reach pseudo steady state at each time step. Finally, it is assumed that gas flows out only through the fracture network and no gas flows out from the matrix/kerogen bulk/desorption directly. We discuss each of the gas storage and transport mechanisms one by one.

All the symbols are explained in the nomenclature. The space distribution of the entire bulk is represented by:

\[ V_b = V_k + V_{in} + V_{pm} + V_f \]  

This can be expressed as respective fractions as:

\[ 1 = f_k + f_{in} + \phi_m + \phi_2 \]

It is to note that matrix and fracture porosities are scaled to entire bulk volume.

### 4.3.1 Kerogen bulk

For the scope of this work, we assume that methane solubility in kerogen bulk is the same as in bitumen (Swami & Settari, 2012; Javadpour et al., 2007) owing to similarity between kerogen and bitumen (Tissot & Welte, 1984). Svrcek & Mehrotra (1982) conducted experiments to determine methane solubility in bitumen. Mehrotra & Svrcek (1982) postulated the following empirical algebraic expression for estimating gas solubility or gas content (m³ of gas at NTP/m³ of bitumen) as a function of pressure and temperature:

\[ G_b = b_1 + b_2 \times p + b_3 \times \frac{p}{T} + b_4 \times \left(\frac{p}{T}\right)^2 \]

Where, \( b_1 = -0.018931 \), \( b_2 = -0.85048 \), \( b_3 = 827.26 \) and \( b_4 = -635.26 \). Also, \( p \) is gas pressure expressed in MPa and \( T \) is temperature in Kelvin.

The diffusion coefficient for methane through bitumen is in the range of \( 10^{-9} \) to \( 10^{-12} \) m²/s (Fisher et al., 2000; Sheikha et al., 2005, Javadpour et al., 2007). Stainforth & Reinders (1990)
and Thomas & Clouse (1990) also determined the diffusion coefficient for gas through kerogen to be in a similar range ($10^{-10}$ to $10^{-13}$ m$^2$/s).

If there are ‘n’ nanopores in the cross section of kerogen (laboratory sample is a cylindrical core with cross section radius $r_c$), the matrix porosity scaled to entire bulk volume can be expressed as:

$$\phi_m = \frac{n \pi r_n^2 L_x}{\pi r_c^2 L_x} = \frac{nr_n^2}{r_c^2}$$  \hspace{1cm} (4.4)

Eq. 4.4 can be rearranged to give an estimate for number of nanopores $n$ as:

$$n = \frac{\phi_m r_c^2}{r_n^2}$$  \hspace{1cm} (4.5)

And the total surface area available for diffusion from kerogen bulk can be written as:

$$\alpha_3 = n 2 \pi r_n L_x = \left(\frac{\phi_m r_c^2}{r_n^2}\right) 2 \pi r_n L_x = \frac{2 \phi_m V_b}{r_n}$$  \hspace{1cm} (4.6)

Mathematically, the gas content (m$^3$ of gas at NTP/m$^3$ of kerogen bulk) for kerogen bulk with pressure $p_k$ is represented as:

$$G_k = b_1 + b_2 \times p_k + b_3 \times \frac{p_k}{T} + b_4 \times \left(\frac{p_k}{T}\right)^2$$ \hspace{1cm} (4.7)

and the gas content in equilibrium with matrix at pressure $p_m$ as:

$$G_m = b_1 + b_2 \times p_m + b_3 \times \frac{p_m}{T} + b_4 \times \left(\frac{p_m}{T}\right)^2$$ \hspace{1cm} (4.8)

Diffusion rate (kg/s) from kerogen bulk into the matrix is dependent upon surface area available for diffusion ($\alpha_3$), diffusion coefficient ($D_k$) and the difference between the actual gas content corresponding to kerogen bulk pressure ($p_k$) and the equilibrium content corresponding to matrix pressure ($p_m$). Mass diffusion rate (kg/s) in the total matrix pore space can then be expressed in analogy with CBM formulation as Eq. 4.9. It is to note that the gas content in kerogen bulk is given by Eq. 4.7 in contrast to given by Langmuir’s isotherm in CBM.

$$\dot{m}_k = -\frac{\partial G_k}{\partial t} \rho_{ntp} V_b f_k = c\alpha_3 D_k (G_k - G_m) \rho_{ntp} V_b f_k$$  \hspace{1cm} (4.9)
In the above equation, negative sign indicates that gas dissolved in kerogen decreases with time as it diffuses into the matrix. Also, \( c \) is a history matching parameter or constant of proportionality with dimensions of \( 1/m^4 \). It is also to note that we assume there is no concentration gradient inside kerogen bulk and it reaches pseudo-steady state at each time step. Initially, both the kerogen bulk and matrix (nanopores) are at initial reservoir pressure and therefore gas diffusion rate is zero. Mathematically, the initial condition can be represented as:

\[
I.C. \rightarrow p_k = p_m = p_i \quad t = 0, \quad 0 \leq x < L_x \quad \ldots \ldots \ldots \ldots (4.10)
\]

Eq. 4.9 also serves as mass balance equation for kerogen bulk. No boundary condition is required since the system is in pseudo steady state.

**4.3.2 Desorption**

Gas is assumed to be adsorbed on the internal surface of nanopores inside kerogen. It is supposed to first desorb from the surface of the nanopores into the matrix pores which then feeds the fracture. This is similar to the ‘Triple Porosity’ formulation in CBM reservoirs (Law et al., 2002; Tan, 2002). Though adsorbed gas is in contact with matrix pressure, initially it may be under saturated and therefore at equilibrium with a lower pressure as observed in many CBM reservoirs (Shi and Durucan, 2005). It’s only when the matrix pressure reaches this lower pressure, generally termed as critical desorption pressure \( (p_{critdes}) \), that the adsorbed gas starts desorbing. Further, adsorbed gas at any stage of depletion has its own equilibrium pressure \( (p_{ad}) \) which is different from the matrix pressure. Once matrix pressure reaches critical desorption pressure and desorption commences, this equilibrium pressure \( (p_{ad}) \) remains higher than the matrix pressure due to a time lag caused by sorption time and possibly phase behavior effects of adsorbed gas (Firoozabadi, 2012).

