DEVELOPMENT AND TESTING OF AN ADVANCED COALBED METHANE
NUMERICAL RESERVOIR SIMULATOR

A Dissertation in
Energy and Mineral Engineering
by
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Submitted in Partial Fulfillment
of the Requirements
for the Degree of
Doctor of Philosophy

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ABSTRACT

A three dimensional, dual-porosity, dual-permeability, two-phase and compositional reservoir simulator with local grid refinement approach is presented. A local grid refinement (LGR) protocol is used for replacing the Peaceman’s wellbore model to simulate complex wellbore geometries while Newton-Raphson procedure is used to find the improvements between each time step. The proposed LGR technique is different than the traditional reservoir simulation methodologies as it uses a high resolution grid system to identify and calculate the performances of complex wellbore structures for which traditional wellbore models are not suitable.

The proposed model generates results that show that the new protocol is capable of accurately calculating the flowrate responses of simple well structures in comparison to available commercial simulators. After that the performances of complex wellbore structures, such as multi-lateral, slanted and undulating wells are compared within different reservoir configurations. Case studies show that the benefits of lateral wells diminish with increasing vertical anisotropy.

Moreover, the local grid refinement technique is a significant undertaking for the computational performance. To deal with this issue, an iterative linear equation solver (GMRES) and advance matrix preconditioners (ParaSails and FASP) are incorporated to the CBM simulator. Furthermore, to increase the computational efficacy of the numerical simulator, two additional subroutines are implemented to have better initial guess at the Newton-Raphson iterations and at the same time to decrease the oscillations experienced
during the Newton-Raphson iterations. These modifications yield significant decreases in the simulation time, where in some cases the simulation time was cut from a week to couple minutes\(^1\).
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### NOMENCLATURE

**Roman**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
</tr>
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<tr>
<td>$A_x$, $A_y$, $A_z$</td>
<td>Cross-sectional flow area perpendicular to flow directions in $x$, $y$, and $z$-directions</td>
<td>$\text{ft}^2$</td>
</tr>
<tr>
<td>$B_g$</td>
<td>Formation volume factor of gas phase</td>
<td>$\frac{\text{RB}}{\text{SCF}}$</td>
</tr>
<tr>
<td>$B_w$</td>
<td>Formation volume factor of water phase</td>
<td>$\frac{\text{RB}}{\text{STB}}$</td>
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<tr>
<td>$c_1$</td>
<td>Curve-fitting coefficient</td>
<td>$\frac{\text{SCF}}{\text{ton}}$</td>
</tr>
<tr>
<td>$c_2$</td>
<td>Curve-fitting coefficient</td>
<td>$\text{psia}$</td>
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<td>$c_m$</td>
<td>Matrix shrinkage compressibility</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
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<td>$c_p$</td>
<td>Pore volume compressibility</td>
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<tr>
<td>$c_t$</td>
<td>Total compressibility</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
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<tr>
<td>$c_{\phi}$</td>
<td>Formation compressibility</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
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<tr>
<td>$c_F$</td>
<td>Compressibility of the fracture</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
</tr>
<tr>
<td>$c_M$</td>
<td>Compressibility of the matrix</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
</tr>
<tr>
<td>$C_f$</td>
<td>Cleat-volume compressibility</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
</tr>
<tr>
<td>$C_g$</td>
<td>Concentration of gas phase</td>
<td>$\frac{\text{lb-mole}}{\text{ft}^3}$</td>
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<tr>
<td>$C_m$</td>
<td>Seidle and Huitt’s matrix swelling coefficient</td>
<td>$\frac{\text{US-ton}}{\text{scf}}$</td>
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<tr>
<td>$c_{\phi}$</td>
<td>Formation compressibility</td>
<td>$\frac{\text{psi}^{-1}}{}$</td>
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<tr>
<td>$D$</td>
<td>Diffusion coefficient</td>
<td>$\frac{\text{ft}^2}{\text{day}}$</td>
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<tr>
<td>$E$</td>
<td>Young’s modulus</td>
<td>$\text{psi}$</td>
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<tr>
<td>$f$</td>
<td>Fraction from $0 - 1$</td>
<td>fraction</td>
</tr>
<tr>
<td>$f_c$</td>
<td>Critical sorption capacity factor</td>
<td>fraction</td>
</tr>
<tr>
<td>$f_l$</td>
<td>Fugacity of component $l$ in gas phase</td>
<td>$\text{psia}$</td>
</tr>
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</table>
\( f_i^0 \) Fugacity of component \( i \) in gas phase at standard state condition \( \text{psia} \)

\( \tilde{f} \) Sorption capacity factor fraction \( g \) Local gravitational acceleration \( \text{ft}^2/\text{sec} \)

\( g_c \) Conversion factor for gravitational acceleration \( \text{lb}_m \cdot \text{ft}/\text{lb}_f \cdot \text{sec}^2 \)

\( G \) Depth from datum to the center of the block \( \text{ft} \)

\( G_A \) Amount of current adsorbed gas \( \text{SCF} \)

\( G_{A,i} \) Amount of original adsorbed gas \( \text{SCF} \)

\( G_c \) Gas content \( \text{SCF}/\text{ton} \)

\( G_f \) Original free gas in the fracture \( \text{SCF} \)

\( G_M \) Original free gas in the matrix \( \text{SCF} \)

\( h \) Thickness \( \text{ft} \)

\( \text{IMBC}_g \) Incremental material balance check for gas phase \( - \)

\( \text{IMBC}_w \) Incremental material balance check for water phase \( - \)

\( k \) Absolute permeability \( \text{perms} \)

\( k_i \) Initial absolute permeability \( \text{perms} \)

\( k_{rg} \) Relative permeability to gas phase fraction \( k_{rw} \) Relative permeability to water phase fraction

\( k_x, k_y, k_z \) Absolute permeability in \( x-, y- \) and \( z- \) directions \( \text{perms} \)

\( K \) Bulk modulus \( \text{psi} \)

\( L_x, L_y, L_z \) Fracture spacing in \( x-, y- \) and \( z- \) directions \( \text{ft} \)

\( m \) Moisture content \( \text{wt. percent} \)

\( m_c \) Critical moisture content \( \text{wt. percent} \)
\begin{verbatim}
M  Constrained axial modulus    psi
M_{g}  Molecular weight of gas  lb/lb-mole
n_{i}^{0}  Pure component adsorption capacity at standard state  SCF/ton
condition
n_{d}  Adsorption capacity of dried coals  mmole/g-coal
n_{w}  Adsorption capacity of wet coals  mmole/g-coal
OGIP  Original gas in place  SCF
OWIP  Original water in place  STB
p  Pressure  psia
p_{cgw}  Capillary pressure  psia
p_{g}  Pressure of gas phase  psia
p_{i}  Initial pressure  psia
p_{sat}  Saturated pressure  psia
p_{w}  Pressure of water phase  psia
p_{D,F}  Dimensionless fracture pressure  -
p_{D,M}  Dimensionless matrix pressure  -
\overline{p_{R}}  Average reservoir pressure  psia
p_{of}  Sandface pressure  psia
p_{L}  Langmuir pressure  psi
q_{g}  Gas flow rate  SCF/day
q_{xp}  Sorption flow rate  SCF/day
q_{w}  Water flow rate  STB/day
q_{D,g}  Dimensionless gas flow rate  -
q_{D,w}  Dimensionless water flow rate  -
\end{verbatim}
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<td>$S_{girr}$</td>
<td>Irreducible Gas saturation</td>
<td>fraction</td>
</tr>
<tr>
<td>$S_w$</td>
<td>Water saturation</td>
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<td>$S_{wirr}$</td>
<td>Irreducible water saturation</td>
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<td>Drainage radius</td>
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<td>$r_w$</td>
<td>Wellbore radius</td>
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<td>Dimensionless radius</td>
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<td>$R$</td>
<td>Gas constant (10.731)</td>
<td>$ft^3 \cdot psi / R \cdot lb \cdot mole$</td>
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<td>Residual of gas flow equation</td>
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<td>$R_{sw}$</td>
<td>Solution gas-water ratio</td>
<td>SCF/STB</td>
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<td>$R_{sw,i}$</td>
<td>Solution gas-water ratio at initial conditions</td>
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<td>Residual of water flow equation</td>
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<tr>
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<td>Darcian velocity of gas phase</td>
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<td>$V_b$</td>
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<td>Bulk volume of the fracture system</td>
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<td>Cumulative water production</td>
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<td>Original free water in the fracture</td>
<td>STB</td>
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<td>$W_M$</td>
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**Greek**

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<td>Matrix shrinkage-swelling coefficient</td>
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<td>$\Delta$</td>
<td>Finite-difference grid size</td>
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<td>$\Delta t$</td>
<td>Finite-difference time step</td>
<td>day</td>
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**Subscripts**

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ACKNOWLEDGEMENTS

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Chapter 1

Introduction

Recent studies show that conventional oil & gas resources are rapidly declining, and many energy companies are searching for alternative resources. Even though, coalbed methane (CBM) has been historically a source of hazard in the mining industry and threatened the lives of underground miners, due to the abundance of coalbed methane reservoirs and with increasing safety measurements, it has become one of the main alternative energy resources for countries like China, Australia and United States (Chakhmakhchev, 2007). In the late 1700's Scotsman William Murdoch recognized the potential of coalbed methane as a source of light in mines. While, an exact date for the first coalbed methane production is lacking; it is believed to begin in 1920's in one of the fields in West Virginia, Ohio or Oklahoma. The first well drilled for coalbed methane production dates to 1950's operations in the San Juan Basin (Scott 2004).

Unlike in sandstone and carbonate reservoirs, gas in coalbed methane reservoirs is stored in the source rock as an adsorbed gas. The volume of gas available for production depends on many parameters, including coal seam thickness, cleat fracture networks and water content. Coalbed methane reserve estimations vary, however the U.S. Geological Survey estimates that the coalbed methane resources in the lower 48 states of the U.S. are in excess of 17.5 trillion cubic feet (USEIA 2010).

First consideration of applying numerical models into reservoir engineering problems dates back to the 1950's. The first useful numerical model for reservoir
simulation was developed in the mid-1950's (Mattax and Dalton, 1990). Like all other reservoirs, numerical reservoir simulators play an important role in coalbed methane reservoir development. The key feature of numerical models is to be able to predict pressure and saturation distributions in reservoirs and hence the performance of wells. One of the challenges in today’s numerical simulators is representing complex well structures (Ding et al. 1998). Current wellbore models lack representation of complex well geometries (Nolen 1990 and Su 1995) and generate erroneous results in predicting the pressure drop around the wellbore (Ding et al. 1998). Moreover, due to complex fluid flow models, performance of the simulators suffers and takes long time to simulate even simple cases. Reservoir dynamics and well geometries of coalbed methane reservoirs make it hard to develop reliable reservoir simulators for reservoir studies and economic analysis.

The complexity of coalbed methane reservoirs makes it necessary to develop specially design computer models with advanced capabilities that include:

- The ability to capture multi-mechanistic fluid flow models, including Fickian and Darcian flow (Ertekin-1986).
- Consideration of the dual porosity and permeability of coalbed reservoirs (Ertekin - 1989).
In this research study, a new means of well representation is introduced to existing CBM simulator. New well representation uses the flow equations and the residual terms to calculate flow rate into wells rather than using wellbore equations to calculate flow rate. Complex wells are described as a combination of high-resolution fine rectangular grid blocks. This technique, also known as local grid refinement, allows capturing flow behavior and pressure distribution around the well more accurately. The technique performs domain decomposition, which creates locally refined sections inside the coarse system and solves both domains simultaneously.

Reservoir simulation is a large mathematical undertaking, incorporating large systems of linear equations. Using local grid refinement technique adds additional burden on the solution since the locally refined region has high resolution, ranging from thousands of grid blocks to millions of grid blocks. In consideration of this, a study has been conducted to find the most efficient mathematical procedures for implementation in the coalbed methane (CBM) simulator. The generalized minimum residual method (GMRES) has been identified as the optimum matrix solution technique. This technique showed significant improvement on simulation run times and memory usage. Even with more efficient matrix solver, the CBM simulator has significant computational power and memory requirements. These requirements restrict the efficacy of this research program as a number of days must be set aside for each simulation run. To overcome this problem, the ParaSails (CASC – 2012) preconditioner and Fast Auxiliary Space Preconditioner (FASP) added to the CBM simulator. For further performance improvement, a parallelized version of the ParaSails preconditioner and the GMRES iterative solver were implemented to the CBM code using message passing interface (MPI) technique.
MPI allows the simulator to use multi-core processors for each simulation run. It is envisaged that this parallel computing approach enables rapid simulation run times. As a result, these improvements increased the efficiency of advanced CBM simulator and simulations could be completed in a short period time. Improvements in CBM simulator allows simulating more realistic reservoir models, which yields better understanding of reservoir conditions. Various complex well architectures are investigated to find out the optimum conditions for methane production from coalbed reservoirs.
Chapter 2

Literature Review

In this chapter, the main discussion will be on the local grid refinement (LGR) approach by reviewing some important background material and presenting some of the existing literature applies to the concepts that are directly related to this work. The concepts are reviewed in the following order:

1. The nature of coalbed methane reservoirs
2. Complex Well Structures
3. Numerical models; improvements (computer speed and storage, and solvers) in reservoir simulations
4. Gridding techniques; grid refinement techniques

2.1 The Nature of Coalbed Methane Reservoirs

Coalbed methane (CBM) is a form of natural gas extracted from coal beds. In recent decades, coalbed methane has become an important source of energy in United States, Canada, and other countries. Australia has rich coal deposits where it is known as coal seam gas (BG Group 2012).

Coalbed methane is distinct from typical sandstone or other conventional gas reservoir, as the methane is stored within the coal by a process called adsorption. Unlike
much natural gas from conventional reservoirs, coalbed methane contains very little heavier hydrocarbons such as propane or butane, and no natural gas condensate.

Coalbed methane reservoirs are dual porosity systems where macro-pores, fractures, serve the role of transporting the fluids (water and gas) to the wellbore and micro-pores serves as the main source of gas storage (King et al. 1986). In most of the coalbed methane reservoirs, micro-pores are not accessible to water and gas in micro-pores are stored in adsorbed form on the surface of the coal matrix system. However, experimental studies (Krooss et al. 2002; Ozdemir, 2004; Jahediesfanjani and Civan, 2006) showed presence of water in the coal matrix is possible and it affects the sorption capacity of the coal. With or without water in the coal matrix, as the pressure in the reservoir drops due to production, the adsorbed gas starts to desorb from the micro-pores. The transportation of gas starting from micro-pores to wellbore can be described in three stages; sorption, diffusion and convection process.

There are several concepts to capture the sorption process. One of the most commonly used techniques is a concept that is introduced by Langmuir in early 1900’s. Langmuir developed the simplest sorption model, where only the sorption pressure and sorption capacity is need for the calculations. Langmuir assumes that;

- The surface of the adsorbent (coal matrix) is uniform and all adsorption sites are equivalent.
- Adsorbed molecules do not interact.
• All adsorption occurs through the same mechanism.

• At the maximum adsorption, only a mono-layer of absorbed molecules is formed.

Even though there are several disadvantages of Langmuir adsorption model, such as; it fails to account for the surface roughness of the absorbate or ignoring the interactions between molecules, these assumptions are seldom true.

As studied by Ertekin et al (1986), the flow process from coal matrix (micro-pores) to fracture system (macro-pores) is dominated by the concentration difference. Early versions of CBM models (King, 1986; Remner et al. 1986; Sung et al. 1986; Sawyer et al, 1990; Manik et al., 2002) were using dual-porosity, single-permeability systems. These models assume that desorbed gas goes directly into the fracture system in the coalbed reservoirs. Because of this assumption, dual-porosity, single-permeability systems suffers drastically with early depletion of the reservoir and the over prediction of gas production and under-prediction of water production in early stages of the reservoir. Since the flow characteristics in fracture and matrix are different, proposed Fickian flow model was implemented to the CBM simulator (Reeves and Pekot, 2001; Cicek, 2003; Thararoop, 2010).
2.2 Complex Well Structures

Predicting the reservoir performance through the reservoir simulations are the major drive for developing numerical reservoir simulators since 1950’s. Reservoir simulation is an important component of economic analysis. Accuracy in well representation, modeling of near wellbore flow convergence, and prediction of total production are important functions of reservoir simulation. The well model is one of the more important components of numerical reservoir simulators since the precision of the fluid flow calculations and bottomhole pressure is directly related to the well model.

In reservoir simulation, wells represent sink and source terms in the reservoir model (Williamson 1981). First introduced by Peaceman (1977 and 1983) and Babu et al. (1991), finite-difference reservoir simulators use the concepts of well index and equivalent well-block radius to represent wells. The main difficulty of well representation in the numerical reservoir simulators is that while the wellbore radius is usually less than 0.5 feet, whereas the corresponding grid block that holds the well has a size ranging from tens of feet to hundreds of feet. Thus, pressure values calculated by the solution of finite-difference approximation of the flow equations do not give the wellbore pressure. Peaceman (1977, 1983) first demonstrated that the pressure of the well block calculated by finite difference gives the block pressure at the equivalent wellbore radius, $r_0$, in a uniform grid system. Peaceman, then, demonstrates that with using this radius, the well block pressure can be related to the wellbore pressure. However, there are some problems with this approach, such as;
• There is not an easy way to determine $r_o$ value for non-square well blocks.

• For not-fully-penetrating wells, the assumption of radial flow geometry at the well block is violated.

• Treatments for block off-centered wells are not accurate.

Therefore, the necessity of having the right model for representing the correct sink/source terms (well model) in flow equations is crucial for numerical reservoir simulation calculations.

As Palmer et. al (1992) discussed, it is crucial to stimulate the coalbed methane reservoirs, since the production profile of gas and water from an unstimulated well will suffer drastically with its absence. Hydraulic fracturing is the most common type of stimulation, and its performance in coal gas reservoirs is studied by several researchers such as Penny et al. (1991), Goktas and Ertekin (1999), Valencia et. al (2005) and Aghighi et al. (2006). Due to unfortunate recent incidents (Switchboard 2011), application of hydraulic fracturing is being restricted in some of the US states and it is even nowadays more difficult to have permission in many states. Companies nowadays use complex well structures to maximize formation accessibility and avoid hydraulic fracturing. Current developments in drilling tools and techniques enable companies to use horizontal and multilateral wells, thus making them common practice in the petroleum industry to improve the economics of production operations.

The ability to control well direction, shape and position is the main advantage of using horizontal wells in coal seam reservoirs (Ertekin et al - 1988). Since the dewatering process in coal seams has the largest effect on gas production, it is crucial to maximize the contact length of the wellbore within the coal seam. Multilateral wells achieve this
maximum contact between the wellbore and the formation while keeping the drilling cost lower. These wells are commonly referred as maximum reservoir contact (MRC) wells (Yang and Deo 2006).

In order to represent advanced wells, models based on fully implicit formulation are required (Larry et al. 2005). Implementation of implicit solution of the wells is a complex procedure and even if it is implemented correctly, current models still suffer from the basic assumptions of Peaceman’s well representation.

2.3 Numerical Models: Improvements in Reservoir Simulator

The main objective of reservoir simulation studies is to predict the future performance of a reservoir with the current knowledge of reservoir properties within a certain levels of uncertainty (Aziz and Settari 1979). During the early 1960’s, numerical reservoir simulators are developed for mainly oil reservoirs (black oil simulators). Early models were used for simulating multi-dimensional reservoirs having multiphase mixtures (mostly oil/water/gas).

After the global oil crisis hit the market and increased the oil prices, companies and researchers sought for alternative resources. This brought the need for more complex numerical models where it can simulate various reservoir processes. During this time many numerical reservoir simulation studies were conducted on thermal stimulation and in-situ combustions (Coats 1978), compositional fluid flow modeling (Kazemi & Cracks 1979), chemical flooding (Bonder et al. 1972) and miscible flooding (Chaudhari 1979).
Additional to the modeling of complex fluid flow dynamics, with the improvements in reservoir monitoring, geologists are now able to create more precise reservoir descriptions using seismic, well logs and core samples. Usually, this additional information yields to have millions of cells to represent the reservoir conditions. Even though, the current computer hardware allows users to store and simulate these reservoir models, there is always a need for better and faster linear equation solvers.

Through the early 1960’s to the mid-1970’s, because of the small scale of the reservoir models, direct solvers using Gauss-Seidel elimination were fast enough for solving the linear equations created in the process of reservoir simulation. However, increase in the number of grid blocks and implementation of complex flow models raised the need for solvers using less memory and performing faster than direct solvers. One of the first iterative solvers was presented in 1981 by Watts. The proposed preconditioned conjugate gradient method was proven to be faster than SIP method in most of the cases. Even though, preconditioned conjugate gradient method is only suitable for symmetric matrices, there are many uses of it in the many industries. In 1992, H. A. van der Vorst saw the lack in conjugate gradient method and published the Bi-Conjugate Stabilized iterative solver which is suitable for solving symmetric and non-symmetric matrixes.

As Yousef Saad (Saad – 2003) states, there is no single matrix solver that will work efficiently for all nonsymmetrical linear systems. The performance of the solver depends on the type of the problem and can differ from case to case. The best way to determine which matrix solver works best for the problem is to test it. In this study, five different matrix solvers were tested. More detailed discussion about the matrix solvers will be presented in Chapter 6.
2.4 Local Grid Refinement

In hydrocarbon reservoirs, sharp pressure differences and rapid fluid movement occur in the vicinity of the well. For small scale reservoir models, the accuracy of the simulation can be improved by using smaller grid block dimensions on and around the well blocks. Therefore, the truncation errors can be minimized and more precise results can be obtained. However, increasing the number of grid block around the well may not be applicable for relatively large scale reservoirs due to memory requirements and time constraints.

Reservoir simulation has been improved by using local grid refinement and adaptive grids (Heinemann, et al. 1983, Quandalle and Besset, 1985, Forsyth and Sammon, 1986, and Pedrosa and Aziz, 1986). Ding and Jeannin (2000 and 2004) emphasized the need to use flexible grid systems due to the scale differences between the reservoir size and wellbore radius. They introduced control volume schemes to improve near-well flow representation in flexible grid systems.

As discussed by Maricic et al (2005) and Roadifer et al (2003), the design of the wellbore is an important factor in degasification of the coalbed methane reservoirs. Local grid refinement allows capturing both path of the well and the pressure transient more accurately. Ertekin and Biterge (1989) developed a numerical reservoir simulator that can integrate static and dynamic local grid refinement techniques. They showed that using local grid refinement, truncation errors around the wells can be reduced drastically. In their studies, they used a local grid refinement technique and were able to match the
flowrate and pressure distribution of the system with the analytical solution of the same problem.