Total gas (kg) adsorbed can be expressed in terms of Langmuir volume \( (G_L) \), Langmuir’s constant \( (b) \) and adsorption pressure \( (p_{ad}) \) as:

\[
G_{ad} = \rho_{ntp} \rho_{bi} V_b G_L \frac{b_{pad}}{1 + b_{pad}} \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.11)
\]

In the above equation, the pressure dependent term can be expressed in a more readily usable form as shown in Eq. 4.12. \( \theta_{ad} \) denotes the fraction of occupied to total available surface
sites for adsorption and is expressed in terms of Langmuir’s constant ($b$) and adsorption equilibrium pressure, $p_{ad}$ (Swami & Settari, 2012) as:

$$\theta_{ad} = \frac{bp_{ad}}{1 + bp_{ad}}$$ \hspace{1cm} (4.12)

Gas rate (kg/s) from desorption into total matrix pore space can be then written as:

$$\dot{m}_{des} = -\frac{\partial G_{ad}}{\partial t} = -\rho_{ntp}\rho_{bi}V_bG_L\frac{\partial \theta_{ad}}{\partial t}$$ \hspace{1cm} (4.13)

In the above equation, negative sign indicates that adsorbed gas content decreases with time as gas desorbs into the matrix. Gas desorption rate will also depend upon the matrix pressure. The lower the matrix pressure, the higher the rate of desorption. Mathematically, it can be expressed as:

$$\dot{m}_{des} = \frac{1}{\tau_2}(G_{ad} - G_{adm}) = \rho_{ntp}\rho_{bi}G_LV_b\frac{\theta_{ad} - \theta_m}{\tau_2}$$ \hspace{1cm} (4.14)

$G_{adm}$ is the equilibrium adsorbed gas content corresponding to matrix pressure ($p_m$) and $G_{ad}$ is the actual gas content corresponding to adsorbed gas pressure, $p_{ad}$ (typically higher than $G_{adm}$). $\tau_2$ is the sorption time and causes the time dependent desorption. It describes the ease of desorption and the lag between the adsorbed gas and matrix (nanopore) pressures. In the extreme case when sorption time approaches zero ($\tau_2 \approx 0$), the system will tend to instant equilibrium between adsorbed phase and matrix. $\theta_m$ is the theoretical fraction of the sites occupied by adsorbed gas corresponding to matrix pressure. $\theta_m$ is related to matrix pressure with a similar Langmuir’s expression as:

$$\theta_m = \frac{bp_m}{1 + bp_m}$$ \hspace{1cm} (4.15)

Initially, adsorbed gas is at critical pressure and the matrix (nanopores) is at initial reservoir pressure. Mathematically, this can be represented as:

1. C. $\rightarrow p_{ad} = p_{critdes}; \ t = 0, \ 0 \leq x < L_x$ \hspace{1cm} ................. \hspace{1cm} (4.16)

1. C. $\rightarrow p_m = p_i; \ t = 0, \ 0 \leq x < L_x$ \hspace{1cm} ................. \hspace{1cm} (4.17)
Eq. 4.13 and 4.14 serve as the mass balance equations for adsorbed gas and the adsorbed gas pressure can be found from them.

4.3.3 Matrix

With the current technology, a good estimate of pore sizes can be obtained for the shale nanopores. One such example has been shown in Figure 4.3. In this case the authors (Javadpour et al., 2007) used high pressure mercury injection technique to find the dominant pore size for fluid flow. After measuring the dominant pore size, absolute Darcy’s permeability can be estimated for circular capillary using the Hagen Poiseuille’s equation.

\[ k_D = \frac{r_n^2}{8} \]

(4.18)

If the representative shape of pores is not circular but some other regular geometrical shape (viz., triangular, rectangular or square), we can still find the Darcy’s permeability (Swami et al., 2013b). Using the base absolute permeability based on pore shape and size, effective Darcy permeability for the porous medium (matrix) can be found as:

\[ k_m = \frac{\phi_m}{\tau_1} k_D \]

(4.19)

With current logging techniques, we can find a good estimate of matrix porosity. Tortuosity (\( \tau_1 \)) can be evaluated from the lab data, if available. For this work, we found an estimate of matrix permeability from Figure 4.4. Though this plot gives only a ballpark figure, it is still good for an initial estimate.

As discussed earlier, matrix essentially means the free gas inside nanopores which are imbedded inside kerogen. We have assumed classical dual porosity model without matrix-to-matrix flow since matrix permeability is too low to cause any inter-matrix block flow. Then, using the mass rate from desorption and diffusion from kerogen bulk, mass balance equation for matrix can be written as:

\[ \dot{m}_k + \dot{m}_{des} - \dot{m}_t = \frac{\partial}{\partial t} (V_b \phi_m \rho_m) \]

(4.20)
\( \dot{m}_t \) (kg/s) is the transfer term accounting for mass flow rate of gas from matrix into fractures. It can be expressed as the source/sink term using Warren and Root’s (1963) formulation.

\[
\dot{m}_t = \frac{\alpha_2 k_{app} (p_m - p_f) \rho_m V_b}{\mu} \quad (4.21)
\]

The matrix to fracture transfer depends on the assumed geometry of the fracture network. For example, for sheet shaped matrix blocks, shape factor \( \alpha_2 \) was postulated by Warren and Root (1963) as:

\[
\alpha_2 = 12 \left( \frac{1}{L_{mz}^2} \right) \quad (4.22)
\]

However, our analysis is valid for any configuration of fractures provided the corresponding shape factor \( \alpha_2 \) is used. In Eq. 4.21, \( k_{app} \) is the apparent permeability (Javadpour, 2009; Swami & Settari, 2012) taking into account slippage at pore walls and Knudsen diffusion.

\[
k_{app} = c_g D_m \mu + F k_m \quad (4.23)
\]

In the above equation, \( D_m \) denotes the effective Knudsen diffusion coefficient for porous medium and is related to Knudsen diffusion coefficient \( D \) by the following expression:

\[
D_m = \frac{\phi_m}{\tau_1} D \quad (4.24)
\]

Also, the slippage factor \( F \) can be expressed as:

\[
F = 1 + \left( \frac{8 \pi R T}{M} \right)^{0.5} \frac{\mu}{p_{avg} r_n} \left( \frac{2}{\alpha_1} - 1 \right) \quad (4.25)
\]

The complete derivation for the apparent permeability has been worked out elsewhere (Javadpour, 2009; Swami & Settari, 2012) and here we use the results directly. Eq. 4.20 can be now expanded using Eqs. 4.9, 4.13 and 4.21 as:
\[ c \alpha_3 D_k (G_k - G_m) \rho_{n tp f k} + \frac{\rho_{n tp} \rho_{b i} G_L}{\tau_2} (\theta_{ad} - \theta_m) - \frac{\alpha_2 k_{app} (p_m - p_f) \rho_m}{\mu} = \phi_m \rho_m c_{mt} \frac{\partial p_m}{\partial t} \] ...

... (4.26)

**4.3.4 Fracture**

For a conventional dual porosity system, we can write the flow equation for fracture pseudo-continuum as shown below with transfer term from matrix.

\[ \frac{\partial}{\partial x} \left( \frac{\mu}{\rho_f k_2} \frac{\partial p_f}{\partial x} V_b \right) + \frac{\alpha_2 k_{app} (p_m - p_f) \rho_m V_b}{\mu} = \frac{\partial}{\partial t} (V_b \phi_2 \rho_f) \] ...

... (4.27)

In the above equation, \( k_2 \) is the pseudo-continuum fracture permeability based on bulk flow area, which can be derived from the intrinsic permeability \( k_f \). Fracture intrinsic permeability can be expressed as a function of fracture width by:

\[ k_f = \frac{w^2}{12} \] ...

... (4.28)

And the permeability scaled to entire bulk volume \( (k_2) \) can be expressed (Swami et al., 2013a) by:

\[ k_2 = k_f w \left( \frac{1}{L_{mz}} \right) \] ...

... (4.29)

In an actual reservoir, fracture network’s permeability is a strong function of reservoir pressure and correspondingly effective stresses (Swami et al., 2013b). But in this case, we do not take any stress dependence on fracture permeability since the laboratory test is done with zero stress boundary conditions and therefore the effective stress in the sample would remain close to zero and fracture permeability would not change much with pressure depletion. The fracture mass conservation equation can then be simplified assuming constant fracture permeability \( (k_2) \) as:

\[ \frac{k_2}{\mu} \frac{\partial}{\partial x} \left( \rho_f \frac{\partial p_f}{\partial x} \right) + \frac{\alpha_2 k_{app} (p_m - p_f) \rho_m}{\mu} = \phi_2 \rho_f c_{ft} \frac{\partial p_f}{\partial t} \] ...

... (4.30)

The initial and boundary conditions can be represented as:
\[ I.C. \quad \rightarrow p_f = p_m = p_i; \quad t = 0, \quad 0 \leq x < L_x \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.31) \]

\[ B.C. 1 \quad \rightarrow p_f = p_{atm}; \quad x = 0, \quad t > 0 \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.32) \]

\[ B.C. 2 \quad \rightarrow \frac{\partial p_f}{\partial x} = 0; \quad x = L_x, \quad t > 0 \quad \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots (4.33) \]

4.4 GAS EVOLUTION CURVE IN LABORATORY

The canister test is widely used in the industry to assess the amount of adsorbed gas in Coal Bed Methane (CBM) reservoirs (Mavor & Nelson, 1977). Of late it has been used for shale gas reservoirs as well (Javadpour et al., 2007). This is done owing to the presence of similar organic matter (kerogen) in coal and shale. It is very important to appreciate the differences between CBM and shale gas. Shale differs from coal in many aspects. Whereas the canister test gives a measure of only adsorbed gas in coal, in shale it gives an estimate of gas coming from all sources: free gas in natural fractures, free gas stored in pores, adsorbed gas and gas dissolved in kerogen bulk. Due to the large fractures in coal, free gas present in fracture network flows out immediately when the canister test commences. So, as the system pressure decreases, only the desorbed gas is obtained. On the contrary, flow in nanopores, gas coming from desorption and gas diffusing from kerogen bulk—all share similar time scales in shale reservoirs. Hence, gas obtained during the canister test does not come only as desorbed gas but as a mixture of the previously mentioned storage mechanisms.

Figure 4.5 shows a gas evolution curve from a shale gas reservoir sample. The example is from Javadpour et al. (2007) and the data is from a Canadian shale gas reservoir. Some water might have been produced while transporting the core from well to surface but negligible water was produced during the test. The four flow behaviors: flow in fractures, matrix, desorption and finally diffusion from kerogen bulk are clearly visible in the plot. Fractures have a very high permeability but very low porosity; hence we see a very rapid initial outflow of gas. This is seen for a very short time, for the first 14 minutes (0.24 hr). Just when fractures are almost completely depleted, the matrix starts feeding the fractures and the pressure is maintained. The matrix dominated flow lasts until about 3.24 hr. The kick observed at 3.24 hr suggests onset of another storage mechanism. It is at this point that the critical pressure is reached for desorption in the
sample and gas starts desorbing from the pore walls into the nanopores. A very interesting phenomenon to observe is the rapid flow of gas. For such a high flow rate, the matrix system needs a high permeability. We believe that the system permeability enhances multifold with desorption. This occurs primarily because of three possible reasons. Figure 4.6 shows a zoomed-in view of a nanopore having adsorbed and free gas. Let’s consider that, in the presence of gas adsorbed on pore walls, the effective diameter for flow is about 1 nm (Figure 4.6a). As the gas desorbs, the methane molecules which have a kinetic diameter of roughly 0.4 nm flow out and expose the entire nanopore for flow (Figure 4.6b). As a result, the effective diameter for flow becomes twice its initial value and the permeability quadruples (Eq. 4.18). Sakhaee-Pour & Bryant (2012) also argue that permeability can increase by up to 8 times as the reservoir pressure falls from 28 MPa to 5 MPa. They attribute it to pore hydraulic diameter increase with desorption. Akkutlu & Fathi (2011) claim that the total pore volume can increase up to 32.4 % as pressure decreases from 4000 psi to atmospheric pressure. They attribute it primarily to the volume occupied by adsorbed gas. Further, recalling from Eq. 4.18, permeability is inversely proportional to tortuosity. As gas molecules desorb, hindrance in the flow path reduces and tortuosity decreases significantly, thereby increasing the permeability. Finally, since adsorption is a surface phenomenon and gas desorbs, the gas molecules travel close the pore surface. Consequently, it is also possible that desorption also create an additional slippage at pore boundaries. As the adsorbed gas depletes, this extra slippage will also decrease and reach its minima towards the end of desorption. Owing to these factors, the matrix permeability increases as desorption continues and reaches its peak when the system is completely devoid of adsorbed gas. Desorption dominated flow regime can be seen from 3.24 to 24.5 hr. Just when the matrix pressure goes down to critical pressure for diffusion, gas starts diffusing from kerogen bulk into the nanopore system. This can be seen from time of 25 hr onwards. As can be appreciated, diffusion is extremely slow but nevertheless a very important process. It results in almost 10 % of the cumulative production at 40 hr.
4.5 Physical and Numerical Models for Laboratory Tests