Ertekin and Goktas (1999) studied LGR technique on cavity completions and extended their results for representation of undulating wells. Cavity completions have been a popular stimulation technique for coalbed methane reservoirs for decades. However, well models, like Peaceman, are not able to represent this kind of completions and gives erroneous results in both flowrate predictions and pressure distribution. Ertekin and Goktas (1999) proved that LGR technique provides a better match against the analytical solution for both the cavity completions and undulating wells.

In this study, a similar technique is utilized to represent horizontal, vertical, and multilateral wells in a dual-porosity, dual permeability coalbed methane reservoir simulation. By applying the LGR technique, it becomes possible to simulate the conditions where multi-lateral wells applied as a replacement of a hydraulic fracturing. The new well representation technique also allows to analyze the effects of well geometry on enhance gas recovery from coalbed methane reservoirs, and ultimate recovery of methane.
Chapter 3

Problem Statement

Well performance, pressure distribution around the wells and well spacing are the main concerns in coalbed methane reservoir development and production predictions. Decreasing the reservoir pressure effectively yields more methane release from the coalbed matrix due to desorption of the methane. Even though, there are many stimulation techniques available, such as cavity completion or fracturing, it has been proven that their effectiveness vary depending on the existing reservoir conditions (Goktas-1999).

Current developments in drilling operations allow companies to utilize multiple branches of horizontal wells or even fishbone-like structures from the same entry point at the surface. However, it is a challenge to represent these complex well structures in numerical reservoir simulations. The widely used Peaceman’s model has been proven to fall short and predicts erroneous flow rates and pressure distributions with complex well geometries (Larry et al. 2005). The basic assumptions of Peaceman’s model such as; presence of radial flow, full penetration of the well block, and the assumption of well location being at the center of the well block distort its applicability to complex flow geometry and do not represent realistic conditions for complex well structures. Even though complex well geometry can be approximated by using relatively small grid blocks
and using Peaceman’s wellbore model, it is known that the convergence under this conditions are hard to achieve and sometimes it is even not possible.

The main goal of this research program is to develop and implement a practical local grid refinement technique to eliminate the need for Peaceman’s well model. By local refinement of the well blocks, it is possible to represent complex well structures within a reservoir model. An in-house advanced numerical reservoir simulator was used to investigate the effects of complex well geometries on the development of coalbed methane reservoirs. Since the current simulator supports dual-porosity, dual-permeability systems with multiphase and multi-component flow, the effects of combination of different well structures was investigated. Locally refined grids were used to calculate the pressure distribution around the well and then more precise flow rates were calculated for given well structures.

Since the high resolution local grid refinement increases the number of grid blocks in the window block, the solution of linear equations in local regions requires extensive memory and computer power. In order to increase the efficacy of the solution procedure, advance iterative solvers are coupled with a better matrix-vector storage technique. Furthermore, parallel programming technique is applied on the matrix solver and matrix preconditioner to decrease the time for generating solution vector.

Another factor on the efficiency of the simulations is the stability of the Newton-Raphson procedure. As Manik (1999) mentioned in his study, the stability of the CBM simulator during multi-component gas injection/recovery simulations are affected adversely due to complex fluid flow equations. In order to overcome this problem, a subroutine is implemented on the reservoir simulator to improve initial guesses of
pressure, saturation and concentration values on Newton-Raphson level. This not only kept simulations more stable, but also helped to achieve faster convergence. Figure 3-1 demonstrates the capabilities of existing and proposed CBM simulator.

The aims of this research can be summarized as follows:

- In order to increase the efficacy of the simulations, an advanced linear equation with two different preconditioners is implemented and parallel processing technique is used for further improvement.

- Local grid refinement technique is implemented and it is proved that this technique can be used as a replacement of well-known Peaceman’s wellbore model.

- Local grid refinement technique is used to simulate complex wellbore geometries and identify the advantages of it under different reservoir conditions.
Table 3-1 Summary of key features in the existing and proposed numerical CBM models

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Chapter 4
Local Grid Refinement

Simulation of coalbed methane reservoirs often needs highly refined grids in local areas of interest to improve simulation accuracy. For example, refined grids may be needed in

- regions where hydraulic gradients change substantially over short distances, as would be common near injecting wells;
- regions requiring detailed representation of heterogeneity, as may be required to simulate faults, lithological displacements caused by faulting, fractures, thin lenses, pinch outs of geologic units, and so on.

Refinement of the finite-difference grid used can be achieved using several methods; the advantages and disadvantages of each are explained below.

Global Grid Refinement

In this case, the entire coarse geological model (Figure 4-1) is refined to create high resolution geological model (Figure 4-2).

Advantages;

- Easy to build the new grid system using the current model
- Can yield reliable results due to minimized truncation errors
- Better representation of fluid flow dynamics throughout the reservoir
Disadvantages;

- Resultant model creates a needless by large number of grid cells outside the area of interest. This will result in extensively large computational power both in storage and time.

**Non-Uniformly Spaced Grid (Conventional Grid Refinement)**

In this method, the grid dimensions vary throughout the reservoir (Figure 4-3). The grid sizes get smaller around the area of interest for better accuracy of the simulation however; gradually increase in size away from this area.
Figure 4 - 2 Global Grid Refinement

Advantages;

- Ideal method for cases where there are not many wells
- Single step matrix solution for the refined area and the coarse system.

Disadvantages;

- Not ideal if there is more than one area of interest in the reservoir domain (ex: existence of few wells to study the behavior of the well structures).
- Can create grid blocks with high aspect ratio, which can lead to numerical errors.
- Creates extra grid blocks in regions which are not critical to the solution which leads to longer simulation times.
Local Grid Refinement (LGR)

In this method, only the area of interest is refined (Figure 4-4). Refined area links to the coarse system and there is a constant information flow between the coarse block and the window block.

Advantages;

- Creates refined grids only in the area of interest
- Having multiple area of interests is not an issue since they will be treated separately
- Easy to design refined grid blocks
- Allows multi-levels of refinement
Disadvantages;

- Constant feedback will be necessary to transfer boundary conditions for the window block
- Window block and the coarse system matrixes are solved separately, however, it is still faster as compared to globally refined or conventional refined models.

![Figure 4 - 4 Local Grid Refinement](image)

One of the first applications of LGR was performed by von Rosenberg (1982). He developed a static multi-level local grid refinement method to minimize truncation errors around the wellbore. His study showed that, using local grid refinement can decrease the truncation errors and leads to more accurate simulation results. Wasserman (1987), on the
other hand, developed a local grid refinement technique where both refined and coarse grid blocks shares the same domain. Even though, his technique requires only one level of Newton-Raphson iteration to solve the entire system, refined and coarse system combined, the numbering scheme utilized makes it difficult to implement on the existing reservoir simulators. Moreover, due to complex data structure of the resultant matrix, as shown in Figure 4-5 and 4-6, the matrix solution performance suffers severely.

![Reservoir Grid Numbering Scheme for Wasserman Local Grid Refinement Procedure](image)

**Figure 4 - 5 Reservoir Grid Numbering Scheme for Wasserman Local Grid Refinement Procedure**
Biterge and Ertekin (1989) developed a new technique which is to a certain extent similar to Wasserman. In their study, they separate the locally refined blocks and the coarse grid system. Locally refined region, window block, surrounded by pseudo grid blocks which hold the corresponding pressure and saturation blocks from the coarse system. In the boundary of the refined grid blocks and pseudo grid blocks, they introduced Dirichlet type boundary conditions. Locally refined regions and coarse grid blocks are solved separately but at the same iteration level.

Similar to Biterge and Ertekin (1989) study, Goktas and Ertekin (1999) implemented the static local grid refinement technique to simulate undulating wells and cavity completions. In their study, they created a locally refined region small enough to represent cavity completions as a combination of several grid blocks. Consequently, they
used the flow equations to calculate the flow going through these small grid blocks. By doing this, they eliminated the need of Peaceman’s equation to calculate flowrate.

In this study, a similar local grid refinement technique that is used by Goktas and Ertekin is applied to simulate the complex well geometries. Figure 4-7 shows an example of the proposed scheme on a vertical well going through a coarse grid block.

As it can be seen from the figure, well blocks are determined through the well path. To be consistent with the wellbore properties, the size of the well blocks determined in such a way that the wellbore and the well blocks have the same volume. Equation 4-1 shows the calculation of the well block dimensions.

\[ \pi r_w^2 h = \Delta x^2 h \]  

\hspace{1cm} (4-1)
Since well blocks have relatively small dimensions (0.44 ft. by 0.44 ft. for a wellbore with 0.25 ft. radius), a smooth transition needs to be established between the well blocks and the rest of the refined region. Moreover, at the boundaries of the refined region a smooth transition is necessary to avoid truncation errors and establish better stability. Equations 4-2, 4-3 and 4-4 are used to calculate the dimensions of the adjacent grid blocks so that the smooth transition between well blocks and refined region and refined region to pseudo grid blocks can be satisfied. Increasing the dimensions of grid blocks gradually allows not only to have a more stable simulation but also to have faster simulations due to reduce number of grid blocks in the window block.

\[
\Delta x_{i+1} = (\Delta x_i)^\alpha \quad \text{where } \alpha > 1.0 \tag{4-2}
\]

\[
\Delta y_{j+1} = (\Delta y_j)^\beta \quad \text{where } \beta > 1.0 \tag{4-3}
\]

\[
\Delta z_{k+1} = (\Delta z_k)^\gamma \quad \text{where } \gamma > 1.0 \tag{4-4}
\]
Chapter 5
Mathematical and Computer Model

In this chapter, the governing equations for the mathematical model and the linearization of those equations will be demonstrated in detail. In this research study, a Cartesian coordinate system is considered for the flow geometry for both the locally refined systems and the coarse grid system. The differential (Eularian) approach is applied on the governing flow equations to derive continuity equation. Figure 5-1 represents the control volume and material balance on the fluid flow through the control volume over time period of $\Delta t$. The material balance can be calculated from Equation 5.1.

$$[\text{mass in}] - [\text{mass out}] + [\text{source/ sink}] = [\text{change in mass}] \quad (5.1)$$

Figure 5 - 1 Finite Volume for Fluid Flow
As mentioned in previous chapters, the early version of the CBM simulator used a dual-porosity, single permeability flow model. During a period of 25 years, the CBM simulator has been improved by the studies of many researchers (King et al., 1986; Remner et al. 1986; Sung et al. 1986; Sawyer et al, 1990; Manik et al., 2002, Reeves and Pekot, 2001; Cicek, 2003 and Thararoop 2010). The existing CBM model has a multi-mechanistic two-phase (gas and water) flow model in a dual-porosity, dual-permeability system and it has the capability to account for water presence in the coal matrix. Facture network and coal matrix equations are solved simultaneously for both water and gas phases. In this development, gas phase is treated as a multi-component system while water phase is assumed to be a single component system. In addition, gas transport is considered to be multi-mechanistic in both fracture and matrix domains while water transport is considered to take place by Darcian flow only.