The physical model is shown in Figure 4.2. As depicted in the equations, only one dimensional flow is considered and the entire flow is assumed to occur through the fractures only. Except for the left face (which is exposed to a constant atmospheric pressure), all the other faces are no-flow boundaries. We took a cylindrical sample with length 0.3 m and radius 0.038 m. The model for the sample was discretized only along the X axis. A pseudo steady state was assumed to exist between kerogen bulk and matrix, adsorbed gas and matrix and finally between matrix and fractures.

The numerical procedure for solving the system of equations for a time step was as follows. First, the fracture equation was solved assuming no pressure support from the matrix. Matrix pressure equation was then solved using the updated fracture pressure value. Corresponding to the new matrix pressure, the mass transfer from adsorbed gas and kerogen bulk dissolved gas was found. These values of desorbed and diffused (from kerogen bulk) gas were substituted in matrix equation and updated matrix pressure values were found. The matrix pressure value was then fed into fracture equation to find the updated pressure profile along the fracture. The process was repeated until a final convergent value set was found. After that we moved to the next time step. For more details on numerical solution algorithm, refer to Appendix 4A.

4.6 Results and Discussions

We used the laboratory experiment of gas evolution carried out by Javadpour et al. (2007) to calibrate our model. Whereas they postulated the different flow regimes and justified the observed production profiles with statistical models, no numerical model was offered which could account for the flow physics. We built our numerical model based on the equations presented earlier. Their laboratory data is reproduced in Figure 4.7. The figure separates the four flow regimes; the first when free gas flows out of the fractures (shown by blue tiles), when matrix starts contributing (shown by red squares), when desorption aids in supplying new gas (shown with green triangles) and finally when diffusion from kerogen bulk kicks in (shown with purple crosses). All the parameters are tabulated in Table 4.1. It is to be noted in Figure 4.5 that
the laboratory curve is not adjusted completely for ‘lost gas’; hence we ignore the lost gas component in this work. As the name suggests, lost gas is the amount of gas which is released (gets lost) while transporting a core from wellbore to surface. Consideration of lost gas will increase the gas estimate in each of the storage mechanism, mostly in the natural fracture system considering that the gas stored in fractures flows out the first as sample is tripped from wellbore to surface.

Our modeling results are plotted in Figure 4.8 along with the experimental data from Javadpour et al.’s work. We assign a relatively high permeability (0.01 mD) and low porosity ($2.0 \times 10^{-3}$) to the fractures. The blue line shows what would happen if fractures were the only storage medium in the system. As can be seen, the fractures deplete very quickly and then the matrix starts feeding the fracture system. The orange line shows the production profile by taking into account only the matrix’s Darcy permeability. From the laboratory measurements, we have an estimate of pore diameter as 7.5 nm, matrix porosity of 0.04 and tortuosity as 5, which corresponds to typical values for shales (Ziarani & Aguilera, 2012). The corresponding matrix absolute permeability comes out to be 56 nD using Eq. 4.18. Quite evidently, the Darcy’s permeability alone is not sufficient to justify the production profile. But if we take into account slippage and Knudsen diffusion, the apparent matrix permeability increases and we can get a better match with the observed data. Apparent permeability is a function of pressure. For this case, it ranges from 200 nD to 500 nD as we move towards the low pressure region (from no-flow boundary at a high pressure of 17.2 MPa to the other end at atmospheric pressure). We observe that slippage and Knudsen diffusion alter matrix permeability very significantly and cause the apparent permeability to become almost 10 times that of Darcy permeability in the low pressure region. The green line shows the production profile corresponding to the matrix contribution when matrix permeability takes into account slippage and Knudsen diffusion. At about 3.24 hr, when the matrix pressure reaches critical desorption pressure ($p_{\text{critdes}}$), gas starts to desorb and feed the matrix; it maintains the pressure and increases the cumulative production. Critical desorption pressure in the case was observed to be 14 MPa. As noted earlier, the gas flow rate becomes higher with the commencement of desorption. It appears that the matrix permeability increases appreciably as desorption continues; desorption increases the effective pore diameter, reduces tortuosity and increases slippage. In this modeling work, we observed that
the average apparent permeability increases gradually from 250 nD to 3000 nD as adsorbed gas is released into the system. It is to be noted that the effect of hydraulic diameter increase on permeability can be calculated quantitatively but the other two effects, i.e., reduction in tortuosity and slippage due to desorption have not been quantified in this work. We observed that the average matrix permeability had to be increased by a factor of about 30 with complete depressurization to get a match with observed data. For a pore diameter of 7.5 nm, an increase in pore diameter with desorption caused the matrix permeability to become only twice of its original value for our set of assumed parameters. Rest of the permeability increase may be in part explained by the two other effects (tortuosity reduction and increase in slippage) but there might be possibly some other physical processes active which have contributed to the observed increase in permeability. After the matrix pressure reaches critical value ($p_{\text{crit,ker}}$, in this case $5 \times 10^5$ Pa) for gas diffusion from kerogen bulk, gas starts diffusing from kerogen bulk into the matrix. We assumed that kerogen occupies roughly 11 % of matrix bulk (v/v) and observed that a diffusion coefficient of $1 \times 10^{-10}$ m$^2$/s matches the observed data. From the laboratory data and modeling work, we conclude that fractures contributed a total of 4 % of the cumulative production, the matrix’s contribution was 78 %, desorption was 7 % and finally gas diffusion from kerogen bulk was 11 %. The original in-place and produced volumes are tabulated in Table 4.2.