5.1 Mathematical Model

5.1.1 Governing Equations

The existing CBM simulator is capable of simulating flow and concentration of ten gas components simultaneously. The following equation is solved using the multi-mechanistic superficial gas velocity. The gas flow equation for component \( l \) in the fracture domain can be written as follows:
The effective area where the diffusive flow happens in the porous media can be represented by the term \( \phi_F S_{g,F} A \). Due to the small fracture spacing in coal, the gas flow equation for the same component “l” in the matrix domain can be written as follows:

\[
\nabla \left( \frac{D_l \phi F S_{g,F}}{5.615} \right) X_{l,F} S_{g,F} \frac{\mu_{g,F}}{B_{g,F}} \nabla \Phi_{g,F} + R_{SW,l,F} \frac{A_k k_{rw,F}}{\mu_w B_{w,F}} \nabla \Phi_{w,F} \right) + \Gamma_{g,l,F} + q_{g,l} + R_{SW,l,F} q_w = \frac{1}{5.615} \frac{\partial}{\partial t} \left[ X_{l,F} \frac{V_p \phi F S_{g,F}}{B_{g,F}} + R_{SW,l,F} \frac{V_p \phi F S_{w,F}}{B_{w,F}} \right] \tag{5.1.1}
\]

In the potential term of the Equation 5.1.1, the depth is assumed to be positive downward from the datum plane; therefore, the flow potentials of gas equation, \( \Phi_{g,F} \) and \( \Phi_{g,M} \) can be expressed as:

\[
\Phi_{g,F} = p_{g,F} - \frac{1}{144 g_c} \frac{g}{\rho_g} G \tag{5.1.3}
\]

\[
\Phi_{g,M} = p_{g,M} - \frac{1}{144 g_c} \frac{g}{\rho_g} G \tag{5.1.4}
\]

The existing CBM model assumes that water flow obeys only the Darcy’s law. Therefore, the flow equation for the water phase can be expressed as follows:

\[
\nabla \left( \frac{A_k k_{rw,F}}{\mu_w B_{w,F}} \nabla \Phi_{w,F} \right) + \Gamma_{w,F} + q_w = \frac{1}{5.615} \frac{\partial}{\partial t} \left[ V_p \phi F S_{w,F} \right] \tag{5.1.5}
\]
Also, the water flow equation from the coal matrix to the fracture network can be expressed by:

\[
\Gamma_{w,M} = \frac{1}{5.615} \frac{\partial}{\partial t} \left[ \frac{V_b \phi_M S_{w,M}}{B_{w,M}} \right]
\]

(5.1.6)

The water flow potentials, \( \Phi_{w,F} \) and \( \Phi_{w,M} \), in Equations (5.1.5) and (5.1.6) can be written as:

\[
\Phi_{w,F} = P_{w,F} - \frac{1}{144} \frac{g}{g_c} \rho_w G
\]

(5.1.7)

\[
\Phi_{w,M} = P_{w,M} - \frac{1}{144} \frac{g}{g_c} \rho_w G
\]

(5.1.8)

For more information about the equations and correlation used in the development of rock and fluid properties please refer to Appendix A.
5.1.2 Auxiliary Equations

The dual-porosity, dual-permeability CBM simulator has at least 4 equations to solve when the system has only one gas component and water phase. The number of unknowns and equations per block increases to 28 in the presence of water and a gas phase with 10 gas components. The total number of unknowns is then calculated as $2 \times NC + 8$. The primary unknowns are $p_{g,F}, p_{g,M}, p_{w,F}, p_{w,M}, S_{g,F}, S_{g,M}, S_{w,F}, S_{w,M}, X_{l,F}$ and $X_{l,M}$, where $l = 1, 2, \ldots, NC$. A set of equal number of equations is required to solve for those unknowns. Equations 5.1.1 to 5.1.6 create $2 \times NC + 2$ equations. The remaining six equations can be obtained from capillary pressure relationships, saturation and mole fraction constraints for the fracture and matrix domains as shown below:

**Capillary pressure relationships:**

$$P_{c_{gW,F}}(S_{g,F}) = p_{g,F} - p_{w,F} \quad (5.1.9)$$

$$P_{c_{gW,M}}(S_{g,M}) = p_{g,M} - p_{w,M} \quad (5.1.10)$$

**Saturation constraints:**

$$S_{g,F} + S_{w,F} = 1 \quad (5.1.11)$$

$$S_{g,M} + S_{w,M} = 1 \quad (5.1.12)$$

**Mole fraction constraints:**

$$\sum_{l=1}^{NC} X_{l,F} = 1 \quad (5.1.13)$$

$$\sum_{l=1}^{NC} X_{l,M} = 1 \quad (5.1.14)$$
5.1.3 Finite-Difference Approximations

As stated earlier, the Eulerian approach is used in this study. Equations 5.1.1, 5.1.2, 5.1.5 and 5.1.6 are used for simultaneous solution of gas pressure, water saturation and gas concentration of each component in fracture network and coal matrix system. These equations include time and space derivatives and the finite difference approximation for these equations are as follows:

Finite-difference approximation for gas phase in fracture network in a 1-D system is:

\[ R_{g,l,F}^{n+1} = \frac{D_{l,F} \phi_{l,F} S_{g,F} A_x}{5.615 \Delta x} \left[ \phi_{l,F} S_{g,F} A_x \right]_{i+1}^{n+1} \left( X_{l,F} \frac{S_{g,F}}{B_{g,F}} \right)_{i+1}^{n+1} - \left( X_{l,F} \frac{S_{g,F}}{B_{g,F}} \right)_{i}^{n+1} \]

\[ - \frac{D_{l,F} \phi_{l,F} S_{g,F} A_x}{5.615 \Delta x} \left[ \phi_{l,F} S_{g,F} A_x \right]_{i-1/2} \left( X_{l,F} \frac{S_{g,F}}{B_{g,F}} \right)_{i}^{n+1} - \left( X_{l,F} \frac{S_{g,F}}{B_{g,F}} \right)_{i-1}^{n+1} \]

\[ + \frac{A_x}{\Delta x} \left[ k_{x,F} \right]_{i+1/2}^{n+1} \frac{1}{\mu_g B_{g,F}} \left( X_{l,F} k_{rg,F} \right)_{up} \left( \phi_{g,F} \right)_{i+1}^{n+1} - \left( \phi_{g,F} \right)_{i}^{n+1} \]

\[ - \frac{A_x}{\Delta x} \left[ k_{x,F} \right]_{i-1/2}^{n+1} \frac{1}{\mu_g B_{g,F}} \left( X_{l,F} k_{rg,F} \right)_{up} \left( \phi_{g,F} \right)_{i}^{n+1} - \left( \phi_{g,F} \right)_{i-1}^{n+1} \]

\[ + \frac{A_x}{\Delta x} \left[ R_{sw,l,F} \right]_{i+1/2}^{n+1} \frac{1}{\mu_w B_{w,F}} \left( X_{l,F} k_{rw,F} \right)_{up} \left( \phi_{w,F} \right)_{i+1}^{n+1} - \left( \phi_{w,F} \right)_{i}^{n+1} \]

\[ - \frac{A_x}{\Delta x} \left[ R_{sw,l,F} \right]_{i-1/2}^{n+1} \frac{1}{\mu_w B_{w,F}} \left( X_{l,F} k_{rw,F} \right)_{up} \left( \phi_{w,F} \right)_{i}^{n+1} - \left( \phi_{w,F} \right)_{i-1}^{n+1} \]

\[ + \Gamma_{g,l,F}^{n+1} + q_{g,l}^{n+1} + R_{sw,l,F} q_{w,l}^{n+1} \]

\[ - \frac{1}{5.615 \Delta t} \left[ \phi_{l,F} S_{g,F} \right]_{i}^{n+1} \left( \phi_{w,F} \right)_{i}^{n+1} + \left( R_{sw,l,F} \phi_{F} S_{w,F} \right)_{i}^{n+1} \]
The right hand side of the above equation includes the flow components for the Fickian flow and the Darcian flow for each gas component. The finite-difference approximation of the gas flow equation in the coal matrix in a 1-D system is given by:

\[
R_{g,i,M}^{n+1} = \Gamma_{g,i,M}^n + q_{srp,i}^{n+1} - \frac{1}{5.615\Delta t} \left[ \left( X_{i,M} V_b \phi_M S_{g,M} \right)^n_i + \left( R_{sw,i,M} V_b \phi_M S_{w,M} \right)^n_i \right] + \frac{1}{5.615\Delta t} \left[ \left( X_{i,M} V_b \phi_M S_{g,M} \right)^n_i + \left( R_{sw,i,M} V_b \phi_M S_{w,M} \right)^n_i \right]
\]

(5.1.15)

The finite-difference approximation of the water equation in the fracture network in a 1-D system is given by:

\[
R_{w,F}^{n+1} = \frac{A_x}{\Delta x} \left[ k_{x,F}^{n+1}_{i+\frac{1}{2}} \frac{1}{\mu_w B_{w,F}} \left( \Phi_{w,F}^{n+1}_{i+1} - \Phi_{w,F}^{n+1}_i \right) \right] - \frac{A_x}{\Delta x} \left[ k_{x,F}^{n+1}_{i-\frac{1}{2}} \frac{1}{\mu_w B_{w,F}} \left( \Phi_{w,F}^{n+1}_i - \Phi_{w,F}^{n+1}_{i-1} \right) \right] + \Gamma_{w,F}^{n+1}_i + q_{wl}^{n+1} - \frac{1}{5.615\Delta t} \left[ \left( V_b \phi_F S_{w,F} \right)^n_i \right] + \frac{1}{5.615\Delta t} \left[ \left( V_b \phi_F S_{w,F} \right)^n_i \right]
\]

(5.1.16)
The finite-difference approximation of the water flow equation in the coal matrix in a 1-D system is given by;

\[
R_{w,M}^{n+1} = \Gamma_{w,M}^{n+1} = \Gamma_{w,M}^{i} - \frac{1}{5.615\Delta t} \left[ \left( \frac{V_b \phi M S_{w,M}}{B_{w,M}} \right)^{n+1} - \left( \frac{V_b \phi M S_{w,M}}{B_{w,M}} \right)^n \right]
\]

(5.1.18)

5.1.4 Calculation of the Transmissibility Terms

Calculation of fluid movement between the grid blocks is one of the most important issues in reservoir simulation. The transmissibility terms represent the fluid movement across the interface between two neighboring grid blocks. The transmissibility equation includes grid block properties, fluid properties and rock properties. The transmissibility term for the gas phase at the interface between grid block \(i\) and \(i+1\) can be calculated as follows:

\[
\frac{A_x}{\Delta x} \left[ \left( k_{x,F} \right)^{n+1}_{i+\frac{1}{2}} \right] \cdot \frac{1}{\mu_g B_{g,F} \left[ k_{rg} \right]_{i+\frac{1}{2}}^{n+1}} \cdot \left[ k_{rg} \right]_{i+\frac{1}{2}}^{n+1}
\]

(5.1.19)

This term can be separated into three parts; including linear, weakly non-linear and strongly non-linear parts. The first part \(\frac{A_x}{\Delta x} \left[ k_{x,F} \right]^{n+1}_{i+\frac{1}{2}}\) (linear) is related to the grid block dimensions and rock permeability. The grid block dimensions are constant. The permeability, however, is a function of pressure as it changes due to the effects of coal
shrinkage and swelling. The harmonic average is used to calculate the first group and it can be written as follows:

\[
\left[ \frac{A_x}{\Delta x} \right]_{i+1 \over 2}^{n+1} k_{x,F} = \frac{2 A_x \Delta x_i A_{x,F}^{n+1} k_{x,F}^{n+1}}{A_x k_{x,F}^{n+1} \Delta x_{i+1} + A_x k_{x,F}^{n+1} \Delta x_i}
\]

(5.1.20)

The weakly non-linear group, which is the second group in Equation 5.1.19, \[ \frac{1}{\mu_g B_{g,F}} \left[ \frac{n+1}{i+1} \right], \] is a function of fluid properties (viscosity and formation volume factor) and pressure. Each property in this group can be calculated using the arithmetic averaging technique as follows:

\[
\left[ \frac{1}{\mu_g B_{g,F}} \right]_{i+1 \over 2}^{n+1} = \frac{1}{2} \left( \mu_g \left| \frac{n+1}{i} \right| + \mu_g \left| \frac{n+1}{i+1} \right| \right) \cdot \frac{1}{2} \left( B_g \left| \frac{n+1}{i} \right| + B_g \left| \frac{n+1}{i+1} \right| \right)
\]

(5.1.21)

The strongly non-linear part, \[ k_{rg,F}^{n+1}_{up}, \] is the third part of the Equation 5.1.19. In this study, the single-point upstream weighting technique is used to determine the gas mole fraction and relative permeability.