A noteworthy point is that in the real field data we might not see such well-defined peaks corresponding to different transport mechanisms as observed in the laboratory data. In the field, the various storage and transport mechanisms may start contributing at different places at the same time due to substantial pressure gradients. Consequently, the peaks observed in laboratory may get obscured in the field due to overlapping of the various storage and transport mechanisms.

Just to see the far reaching effect of diffusion from kerogen bulk, we ran the simulation for 40 days (~ 1000 hr). Results are reproduced in Figure 4.9. We observed that cumulative production peaks out at about 15 days into approximately 8,000 cc of gas. It is noted that fractures contributed a total of 3 % to the cumulative production, matrix’s contribution was 63.5 %, desorption 6 % and finally gas diffusion from kerogen bulk accounted for 27.5 % in this case. This result re-emphasizes that diffusion is comparatively a slow process but definitely not
insignificant. It dominates the flow behavior towards the latter part of reservoir life. All the other
transport mechanisms for storage mechanisms (viz. fractures, matrix and gas desorption) are
relatively fast and deplete in the first 30 hours or so. It is the diffusion from kerogen bulk which
carries out until about 15 days. This suggests further research to see if diffusion can somehow be
made faster. If that could be done, both the in-place resource and reserves could be increased
appreciably.

4.7 CONCLUSIONS

In this work we separated the different flow mechanisms observed in a laboratory scale
shale gas production test. We were able to match the production data with numerical model by
taking into account the physics at the molecular level. The final conclusions are:

1. Shale gas reservoirs contain gas stored via four storage mechanisms: fractures, matrix
   pores, adsorbed phase and dissolved in kerogen bulk.

2. Effect of slippage and Knudsen diffusion is important and it increases the matrix apparent
   permeability quite significantly. Apparent permeability should therefore be considered in
   reservoir simulators.

3. An appreciable amount of gas is stored in the organic fraction of the shale, i.e., kerogen
   as both free gas in its nanopores and as dissolved gas in the kerogen bulk. Gas diffusion
   from kerogen bulk is a slow process but it is not negligible compared to matrix flow or
   desorption. It kicks in after matrix pressure falls below a certain critical pressure and
   helps sustain the production thereafter.

4. To match the laboratory data a substantial increase in matrix permeability with desorption
   is required. This warrants further research.

5. This model should be verified against more shale gas evolution tests to reach a conclusive
   estimate of governing parameters.

   It is important to point out that while the model captures the onset of different
   contributing storage and transport mechanisms as observed in the laboratory data and provides
   estimates of the physical parameters, it is somewhat simplified and therefore the characterization
obtained by the history match may be further improved. In reality, all the faces of the sample may be open to flow while in our model we assumed only one face to be open to flow. Additionally, we do not have all the reservoir data of the sample against which we have calibrated our model. Further, we used values for methane solubility in kerogen assuming kerogen’s equivalence to bitumen. In reality the two could be different. Methane content of a particular kerogen will also depend upon its type and maturity (Ross & Bustin, 2009). Although the model presented can be used for field scale simulation work, its parameters can be further calibrated with more laboratory tests where reservoir data is known.

4.8 NOMENCLATURE

AFM = Atomic Force Microscope
b = Langmuir’s constant, Pa$^{-1}$
c = History matching parameter/constant of proportionality, 1/m$^4$
cc = cubic centimeters
$\gamma$ = Fracture compressibility, Pa$^{-1}$
$\gamma_t$ = Total fracture compressibility, Pa$^{-1}$. $\gamma_t = \gamma_g + \gamma_f$
$\gamma_g$ = Gas compressibility Pa$^{-1}$
$\gamma_m$ = Total matrix compressibility, Pa$^{-1}$. $\gamma_m = \gamma_g + \gamma_r$
$\gamma_r$ = Rock compressibility, Pa$^{-1}$
D = Knudsen diffusion constant, m$^2$/s
$D_k$ = Diffusion constant for gas diffusion through kerogen bulk, m$^2$/s
$D_m$ = Matrix’s Knudsen diffusion constant (accounting for porosity and tortuosity), m$^2$/s
$\phi_i$ = Fraction of inorganic matter in total bulk volume, dimensionless fraction
$\phi_k$ = Fraction of kerogen (organic matter) in total bulk volume, dimensionless fraction
F = Gas slippage factor, dimensionless
$G_{ad}$ = Adsorbed gas content corresponding to adsorbed gas pressure ($p_{ad}$), kg
$G_{adm}$ = Pseudo adsorbed gas content corresponding to matrix pressure ($p_m$), kg
$G_b$ = Gas content dissolved in bitumen, m$^3$ of gas at NTP/m$^3$ of bitumen
\( G_k \) = Gas content dissolved in kerogen bulk (based on empirical law for methane solubility in bitumen), m³ of gas at NTP/m³ of kerogen bulk

\( G_L \) = Langmuir’s volume, NTP m³ of gas/kg of shale sample

\( G_m \) = Pseudo gas content (equilibrium gas dissolved corresponding to matrix pressure based on Langmuir empirical law), taken here from methane solubility in bitumen, m³ of gas at NTP/m³ of kerogen bulk

\( k_2 \) = Fracture permeability scaled to total bulk volume, m²/s

\( k_{app} \) = Apparent permeability of matrix accounting for slippage and Knudsen diffusion, m²

\( k_D \) = Darcy permeability, m²

\( k_f \) = Fracture intrinsic permeability, m²/s

\( k_m \) = Matrix’s Darcy permeability (accounting for porosity and tortuosity), m²