If \[ \Phi_{g,F}^{n+1}_i < \Phi_{g,F}^{n+1}_{i+1}, \] then \[ k_{rg}^{n+1}_{up} = k_{rg}^{n+1}_i \] else \[ k_{rg}^{n+1}_{up} = k_{rg}^{n+1}_{i+1} \]

(5.1.22)
Similar to the transmissibility terms of Darcian flow, the transmissibility group of the Fickian flow, 
\[ D_{l,F} \frac{A_x}{\Delta x_{i+\frac{1}{2}}} \] in Equation 5.1.15, can be calculated assuming that diffusivity coefficient is constant.

\[
\frac{A_x}{\Delta x_{i+\frac{1}{2}}} = D_{l,F} \frac{2 A_x |_{i} A_x |_{i+1}}{\Delta x_{i+1} + A_x |_{i+1} \Delta x_{i}}
\]

(5.1.23)

In addition, a harmonic average is used for the calculations of the non-linear term.

\[
\frac{\phi_F S_{g,F} |_{i+\frac{1}{2}}}{\phi_F S_{g,F} |_{i}} = \frac{2 (\phi_F S_{g,F} |_{i}) (\phi_F S_{g,F} |_{i+1})}{(\phi_F S_{g,F} |_{i}) + (\phi_F S_{g,F} |_{i+1})}
\]

(5.1.24)

Calculations of the transmissibility terms in the water phase flow equations (Equation 5.1.17) are analogous to Equations 5.1.19, 5.1.20 and 5.1.21. The harmonic averaging technique is used to calculate the group of grid block dimensions and permeability and the arithmetic averaging technique is used for the weakly non-linear fluid properties including viscosity and formation volume factor.

In addition, Manik et al. (2002) suggested using single-point upstream weighting technique to calculate the gas mole fractions at the interface between two blocks.

If \( \Phi_{g,F} |_{i}^{n+1} < \Phi_{g,F} |_{i+1}^{n+1} \), then \( X_{i}^{n+1} |_{u} = X_{i}^{n+1} |_{i} \) else \( X_{i}^{n+1} |_{u} = X_{i}^{n+1} |_{i+1} \)

(5.1.25)
5.1.5 Source/Sink Terms

In the dual-porosity, dual-permeability CBM reservoir system, the source/sink terms can be categorized under two groups including the implicit and explicit source/sink terms.

5.1.5.1 Implicit Source/Sink Terms

Unlike sandstone and carbonate reservoirs, methane in coalbed reservoirs stored as an absorbed gas. Chawathe et al. (1996) studied the transport phenomena of methane from coal matrix to fracture systems and developed Equation 5.1.16. In this equation, the term $\Gamma_{g,l,F}^{n+1}$ represents gas transfer from the coal matrix to the fracture system. He proposed the following implicit source relationship to describe the gas transfer:

$$\Gamma_{g,l,F}^{n+1} = X_{l,up}^{n+1} \sigma V_b|_l \left( \frac{T_{sc}}{T_{psc}} \right) \left[ \frac{k_{rg,up}|_l^{n+1}}{h_g(z_{g,F}^{n+1})} \right] \left[ \frac{(p_{g,M}|_l^{n+1})^2 - (p_{g,F}|_l^{n+1})^2}{2} \right]$$

$$+ \sigma V_b|_l \left( \frac{T_{sc}}{T_{psc}} \right) \cdot D_{l,M} \left[ X_{l,M} \frac{p_{g,M}|_l^{n+1} - s_{g,M}|_l^{n+1}}{Z(p_{g,F}|_l^{n+1})} - X_{l,F} \frac{p_{g,F}|_l^{n+1} - s_{g,F}|_l^{n+1}}{Z(p_{g,F}|_l^{n+1})} \right]$$

(5.1.26)

In the above equation, arithmetic average is used for calculating the average pressures in the matrix and the fracture system. As can be noted from the equation, in the calculation of interporosity terms, $\Gamma_g$ and $\Gamma_w$, the diffusivity constant of the matrix system is used. The reason behind this approach is that the diffusive flow is dominant in
the coal matrix and not in fracture system. Similar calculations can be performed on the permeability term, however, in the case of permeability; geometric average should be used to calculate the average value. In this study, the shape factor, $\sigma$, developed by Chang (1993) for unsteady flow in fractured rock is used:

$$\sigma = \pi^2 \left( \frac{1}{l_x^2} + \frac{1}{l_y^2} + \frac{1}{l_z^2} \right)$$  \hspace{1cm} (5.1.27)

In Equation 5.1.27, $L_x$, $L_y$ and $L_z$ are the lengths of the coal matrix (fracture spacing) in $x$-, $y$- and $z$-directions, respectively. The gas mole fraction and relative gas permeability are determined using the one-point upstream weighting technique as:

If $p_{g,M}^{n+1}_i \geq p_{g,F}^{n+1}_i$ then $X_{i,up}^{n+1}_i = X_{i,M}^{n+1}_i$ and $k_{r,g,up}^{n+1}_i = k_{r,g,M}^{n+1}_i$

else $X_{i,up}^{n+1}_i = X_{i,F}^{n+1}_i$ and $k_{r,g,up}^{n+1}_i = k_{r,g,F}^{n+1}_i$  

$$\text{(5.1.28)}$$

Assuming that all the gas transferred from the matrix goes into the fracture, one can obtain the following equation:

$$\Gamma_{g,l,M}^{n+1}_i = -\Gamma_{g,l,F}^{n+1}_i$$  \hspace{1cm} (5.1.29)

The water transfer term, $\Gamma_{g,l,F}^{n+1}_i$, in Eq.(5.1.18) can be written as:

$$\Gamma_{w,F}^{n+1}_i = \sigma V_b_i \left( \frac{k_{r,w,up}^{n+1}_i k_M^{n+1}_i}{\mu_w (p_M^{n+1}_i - p_{w,F}^{n+1}_i)} \right) \left( p_{w,M}^{n+1}_i - p_{w,F}^{n+1}_i \right)$$  \hspace{1cm} (5.1.30)
Similar to the calculations performed on gas phase, the average pressure in the water phase, $\overline{p_w}_i^{n+1}$, is also calculated by using the arithmetic average of water pressures in the fracture and matrix systems. Water relative permeability is calculated by using single-point upstream weighting as it is done for the gas phase.

\begin{equation}
\text{If } p_{w,M}^i |_{i}^{n+1} \geq p_{w,F}^i |_{i}^{n+1} \text{ then } k_{rw,up}^i |_{i}^{n+1} = k_{rw,M}^i |_{i}^{n+1} \\
\text{else } k_{rw,up}^i |_{i}^{n+1} = k_{rw,F}^i |_{i}^{n+1}
\end{equation}

(5.1.31)

As it was assumed for the gas phase, water in the matrix system goes directly into the fracture system:

$$\Gamma_{w,M}^i |_{i}^{n+1} = -\Gamma_{w,F}^i |_{i}^{n+1}$$

(5.1.32)

### 5.1.5.2 Explicit Source/Sink Terms

In this study, explicit source and sink terms are introduced by two different methods. The first option to calculate these terms is using the Peaceman model and gas sorption rate term developed by King et al. (1986), the second method is using local grid refinement technique to calculate the flowrate for the well block (Goktas, 1999; Hu, 2011).

In the existing CBM simulator, the following equations are implemented to calculate gas and water phase flow rates using Peaceman’s equation and King et al. (1986) model.
a. Flowrate Calculations by Peaceman and King et al.

Gas flow rate term

The gas flow rate term, $q_{g,i}^{n+1}$, in Equation 5.1.16 can be expressed by the Peaceman’s wellbore equation as follows:

$$q_{g,i}^{n+1} = -X_{i,F}^{n+1} \frac{2\pi T_{sc}}{T_{psc}} \left( \frac{k_{rg,F}^{n+1} k_F^{n+1}}{\mu_g} \ln \left( \frac{r_e}{r_{w,l}} \right) \right)$$

$$- \frac{2\pi T_{sc}}{T_{psc}} D_{i,F} h_i X_{i,F} \left( \frac{p_{g,F}^{n+1} S_{g,F}^{n+1}}{Z(p_{g,F}^{n+1})} - \frac{p_{w,f}^{n+1} S_{g,F}^{n+1}}{Z(p_{w,f}^{n+1})} \right) \ln \left( \frac{r_e}{r_{w,l}} \right) + S_i$$

(5.1.33)

The average fracture permeability, $k_F$, is calculated using the geometric mean of the permeabilities in the plane that is perpendicular to the well.

Water flow rate term

The water flow rate term, $q_w$, in equation 5.1.18 can be written as:

$$q_w^{n+1} = -2\pi k_{rw,F}^{n+1} k_F^{n+1} h_i \left( \frac{p_{w,F}^{n+1} - p_{w,f}^{n+1}}{\mu_w} \right)$$

$$- \frac{2\pi T_{sc}}{T_{psc}} D_{i,F} h_i X_{i,F} \left( \frac{p_{g,F}^{n+1} S_{g,F}^{n+1}}{Z(p_{g,F}^{n+1})} - \frac{p_{w,f}^{n+1} S_{g,F}^{n+1}}{Z(p_{w,f}^{n+1})} \right) \ln \left( \frac{r_e}{r_{w,l}} \right) + S_i$$

(5.1.34)
Gas sorption rate term

A non-equilibrium sorption rate calculation was first proposed by King et al. (1986). This model calculates the sorption rate term of coal systems depending on time and pressure using a first-order kinetic equation as follows:

\[
\frac{dV_{a,l}}{dt} = \frac{1}{\tau} (V_{a,l} - V_{e,l}) \tag{5.1.35}
\]

\(V_{a,l}\) and \(V_{e,l}\) are the amounts of gas adsorbed and adsorption capacity of the gas component \(l\), respectively, and \(\tau\) is the pseudo-steady state sorption time constant, which represents the time delay of adsorbed/desorbed gas transport through the micropores in the coal matrix. Rearranging Equation 5.1.35 will yield:

\[
\int_{V_{a,l}}^{V_{a,l}|^{n+1}} \frac{dV_{a,l}}{(V_{a,l} - V_{e,l})} = \int_{t^n}^{t^{n+1}} \frac{dt}{\tau}
\]

\(\tag{5.1.36}\)

Manik et al. (2002) proposed that the above equation could be rearranged and integrated to solve for adsorption capacity term, \(V_{a,l}\) at time level \(n + 1\). The equation below shows the final form used in this study for the instantaneous sorption calculation:

\[
V_{a,l}|^{n+1} = V_{a,l}|^{n} \exp \left(-\frac{\Delta t}{\tau}\right) + V_{e,l}|^{n+1} [1 - \exp \left(-\frac{\Delta t}{\tau}\right)]
\]

\(\tag{5.1.37}\)

The gas sorption rate for gas component \(l\) can be calculated as:

\[
q_{srp}|^{n+1} = \frac{V_{a,l}|^{n+1} - V_{a,l}|^{n}}{\Delta t}
\]