\( L_x \) = Length of sample in X direction, m

\( L_{mz} \) = Length of matrix block (for dual porosity model) / separation between fractures in Z direction, m

\( m_{des} \) = Desorptive mass transfer rate to matrix, kg/s

\( m_k \) = Mass transfer rate from kerogen bulk to matrix, kg/s

\( m_t \) = Mass transfer rate from matrix to fractures, kg/s

\( M \) = Molecular mass, kg/mol

\( n \) = No. of nanopores in sample

\( NTP \) = Normal temperature and pressure conditions. Normal temperature is defined as 273 K and normal pressure as 1.01325×10⁵ Pa

\( p \) = Pressure, Pa

\( p_{ad} \) = Adsorbed gas phase pressure, Pa

\( p_{critdes} \) = Critical matrix pressure at which desorption begins, Pa

\( p_{critker} \) = Critical matrix pressure at which gas begins diffusing from kerogen bulk into matrix, Pa

\( p_i \) = Initial reservoir pressure, Pa

\( p_k \) = Pressure of gas dissolved in kerogen bulk, Pa

\( p_m \) = Matrix pressure (pressure of free gas in nanopores), Pa
\( r_c \) = Radius of the core, \( \text{m} \)
\( r_n \) = Pore radius, \( \text{m} \)
\( R \) = Universal Gas constant, 8.314 \( \text{J/K/mol} \)

SEM = Scanning Electron Microscope

\( T \) = Temperature, \( \text{K} \)

\( V_b \) = Bulk volume, \( \text{m}^3 \)
\( V_f \) = Volume occupied by fractures, \( \text{m}^3 \)
\( V_{in} \) = Inorganic matter volume, \( \text{m}^3 \)
\( V_k \) = Kerogen (organic matter) bulk volume, \( \text{m}^3 \)
\( V_{pm} \) = Pore volume (occupied by nanopores inside kerogen), \( \text{m}^3 \)

\( w \) = Fracture width, \( \text{m} \)

\( z \) = Gas compressibility factor, dimensionless

**GREEK LETTERS**

\( \alpha_1 \) = Fraction of molecules striking pore wall which are diffusely reflected, dimensionless

\( \alpha_2 \) = Warren & Root’s shape factor, \( 1/\text{m}^2 \)

\( \alpha_3 \) = Total surface area of all the nanopores in sample, \( \text{m}^2 \)

\( \mu \) = Gas viscosity, \( \text{Pa.s} \)

\( \rho_f \) = Gas density corresponding to fracture pressure, \( \text{kg/m}^3 \)

\( \rho_m \) = Gas density corresponding to matrix pressure, \( \text{kg/m}^3 \)

\( \rho_{bi} \) = Bulk density of shale at initial reservoir pressure, \( \text{kg/m}^3 \)

\( \tau_1 \) = Tortuosity, dimensionless

\( \tau_2 \) = Sorption time, \( \text{s} \)

\( \phi_m \) = Matrix porosity (scaled to total bulk volume), fraction

\( \phi_2 \) = Fracture porosity (scaled to total bulk volume), fraction

\( \theta_{ad} \) = Fraction of total surface sites (available for adsorption) occupied by molecules, dimensionless

\( \theta_m \) = Pseudo fraction variable corresponding to matrix pressure, dimensionless
4.9 ACKNOWLEDGEMENT

We wish to thank Dr. Chris Clarkson at University of Calgary for his valuable comments and discussions. We also wish to acknowledge the financial aid from the consortium for Shale Gas Modeling at University of Calgary for supporting the research funding.

4.10 REFERENCES


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4.11 Figures

Figure 4.1: SEM image of shale gas reservoir (Ambrose et al., 2010)

Figure 4.2: Physical model to model the flow in shale sample. A.) shows the discretized sample along X axis. Also, fractures and kerogen can be seen interbedded inside the inorganic matter. Except for the left face, all the other faces are no flow boundaries. B.) Zoomed in view. Gas can be seen stored as i) free gas in natural fractures, ii) free gas in nanopores, iii) adsorbed and iv) dissolved in kerogen bulk.
**Figure 4.3:** An example of determination of pore sizes by mercury injection test (Javadpour et al., 2007)

**Figure 4.4:** Chart relating pore throat, porosity and permeability (Rahmanian et al. 2007)
Figure 4.5: Gas evolution test for shale sample (Javadpour et al., 2007)

a. Adsorbed and free gases inside a nanopore. Size of Methane molecule is quite comparable to nanopore size. Due to adsorbed gas, the effective hydraulic diameter of the pore can be very small compared to actual diameter.

b. As gas desorbs, it increases pore’s hydraulic diameter significantly, reduces tortuosity gets and causes extra slippage at the boundary; thereby increasing the matrix permeability many folds.

Figure 4.6: Adsorbed and free gases inside a nanopore. As gas desorbs, it increases the effective diameter available for flow, reduces tortuosity and causes extra slippage at the boundary; thereby increasing the matrix permeability manyfold.
**Figure 4.7:** Dissociation of experimental data (Javadpour et al., 2007) into four flow regimes; fractures, matrix (nanopores), desorption and diffusion from kerogen bulk.

**Figure 4.8:** Extrapolation of various storage and transport mechanisms. Also superimposed are the experimental results from Javadpour et al.’s (2007) work.
Figure 4.9: Simulation results for cumulative gas recovery after 40 days (~1000 hr). Fractures, matrix (nanopores) and adsorbed gas deplete within first 30 hours and diffusion from kerogen bulk is the only contributing mechanism thereafter.