\(\tag{5.1.38}\)
Calculations of multi-component sorption

According to Myers and Prausnitz (1965), the following equations are developed and implemented based on the thermodynamic equilibrium between gas components in the free and the absorbed phase. The equilibrium coefficient between phases can be calculated by;

\[ f_i = f_i^0 Y_i \]  
(5.1.39)

and

\[ pX_i \phi_i = p_i^0 \phi_i^0 Y_i \]  
(5.1.40)

where \( f_i^0 \) is fugacity of pure component \( l \) in the gas phase at standard conditions, \( p_i^0 \) is pressure at a standard state condition of pure component \( l \) in the adsorbed phase and \( \phi_i^0 \) is pure component fugacity coefficient at standard conditions. The flowing relationship demonstrates the spreading pressure group at the standard state, \( \psi_i^0 \), and the pure adsorption capacity, \( n_i^0 \):

\[ \psi_i^0 = \int_{0}^{n_i^0} \frac{n_i^0}{f_i} df_i \]  
(5.1.41)

where \( f_i \) is fugacity of component \( l \) in gas phase. At standard conditions, spreading pressure values for all components are equal; therefore, one can obtain:

\[ \psi_1^0 = \psi_2^0 = \ldots = \psi_{NC}^0 \]  
(5.1.42)

Principal unknowns in the multi-component sorption calculations are \( Y_1, Y_2 \ldots Y_{NC} \) and \( f_1^0, f_2^0, \ldots, f_{NC}^0 \), number of unknowns equals to \( 2 \times \text{Number of Gas Component} \). Equations (5.1.39), (5.1.40) and (5.1.42) provide \( 2 \times \text{Number of Gas Component} - 1 \) equations; therefore, the mole fraction constraint of the adsorbed phase is also used.
\[
\sum_{i=1}^{NC} Y_i = 1 \quad (5.1.43)
\]

Manik et al. (2002) developed an iterative technique and implemented on CBM simulator to solve the unknowns described above:

\[
\mathcal{R}(\psi^0) = \sum_{i=1}^{NC} Y_i - 1 = \sum_{i=1}^{NC} \left( \frac{f_i}{f_i^0} \right) - 1 = 0 \quad (5.1.44)
\]

Equation (5.1.44) can be solved by using the Newton-Raphson procedure as follows:

\[
\psi^0 \bigg|^{k+1} = \psi^0 \bigg|^{k} - \frac{\mathcal{R}(\psi^0)}{d\mathcal{R}(\psi^0)/d\psi^0} \bigg|^{k} \quad (5.1.45)
\]

Substituting Equation 5.1.41 into the derivative \( \mathcal{R}(\psi^0)/d\psi^0 \), one can obtain:

\[
\frac{d\mathcal{R}(\psi^0)}{d\psi^0} = \frac{d}{d\psi^0} \left[ \sum_{i=1}^{NC} \left( \frac{f_i}{f_i^0} \right) - 1 \right] = \sum_{i=1}^{NC} \left[ - \frac{f_i}{(f_i^0)^2} \frac{df_i^0}{d\psi^0} \right] \quad (5.1.46)
\]

where

\[
\frac{df_i^0}{d\psi^0} = \frac{f_i^0}{n_i^0} \quad (5.1.47)
\]

Substituting Equations 5.1.46 and 5.1.47 into Equation 5.1.45 gives:

\[
\psi^0 \bigg|^{k+1} = \psi^0 \bigg|^{k} - \frac{\sum_{i=1}^{NC} \left[ \frac{f_i}{f_i^0} \right] - 1}{\sum_{i=1}^{NC} \left[ \frac{f_i}{f_i^0 n_i^0} \right]} \quad (5.1.48)
\]

According to Manik et al.’s development (2002), one can start solving Equations 5.1.49 and 5.1.50 to calculate the fugacity of the free gas phase of component \( l \) using;
\[ \ln \varphi_i = -\ln(Z - B) + \frac{A}{2.829427125B} \left[ \frac{\Sigma_{j=1}^{N} A_{ij} X_j}{A} - \frac{B_i}{B} \right] + \ln \left[ \frac{Z - 0.414213562B}{Z + 2.414213562B} \right] + \frac{B_i}{B} (Z - 1) \] 

(5.1.49)

and

\[ f_i = \varphi_i X_i P \] 

(5.1.50)

After that adsorption capacity, \( n_i \), can be calculated for a specific pressure range by:

\[ n_i = \frac{c_1 f_i}{c_2 + f_i} \] 

(5.1.51)

where \( c_1 \) and \( c_2 \) are curve-fitting coefficients. An expression for spreading pressure can be calculated by substituting Equation 5.1.51 into Equation 5.1.41:

\[ \psi_i^0 = \int_0^{f_i^0} \frac{c_1}{c_2 + f_i} df_i = c_1 \ln \left( \frac{c_2 + f_i^0}{c_2} \right) \] 

(5.1.52)

Rewriting the above equation to solve for fugacity of component \( l, f_i^0 \):

\[ f_i^0 = c_2 \exp \left( \frac{\psi_i^0}{c_1} \right) - c_2 \] 

(5.1.53)

Finally, \( n_i^0 \) can be calculated as:

\[ n_i^0 = \frac{c_1 f_i^0}{c_2 + f_i^0} \] 

(5.1.54)

The convergence criterion for Equation 5.1.48 is:

\[ \left| \psi_i^{(k+1)} - \psi_i^{(k)} \right| \leq 10^{-15} \] 

(5.1.55)
b. Flowrate Calculations by Residual Approach

A first theoretical study of the numerical productivity index (PI) was made by Peaceman in 1978. The formula provided by Peaceman (1983), which is accurate for fully penetrating vertical wells in uniform grid blocks, is widely used in reservoir simulation. However, this formula cannot be directly used in more complex cases such as advanced wells or flexible gridding techniques. This topic has been investigated by various authors (Lee 1989, Peaceman 1990 and 1993, Babu et al. 1991, Palagi and Aziz 1991, Mochizuki 1995, Ding et al. 1994, 1995 and 1996) and published work looking at complex well modeling. Even though these studies improved the accuracy of the simulation for black-oil models, there has been limited improvement for coalbed methane reservoirs. Since the coalbed methane reservoirs are dual-porosity systems, more accurate pressure distribution is necessary for exact calculation of the sorption terms calculations.

As mentioned earlier, coalbed methane reservoirs are dual-porosity domains. Methane is stored as an adsorbed gas in the coal matrix and desorption is directly related to the block pressure. The proposed CBM model used a local grid refinement technique to capture the most accurate pressure distribution around the well. Then, the residual term is calculated for each well block in a locally refined area and is used for determining fluid flow into the well.

As it can be seen from Figure 5-1, the well blocks presented in black color and the shaded blocks represent the grid blocks that are small enough to have the same pressure values of the well. Since there is no accumulation occurs in these grid blocks, the amount of fluid flow through these grid blocks is used in total flowrate calculations as follows;
In this equation, \( q_i \) can be calculated by solving equation 5.1.57, and assuming there will be no accumulation or depletion within or from the well block.

\[
q_{g, total} = \sum q_{g, l, i}
\]

(5.1.56)

\[
\nabla \cdot \left( \frac{D_{l,F} \Phi_F S_{g,F} A}{5.615} \nabla \left( X_{l,F} \frac{S_{g,F}}{B_{g,F}} \right) + X_{l,F} \frac{A k r_{g,F}}{\mu_g B_{g,F}} \nabla \Phi_{g,F} R_{sw,l,F} \frac{A k F k r_{w,F}}{\mu_w B_{w,F}} \nabla \Phi_{w,F} \right)
\]

\[+ \Gamma_{g,l,F} + q_{g,l} + R_{sw,l,F} q_w = \frac{1}{5.615} \frac{\partial}{\partial t} \left[ X_{l,F} \frac{v_h \Phi_{p,F} S_{g,F}}{B_{g,F}} + R_{sw,l,F} \frac{v_h \Phi_{p,F} S_{w,F}}{B_{w,F}} \right]
\]

(5.1.57)

Since the pressure in pseudo-well blocks and well blocks will be at the specified pressure, the coefficient matrix for the \( P_{s,F} \) specified well conditions can be constructed as demonstrated in Figure 5-3. Once the solution is achieved, the above equation will be used to calculate the flowrate from each grid block and then total flowrate from the well can be calculated by using Equation 5.1.56.
Figure 5 - Numbering Scheme in a Locally Refined Region

- **Well Blocks**
- **Pseudo-Well Blocks**
- **Reservoir Blocks**
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Figure 5 - 3 Local Grid Refinement - Grid Coefficient Matrix for $P_{a}$ Specified Conditions
5.1.6 Shrinkage and Swelling Effect

In Coalbed Methane Reservoirs (CBM), water can be found in two forms (1) bound water, which is considered as immobile and is bonded to the coal surface, and (2) bulk water, which is considered to be mobile and can be present in the coal matrix. As discussed by authors, Joubert et al., 1973; Clarkson and Bustin, 2000; Krooss et al., 2002; Ozdemir, 2004; Jahediesfanjani and Civan, 2006, and Thararoop, 2010 bound water affects the sorption capacity of the coal, since it covers the surface area that would otherwise be occupied by methane molecules. The term critical moisture content, $m_c$, refers to the maximum amount of bound water that can be presented in the coal matrix.

Thararoop (2010) conducted a study on coal shrinkage and swelling due to water presence in coal matrix and developed a model for the CBM simulator. The current CBM model includes this effect. The coal matrix permeability and porosity are calculated by the following equation. Further information about the development of this equation can be found in Appendix–B.

\[
\frac{k}{k_i} = \left(\frac{\phi}{\phi_i}\right)^3 = \left\{ e^{c_p(p-p_i)} + \sum_{l=1}^{NC} \left[ \frac{I_l \phi_l \rho V_m}{\phi_i} \left( \frac{Y_{li} p_l}{p_l + p} - \frac{Y_l p}{p_l + p} \right) \right] \right\}^3 \quad (5.1.58)
\]

5.1.8 Generalized Newton-Raphson Procedure

The dual-porosity, dual-permeability, multi-phase, multi-component CBM simulator contains highly non-linear equations for the solution of a given system. In order to solve this large mathematical undertake, the generalized Newton-Raphson method is implemented. In every Newton-Raphson iterations, the flow equations are linearized and then solved simultaneously by using GMRES matrix solver. There are totally $NB \times 2 \times$
$(NGC + 1)$ primary unknowns to be solved in each iteration. The following equations are the linearized form of the residual equations and are used for creating the coefficient matrix for the solution matrix.