4.12 TABLES

Table 4.1: Values of Variables Used in This Paper

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Units</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_1$</td>
<td>0.8</td>
<td>Dimensionless</td>
<td>Shabro et al. (2011)</td>
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<td>Reservoir temperature, T</td>
<td>423</td>
<td>K</td>
<td>Shabro et al. (2011)</td>
</tr>
<tr>
<td>Viscosity, $\mu$</td>
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<td>Pa.s</td>
<td>Shabro et al. (2011)</td>
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<td>Nano pore radius, $r_n$</td>
<td>$7.5 \times 10^{-9}$</td>
<td>m</td>
<td>Measured in lab. Match from</td>
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<tr>
<td>Shale matrix absolute permeability, $k_m$</td>
<td>56</td>
<td>nD</td>
<td>Measured in lab. Match from</td>
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<tr>
<td>Diffusion coefficient in kerogen bulk, $D_k$</td>
<td>$1.00 \times 10^{-10}$</td>
<td>m$^2$/s</td>
<td>Stainforth &amp; Reinders (1990) and Thomas &amp; Clouse (1990). Match from modeling</td>
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<td>Knudsen diffusion coefficient, $D$</td>
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<td>Initial reservoir pressure, $p_i$</td>
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<td>Atmospheric pressure, $p_{atm}$</td>
<td>1.01325$ \times 10^5$</td>
<td>Pa</td>
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### Table 4.2: Original Gas In Place and Produced Gas Volumes

<table>
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<tr>
<th>Storage Mechanism</th>
<th>Initial Gas in Place (IGIP), cc NTP</th>
<th>Contribution in IGIP, %</th>
<th>After 52.5 hr (experimental results)</th>
<th>After 15 days (model’s prediction)</th>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Gas produced, cc NTP</td>
<td>Contribution in total production, %</td>
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<td></td>
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<td>Gas produced, cc NTP</td>
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<td></td>
<td></td>
<td></td>
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<td>Contribution in total production, %</td>
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<tr>
<td>Fractures</td>
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<td>3</td>
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<td>Matrix (nanopores)</td>
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<td>Adsorbed</td>
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<td>Kerogen bulk</td>
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</table>

4.13 Appendix 4A

The following flowchart depicts the procedure followed for solving the couple equations:
Initialize the model with respective initial condition for each storage medium and boundary condition for the fractures’ equation.

Is it first time step?

Yes

Is it first iteration?

Yes

Solve Eq. 4.30 for $p_f$ assuming no mass flux from matrix to fractures

No

Is it first iteration for subsequent time steps?

Yes

Solve Eq. 4.30 for $p_f$ assuming mass flux from matrix to fractures corresponding to $p_m$ from inner loop

No

Solve Eq. 4.30 for $p_f$ assuming mass flux from matrix to fractures same as at previous time step

Convergence achieved for $p_f$, $p_m$, $p_{ad}$ and $p_k$ (with at least one cycle on inner loop)?

Yes

Inner Loop

Convergence achieved for $p_m$, $p_{ad}$ and $p_k$?

No

Solve Eq. 4.26 for $p_m$ while accounting for mass flux from desorption and diffusion from kerogen bulk. Solve Eq. 4.9 and 4.14 to update $p_k$ and $p_{ad}$. Desorption and diffusion are inactive as long as $p_m < p_{critdes}$ and $p_m < p_{critdiff}$ respectively.

Move to next time step

No

Start
The following algorithm details procedure for solving the coupled equations numerically.  

**Step 1:** The developed numerical model consists of 100 grid cells, each identical with respect to gas content in different storage media (natural fractures, matrix pores, adsorbed and dissolved in kerogen bulk) and reservoir properties (porosity, pore size, pores’ number density, fractures’ width etc.).

**Step 2:** Assign respective boundary conditions; right boundary to be a no flow boundary and left one at constant atmospheric pressure (Refer to Figure 4.2). Assign initial conditions for different storage media as detailed in Table 4.1.

**Step 3:** Discretize the fracture equation using finite difference method and solve to find pressure profile in the fracture pseudo-continuum (Eq. 4.30) at a particular time step while assuming that for the *first iteration,*

3a: No mass flux from matrix to fractures for the *first time step* calculation

3b: Mass flux from matrix to fractures is the same as calculated at previous time step for *all the time steps* after the first one

**Step 4:** Solve Eq. 4.26 to find pressure profile in matrix (nanopores) while accounting for mass flux from kerogen bulk and desorption, corresponding to pressure profile calculated for gas in the fracture system in Step 3

**Step 5:** At each iteration, perform a mass balance on gas dissolved in kerogen (Eq. 4.9) and as adsorbed phase (Eq. 4.14) and hence update the gas pressures (in kerogen bulk and adsorbed phase).

**Step 6:** Iterate at Step 4 and 5 until a convergent value set is found for gas pressures in matrix (nanopores), adsorbed and kerogen bulk

**Step 7:** Iterate from Step 3 to 6 until we achieve convergence on gas pressures in fractures, matrix (nanopores), adsorbed and kerogen bulk.

**Step 8:** Update the gas content in each of the storage media (Eq. 4.9 for kerogen bulk, Eq. 4.14 for adsorbed gas) corresponding to convergent pressure value set found in Step 7, and move to the next time step.

Note that there are two iterative loops on four pressure systems. Corresponding to gas pressure in the fracture system with the first iteration, the inner loop works on gas pressure for matrix (nanopores) pressure, adsorbed phase and gas dissolved in kerogen. The outer loop then updates
the pressure profile in fractures and then inner loop is invoked again. The two loops continue iterating until a final convergence is achieved for all the four pressure systems. For each of the iteration loops we have kept a convergence criterion as follows for each of the storage media:

\[ \frac{p_s(\text{itr}) - p_s(\text{itr} - 1)}{p_s(\text{itr} - 1)} < 1 \times 10^{-9} \]

Where \( p_s(\text{itr}) \) refers to iteration pressure for each of the storage medium. ‘\( \text{itr} \)’ refers to iteration number and subscript ‘\( s \)’ refers to storage medium, \( s = f \) for fractures, \( s = m \) for matrix pores, \( s = ad \) for adsorbed gas and \( s = k \) for kerogen bulk.
CHAPTER FIVE: SUMMARY AND CONCLUSIONS

5.1 Summary

Shale reservoirs are playing a very important role in the North American energy mix and they are expected to play an even greater role in many countries throughout the world. As more and more horizontal wells are drilled and hydraulically fractured to tap this abundant resource, there is a greater need to understand the storage and transport mechanisms in shale gas resources. This understanding will help the reservoir simulators to emulate the flow behavior better and make better predictions about the productivity. The knowledge of storage mechanisms will also influence the way reserves are booked. In this research work, we tried to identify the various storage and transport mechanisms active in shale gas reservoirs. We set out the following aims for this research work:

1. To assess the impact of extremely small size of shale matrix pores on transport mechanism inside the pores and validate various formulations available in the literature on both theory and against experimental results.