\[
\begin{align*}
\left[R_{g,l,F}ight] & = \\
& - \left[\frac{\partial R_{g,l,F}}{\partial p_{g,F}}\right]_{m}^{(k)} \left[\Delta p_{g,F}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial p_{g,M}}\right]_{m}^{(k+1)} \left[\Delta p_{g,M}\right]_{n+1}^{(k+1)} \\
& + \left[\frac{\partial R_{g,l,F}}{\partial S_{w,F}}\right]_{m}^{(k)} \left[\Delta S_{w,F}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial S_{w,M}}\right]_{m}^{(k+1)} \left[\Delta S_{w,M}\right]_{n+1}^{(k+1)} \\
& \quad + \left[\frac{\partial R_{g,l,F}}{\partial X_{1,F}}\right]_{m}^{(k)} \left[\Delta X_{1,F}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial X_{2,F}}\right]_{m}^{(k+1)} \left[\Delta X_{2,F}\right]_{n+1}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,l,F}}{\partial X_{NC-1,F}}\right]_{m}^{(k+1)} \left[\Delta X_{NC-1,F}\right]_{n+1}^{(k+1)} \\
& \quad + \left[\frac{\partial R_{g,l,F}}{\partial X_{1,M}}\right]_{m}^{(k+1)} \left[\Delta X_{1,M}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial X_{2,M}}\right]_{m}^{(k+1)} \left[\Delta X_{2,M}\right]_{n+1}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,l,F}}{\partial X_{NC-1,M}}\right]_{m}^{(k+1)} \left[\Delta X_{NC-1,M}\right]_{n+1}^{(k+1)} \\
& - \left[\frac{\partial R_{g,l,F}}{\partial p_{g,F}}\right]_{2}^{(k)} \left[\Delta p_{g,F}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial p_{g,M}}\right]_{2}^{(k+1)} \left[\Delta p_{g,M}\right]_{n+1}^{(k+1)} \\
& \quad + \left[\frac{\partial R_{g,l,F}}{\partial S_{w,F}}\right]_{2}^{(k)} \left[\Delta S_{w,F}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial S_{w,M}}\right]_{2}^{(k+1)} \left[\Delta S_{w,M}\right]_{n+1}^{(k+1)} \\
& \quad + \left[\frac{\partial R_{g,l,F}}{\partial X_{1,F}}\right]_{2}^{(k+1)} \left[\Delta X_{1,F}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial X_{2,F}}\right]_{2}^{(k+1)} \left[\Delta X_{2,F}\right]_{n+1}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,l,F}}{\partial X_{NC-1,F}}\right]_{2}^{(k+1)} \left[\Delta X_{NC-1,F}\right]_{n+1}^{(k+1)} \\
& \quad + \left[\frac{\partial R_{g,l,F}}{\partial X_{1,M}}\right]_{2}^{(k+1)} \left[\Delta X_{1,M}\right]_{n+1}^{(k+1)} + \left[\frac{\partial R_{g,l,F}}{\partial X_{2,M}}\right]_{2}^{(k+1)} \left[\Delta X_{2,M}\right]_{n+1}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,l,F}}{\partial X_{NC-1,M}}\right]_{2}^{(k+1)} \left[\Delta X_{NC-1,M}\right]_{n+1}^{(k+1)} \\
& \quad + \ldots +
\end{align*}
\]
where \( l = 1, 2, \ldots, \text{NC} \) and \( m = 1, 2, \ldots, \text{NB} \).
Similarly, one can obtain the linear gas residual equation for the matrix system for block $m$ as follows:

$$
\left[R_{g,j,M}\right]_{m}^{(k)} =
$$

\[
-\left[\frac{\partial R_{g,j,M}}{\partial p_{g,F}}\right]_{m}^{(k)} \left[\Delta p_{g,F}\right]_{m}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial p_{g,M}}\right]_{m}^{(k)} \left[\Delta p_{g,M}\right]_{m}^{(k+1)} + \\
\left[\frac{\partial R_{g,j,M}}{\partial S_{w,F}}\right]_{m}^{(k)} \left[\Delta S_{w,F}\right]_{m}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial S_{w,M}}\right]_{m}^{(k)} \left[\Delta S_{w,M}\right]_{m}^{(k+1)} + \\
\left[\frac{\partial R_{g,j,M}}{\partial X_{1,F}}\right]_{m}^{(k)} \left[\Delta X_{1,F}\right]_{m}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial X_{2,F}}\right]_{m}^{(k)} \left[\Delta X_{2,F}\right]_{m}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,j,M}}{\partial X_{NC-1,F}}\right]_{m}^{(k)} \left[\Delta X_{NC-1,F}\right]_{m}^{(k+1)} + \\
\left[\frac{\partial R_{g,j,M}}{\partial X_{1,M}}\right]_{m}^{(k)} \left[\Delta X_{1,M}\right]_{m}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial X_{2,M}}\right]_{m}^{(k)} \left[\Delta X_{2,M}\right]_{m}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,j,M}}{\partial X_{NC-1,M}}\right]_{m}^{(k)} \left[\Delta X_{NC-1,M}\right]_{m}^{(k+1)} \\
-\left[\frac{\partial R_{g,j,M}}{\partial p_{g,F}}\right]_{2}^{(k)} \left[\Delta p_{g,F}\right]_{2}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial p_{g,M}}\right]_{2}^{(k)} \left[\Delta p_{g,M}\right]_{2}^{(k+1)} + \\
\left[\frac{\partial R_{g,j,M}}{\partial S_{w,F}}\right]_{2}^{(k)} \left[\Delta S_{w,F}\right]_{2}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial S_{w,M}}\right]_{2}^{(k)} \left[\Delta S_{w,M}\right]_{2}^{(k+1)} + \\
\left[\frac{\partial R_{g,j,M}}{\partial X_{1,F}}\right]_{2}^{(k)} \left[\Delta X_{1,F}\right]_{2}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial X_{2,F}}\right]_{2}^{(k)} \left[\Delta X_{2,F}\right]_{2}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,j,M}}{\partial X_{NC-1,F}}\right]_{2}^{(k)} \left[\Delta X_{NC-1,F}\right]_{2}^{(k+1)} + \\
\left[\frac{\partial R_{g,j,M}}{\partial X_{1,M}}\right]_{2}^{(k)} \left[\Delta X_{1,M}\right]_{2}^{(k+1)} + \left[\frac{\partial R_{g,j,M}}{\partial X_{2,M}}\right]_{2}^{(k)} \left[\Delta X_{2,M}\right]_{2}^{(k+1)} + \ldots + \left[\frac{\partial R_{g,j,M}}{\partial X_{NC-1,M}}\right]_{2}^{(k)} \left[\Delta X_{NC-1,M}\right]_{2}^{(k+1)} \right]++]
\[
\begin{align*}
&\left\{\frac{\partial R_{g,l,M}}{\partial p_{g,F}}\right\}_{m}^{(k)} \left[ \Delta p_{g,F} \right]_{NB}^{(k+1)} + \left[ \frac{\partial R_{g,l,M}}{\partial p_{g,M}} \right]_{m}^{(k+1)} \left[ \Delta p_{g,M} \right]_{NB}^{(k)} \\
&+ \left[ \frac{\partial R_{g,l,M}}{\partial S_{w,F}} \right]_{m}^{(k+1)} \left[ \Delta S_{w,F} \right]_{NB}^{(k+1)} + \left[ \frac{\partial R_{g,l,M}}{\partial S_{w,M}} \right]_{m}^{(k)} \left[ \Delta S_{w,M} \right]_{NB}^{(k+1)} \\
&+ \left[ \frac{\partial R_{g,l,M}}{\partial X_{1,F}} \right]_{m}^{(k)} \left[ \Delta X_{1,F} \right]_{NB}^{(k+1)} + \left[ \frac{\partial R_{g,l,M}}{\partial X_{2,F}} \right]_{m}^{(k+1)} \left[ \Delta X_{2,F} \right]_{NB}^{(k)} \\
&+ \ldots + \left[ \frac{\partial R_{g,l,M}}{\partial X_{NC-1,F}} \right]_{m}^{(k+1)} \left[ \Delta X_{NC-1,F} \right]_{NB}^{(k+1)} \\
&+ \left[ \frac{\partial R_{g,l,M}}{\partial X_{1,M}} \right]_{m}^{(k)} \left[ \Delta X_{1,M} \right]_{NB}^{(k+1)} + \left[ \frac{\partial R_{g,l,M}}{\partial X_{2,M}} \right]_{m}^{(k+1)} \left[ \Delta X_{2,M} \right]_{NB}^{(k)} \\
&+ \ldots + \left[ \frac{\partial R_{g,l,M}}{\partial X_{NC-1,M}} \right]_{m}^{(k+1)} \left[ \Delta X_{NC-1,M} \right]_{NB}^{(k+1)} \right}\}
\end{align*}
\]

(5.1.60)

where \( l = 1, 2, \ldots, NC \) and \( m = 1, 2, \ldots, NB \).
The linearization of the residual equations for water flow in the fracture system yields the following linear equation for block \( m \).

\[
\begin{align*}
[R_{w,F}]^{(k)}_{m_{n+1}} &= \left( -\frac{\partial R_{w,F}}{\partial p_{g,F}} \right)^{n+1}_{m} \Delta p_{g,F}^{(k+1)}_{n+1} + \left( -\frac{\partial R_{w,F}}{\partial p_{g,M}} \right)^{n+1}_{m} \Delta p_{g,M}^{(k+1)}_{n+1} \\
+ \left( \frac{\partial R_{w,F}}{\partial S_{w,F}} \right)^{n+1}_{m} \Delta S_{w,F}^{(k+1)}_{n+1} + \left( -\frac{\partial R_{w,F}}{\partial S_{w,M}} \right)^{n+1}_{m} \Delta S_{w,M}^{(k+1)}_{n+1} \right) \\
+ \left( \frac{\partial R_{w,F}}{\partial p_{g,F}} \right)^{n+1}_{m} \Delta p_{g,F}^{(k+1)}_{2} + \left( -\frac{\partial R_{w,F}}{\partial p_{g,M}} \right)^{n+1}_{m} \Delta p_{g,M}^{(k+1)}_{2} \\
+ \left( \frac{\partial R_{w,F}}{\partial S_{w,F}} \right)^{n+1}_{m} \Delta S_{w,F}^{(k+1)}_{2} + \left( -\frac{\partial R_{w,F}}{\partial S_{w,M}} \right)^{n+1}_{m} \Delta S_{w,M}^{(k+1)}_{2} \right) + \ldots + \\
+ \left( \frac{\partial R_{w,F}}{\partial p_{g,F}} \right)^{n+1}_{m} \Delta p_{g,F}^{(k+1)}_{NB} + \left( -\frac{\partial R_{w,F}}{\partial p_{g,M}} \right)^{n+1}_{m} \Delta p_{g,M}^{(k+1)}_{NB} \\
+ \left( \frac{\partial R_{w,F}}{\partial S_{w,F}} \right)^{n+1}_{m} \Delta S_{w,F}^{(k+1)}_{NB} + \left( -\frac{\partial R_{w,F}}{\partial S_{w,M}} \right)^{n+1}_{m} \Delta S_{w,M}^{(k+1)}_{NB} \right) \\
\end{align*}
\]