2. To develop a theoretical model for gas flow in one nanopore while capturing the non-Darcy flow mechanisms inside the pore, gas desorption from the pore surface and gas diffusion from kerogen bulk.

3. To upscale the pore scale model to laboratory scale numerical model for ‘quad porosity’ system including the gas stored inside the natural fractures, matrix pores, adsorbed and dissolved in kerogen bulk. This numerical model should be in a form to be readily incorporated inside a reservoir simulator.

With the research conducted during this graduate studies, we achieved all the above mentioned objectives. A brief summary of work conducted to achieve each of the objectives is provided below:

1. We reviewed various correlations available in literature for non-Darcy transport in shale nanopores. Whereas most of the correlations are based on experiments conducted upon tight gas reservoirs, a few of the experiments were conducted on shale reservoirs as well. In addition, some of the correlations are based on flow simulation of rarefied media and
are theoretical in nature. We compared the predictions made by different correlations against actual laboratory data from Mesaverde formation in Western US (studied by Byrnes et al., 2009). We found that apparent permeability increases significantly as reservoir pressure falls or pore radii decrease. A more suitable parameter to capture the apparent permeability change is found to be Knudsen number. It takes into account the reservoir pressure, temperature, pore radius and porosity. We observed that the apparent permeability could be as much as 1000 times of absolute Darcy permeability as Knudsen number changes from 0.1 to 100 in Mesaverde formation. We found that the correlations postulated by Jones & Owens (1980), Sampath & Keighin (1982), Florence et al. (2007) and Javadpour et al. (2007) give a good match with the measured laboratory data but only the Javadpour et al.’s correlation fits well on theoretical basis too. Further, we found that the apparent permeability casts significant effect on cumulative production prediction. For a 100 ft matrix block, we observed that taking into account the apparent permeability predicted the cumulative production to be 40% higher than the case when it was not taken into account over a reservoir production period of 30 years.

2. The next step was to investigate the gas flow origins in shale reservoirs and develop a pore scale model for flow in a single pore in shale. We developed a theoretical flow model where we captured non-Darcy transport mechanism, gas desorption, and gas diffusion from kerogen bulk. We found theoretically that contrary to the conventional belief, gas dissolved in kerogen bulk is quite significant compared to free gas stored in matrix and adsorbed phase. Furthermore, we found that the gas diffusion from kerogen bulk into shale matrix can affect the pressure transients and cumulative production quite significantly.

3. After having built a theoretical model for pore scale flow, further step was to build a laboratory scale model incorporating the ‘quad porosity’ or four storage mechanisms and various transport mechanisms. We built the model accordingly and calibrated it against a laboratory evolution dataset from a Canadian shale gas reservoir. We found from this work that gas stored as adsorbed phase and dissolved in kerogen bulk is significant, but gas desorption and diffusion from kerogen are triggered only after the reservoir pressure reaches critical desorption and critical diffusion pressures respectively.
From this research, we concluded that the gas dissolved in kerogen bulk is quite significant and should be taken into account while reporting Original Gas in Place and calculating pressure transients. Finally, the ‘quad porosity’ model developed in this work can be readily incorporated in a commercial simulator after calibrating against more field data.

5.2 Major Contributions

Three SPE papers were developed which were based on the research work conducted during this graduate research. One of the papers (SPE 155756) has been in SPE’s top download list for the last 6 months continuously. It has also been identified as the recommended reading in *Journal of Petroleum Technology* (Oct. 2012) to gain better understanding of the transport physics in shale reservoirs. Further, I presented this work at 2011 SPE Canadian Regional Student Paper Contest at Masters’ level where I won the first prize. Based on my performance there, I was nominated to represent Canada at the 2012 SPE International Student Paper Contest where I won the second prize.

More than the academic achievements, we see that this work (SPE 155756) is being accepted as an important reference for research on shale gas transport mechanisms.

5.3 Directions for Future Research

Although our mathematical model is quite robust in its approach, there are certain parameters which we have approximated due to lack of data. As a future research, we would like to recommend following:

1. We assumed methane solubility in kerogen bulk to be the same as in bitumen. They are very similar but there might be some differences in values. We recommend measuring methane solubility in kerogen bulk. This may impact the results.

2. We assumed certain parameters while modeling and matching the results of numerical model with laboratory results. In particular, the critical pressures for gas desorption and diffusion from kerogen bulk were found from the match from modeling. We recommend actually measuring these parameters for a better understanding of the physics.
3. With our modeling, we observed a very high increase in matrix permeability with desorption. This effect may or may not be a universal phenomenon and warrants further research.

4. The model developed in chapter 4 should be verified against more gas evolution tests on shale to arrive at a more confident estimate of governing parameters.

5. We did not take into account the phase behavior effects (if any) due to nanopore size and/or adsorbed gas (Firoozabadi, 2012). The PVT considerations demand further research to improve the model further.

6. We assumed a single pore size for nanopores inside the kerogen. In reality there is a huge range of pore sizes and hence permeabilities (Behar & Vandenbroucke, 1987; Bowker, 2003; Wang & Reed, 2009). Consideration of different pore sizes and permeabilities will affect the model’s prediction.

7. We assumed a single phase flow, while in reality there may be mobile water and possibly also condensate associated with the gas. Consideration of other fluids will affect the volumes in place (initial saturations) and transport mechanisms (due to relative permeability effects).

8. In this work, we neglected effect of inorganic matter (clay, silica and siltstone) present in shale. There might be some gas associated with it. Hence, its consideration might affect the results and interpretation. Also it will impact the assumption of kerogen bulk being connected to natural or created fractures and the model has to be modified to accommodate the same.

9. A high rank shale kerogen material may have more small nanopores (<2 nm) and in that case the adsorbed gas component may be much higher than what we observed/assumed in our work (Ross & Bustin, 2009).
BIBLIOGRAPHY


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