(5.1.61)

where \( m = 1, 2, \ldots, NB \).
Similarly, one can obtain the linearized water residual equation for the matrix system for block $m$ as follows:

$$
\begin{align*}
[R_{w,M}]_{m}^{(k)}_{n+1} &= \\
&= - \left\{ \left[ \frac{\partial R_{w,M}}{\partial p_{g,M}} \right]_{m}^{(k)}_{n+1} \left[ \Delta p_{g,M} \right]_{n+1}^{(k)}_{n+1} + \left[ \frac{\partial R_{w,M}}{\partial p_{g,M}} \right]_{m}^{(k)}_{n+1} \left[ \Delta p_{g,M} \right] \right\} + \\
&+ \left\{ \left[ \frac{\partial R_{w,M}}{\partial S_{w,F}} \right]_{m}^{(k)}_{n+1} \left[ \Delta S_{w,F} \right]_{n+1}^{(k+1)} + \left[ \frac{\partial R_{w,M}}{\partial S_{w,F}} \right]_{m}^{(k)}_{n+1} \left[ \Delta S_{w,M} \right] \right\} \\
&- \left\{ \left[ \frac{\partial R_{w,M}}{\partial p_{g,M}} \right]_{2}^{(k)}_{n+1} \left[ \Delta p_{g,M} \right]_{n+1}^{(k+1)}_{n+1} + \left[ \frac{\partial R_{w,M}}{\partial p_{g,M}} \right]_{2}^{(k)}_{n+1} \left[ \Delta p_{g,M} \right]_{n+1}^{(k+1)}_{n+1} \right\} \\
&+ \left\{ \left[ \frac{\partial R_{w,M}}{\partial S_{w,F}} \right]_{2}^{(k)}_{n+1} \left[ \Delta S_{w,F} \right]_{n+1}^{(k+1)}_{n+1} + \left[ \frac{\partial R_{w,M}}{\partial S_{w,F}} \right]_{2}^{(k)}_{n+1} \left[ \Delta S_{w,M} \right]_{n+1}^{(k+1)}_{n+1} \right\} + \ldots + \\
&- \left\{ \left[ \frac{\partial R_{w,M}}{\partial p_{g,M}} \right]^{(k)}_{NB} \left[ \Delta p_{g,M} \right]^{(k+1)}_{NB} + \left[ \frac{\partial R_{w,M}}{\partial p_{g,M}} \right]^{(k)}_{NB} \left[ \Delta p_{g,M} \right]_{NB} \right\} + \\
&+ \left\{ \left[ \frac{\partial R_{w,M}}{\partial S_{w,F}} \right]^{(k)}_{NB} \left[ \Delta S_{w,F} \right]_{NB}^{(k+1)} + \left[ \frac{\partial R_{w,M}}{\partial S_{w,F}} \right]^{(k)}_{NB} \left[ \Delta S_{w,F} \right]_{NB} \right\} \\
&+ \ldots + \\
&= (5.1.62)
\end{align*}
$$

where $m = 1, 2, \ldots, NB$. 
5.2 Computer Model

The current CBM model is capable of simulating the multi-mechanistic, dual-porosity, dual-permeability numerical flow model of coalbed methane reservoirs accounting for coal shrinkage and swelling effects and able to apply local grid refinement to the well blocks. The part of the code that is responsible for reading the input data, calculating the linearized residual equations and writing the incremental output file is developed in C++. The proposed advanced CBM simulator utilizes GMRES iterative solver, and it is working in conjunction with ParaSails matrix pre-conditioner and FASP preconditioner. Both the GMRES solver and the Parasails pre-conditioner are developed using C language and parallel computing with using message passing interface method (MPI). The library file for FASP preconditioner and GMRES iterative solver is obtained from the Mathematical Department of the Pennsylvania State University. Current FASP solver works only on a single CPU, however, the tests shows that FASP solves the linear system faster than the parallelized GMRES and ParaSails preconditioner.

The proposed model is capable of simulating inner boundary conditions at the well with water flowrate, gas flowrate, and sandface pressure specification. Injected gas mole fraction is also permitted for the injection wells. The proposed model is also capable of simulating the conditions of vertical and horizontal wells that penetrates more than one grid block using both Peaceman model and local grid refinement technique. Further investigations will be performed to add the ability to simulate multilateral wells, slanted wells and more complex well structures by using local grid refinement.
Application of many parameters, such as coal shrinkage and swelling effect, local grid refinement, well criteria changes (such as production to injection, or injection to production) can be controlled with the input file. The input file can be edited using any text editor.

The main portion of the CBM simulator is developed using C++, the matrix preconditioners and the GMRES solver utilize C programming language. The CBM code consists of 207 functions in 22 different code files, whereas the previous version of the CBM simulator had 24 functions in 6 code files. The following functions represent some of the recently added functions to introduce local grid refinement, iterative solver, stabilization functions and matrix preconditioner.

**Main Program**

The main program control all the other subroutines, including creating the LGR modules, calling modules for pressure and distribution calculations, calling functions for flow calculation, time step size determination and calling subroutines for writing output files.

**Subroutine Read**

This subroutine reads all the rock and fluid properties of the reservoir. Moreover, it reads the specifications for well, well criterion, LGR identifier for the well that are going to be simulated using LGR, and reads well path for the complex well configurations.
**Subroutine lgrcreator**

This subroutine identifies the well blocks and creates the locally refined grid blocks. The subroutine is capable of effectively creating the grid blocks by checking the starting and ending point of each well.

**Subroutine pswupdate**

This subroutine is responsible for transferring the pressure and saturation values between the window block and the coarse grid system after each newton raphson iteration.

**Subroutine initvar**

This subroutine tracks the changes of each iteration and prepares the initial guesses for pressure, saturation and gas fractions value for the next time step.

**Subroutine lgrnewtonraphson**

This subroutine calculates the residual terms, the partial derivative terms, constructs the jacobian matrix and calls the matrix solver for calculating the solution vector for pressure specified wells. After getting the solution vector, it also calls the initvar subroutine to track and calculate the initial values for the next time step.

**Subroutine NRFlow**

This subroutine is very similar to lgrnewtonraphson subroutine but instead of pressure specification, it is called in the case of flowrate specified wells.

**Subroutine calcq**

This subroutine calculates the flowrates that are transferred between the LGR system and coarse grid system.
Chapter 6

Computational Performance Issues

In this chapter, one of the more important parts of this research study is discussed. Reservoir simulation is a large mathematical undertaking, incorporating large systems of linear equations. Implementing an efficient solver is not only necessary for faster results, but also necessary to run more realistic cases. This chapter will discuss the enhancements made on the simulator including:

- Improvements on Newton-Raphson iterations
- Implementation of an alternative matrix storage scheme
- Implementation of an iterative solver, GMRES
- Implementation of a matrix preconditioner
- Parallelization of matrix solver and matrix preconditioner

6.1 Improvements on Newton-Raphson

CBM simulator has capability to solve multi-mechanistic, multiphase flow with multiple gas components. Principal unknowns for a simple case, where only one gas component exists in gas phase, has principal unknowns of $p_{g,f}, p_{g,m}, S_{w,f}$, and $S_{w,m}$. Principal unknowns of $X_{i,f}$ and $X_{i,m}$ will be included in case where more than one gas component exists in the gas phase.
Since pressure function behaves as a parabolic function and saturation function behaves as a hyperbolic function, the convergence of Newton-Raphson iterations can be problematical and convergence is not guaranteed if the time-step size is too large. In order to increase the stability of the system and guaranteed faster convergence two techniques were implemented. First one involves incorporation of a subroutine that predicts a better set of initial guesses for pressure and saturation distributions. Second one is the implementation of a subroutine which controls the improvements in each Newton-Raphson iteration to result in a smooth convergence and to avoid oscillations around the solution.

6.1.1 Initial Guess Subroutine

In numerical analysis, the idea of using Newton-Raphson is to approximate the solution by using its tangent line at the initial guess and compute the x-intercept of this tangent line for the next guess (Equation 6.1).

\[ x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \]  

(6.1)

This x-intercept will typically be a better approximation to the function's root than the original guess, and the method can be iterated until a desired convergence factor is achieved. The method will usually converge, provided this initial guess is close enough to the unknown root, and that \( f'(x_0) \neq 0 \). Furthermore, the convergence is at least quadratic in the neighborhood of the root, which intuitively means that the number of
correct digits roughly at least doubles in every step. Figure 6-1 shows the path how
function \( f(x) = \cos(x) - x^3 \) behaves under different initial guesses.

As it can be seen from the above graph, initial guesses \( x = -1 \) and \( x = 1 \) follows
different paths and requires different number of iterations to converge to the root of the
function. Depending on the initial guess, the Newton-Raphson method may fail or
experience difficulty to converge to the solution as it is for the initial guess of \( x = -1 \).
This difficulty can be eliminated by a better initial guess, in this case \( x = 1.1 \), and
convergence can be guaranteed.

In the previous version of the CBM simulator, the initial guess for the pressure
and saturation values were gathered from the previous successive convergences. Even
though it is acceptable for many cases, this procedure increases the number of iterations to find the roots for the next time step. In the current CBM model, a new subroutine is implemented into the simulator to track changes between each Newton-Raphson iteration and prepare a better initial guess for the next time step. Figure 6-2 demonstrates an example of how initial guess of the pressure of the grid block can be estimated for the next time step. By implementing this subroutine, total simulation time can be cut to 20 – 40%, since the number of Newton-Raphson iterations are reduced significantly.

![Figure 6 - 2 Current Model Initial Guess Calculations](image-url)
6.1.2 Stabilization of Oscillations

Even though, assigning better initial guesses helped the convergence in Newton-Raphson level, the CBM simulator was still suffering from the oscillations around the solution. For hyperbolic equations, it might be inevitable to have oscillations. As it can be seen from Figure 6-3, if an initial guess of $x = 1$ or $x = 0$ is used for the solution of the function $f(x) = x^3 - 2x + 2$, Newton-Raphson starts oscillating between $x = 0$ and $x = 1$ (local minimum). One way to eliminate this kind of behavior from CBM simulator is to track the water and gas residuals for every grid block for each iteration and identify the points where oscillation occurs. Once the grid blocks are identified, modifications on the improvements can be made by damping the improvements. In order guarantee the convergence and avoid oscillations, the CBM simulator tracks the Newton-Raphson improvements for each grid block for the previous two consecutive iterations. Once the system recognizes an oscillation, then it calculates the damping factor for each individual grid block and modifies the solution vector by using damping factors. Even though these modifications helped to eliminate most of the oscillation problems, it is still difficult to discard it completely. In some cases, it is a challenge to eliminate the oscillations after the time step size increases. When the time step size is increased, the initial guesses for the saturation and pressure values somewhat off of the exact solution which causes oscillations. This problem is dealt with by controlling the increase on time step sizes.

In CBM simulator, the user inputs the maximum time step size for the simulations, however, the simulations starts with very small time step size of 0.00001 days. The time step size is reset to this value whenever there is a change in well criteria.
The main reason to reset time step size is to keep the numerical stability of the local grid system. The stability of the window block is highly depended on the time step size and having a large time step creates problems, such as oscillations or errors in the calculation of pressure and saturation distributions.

The CBM simulator starts with 0.00001 days with an initial time step size and keeps increasing it till it hits the time step size of 0.1 days or fails to converge within the maximum number of iterations allowed. Once it reaches one of the aforementioned two control criteria, then simulator starts tracking the number of iterations it takes for each time step. In order to increase the time step size, CBM simulator needs at least ten consecutive time steps completed with two or less Newton-Raphson iterations. Once this criterion is achieved, the CBM simulator will increase the time step size by 30%. The sensitivity analysis on limiting the growth in time step size showed 80% reduction on oscillations and in the meantime increases the simulation performance by 20%. At this point, it should be noted that the modules that predict the initial guesses for the Newton-Raphson iterations performs better if the time step sizes between each iteration are similar. By limiting the growth on time step size both the stability of the system and the performance of the initial guesses increase.
6.2 Matrix Storage Schemes

One of the biggest problems in dealing sparse matrix is storage of the coefficient matrix, $A$, effectively. As mentioned earlier, current CBM model is capable of simulating dual-porosity, dual-permeability system with having water phase and gas phase (multi-component) in a three dimensional reservoir. This complex flow model and reservoir structure creates an extensively populated sparse matrix as a coefficient matrix. Since the size of the coefficient matrix increases logarithmically with increasing number of number of active grid blocks, it is necessary to implement and use an efficient matrix storage
technique. The previous CBM model used Gaussian Elimination method as a matrix solver and as a requirement of this solution technique, all the values between the outer most diagonals had to be stored in the coefficient matrix. Even though the entire coefficient matrix is not stored and all the zero values outside the outer most diagonals are eliminated, due to the complexity of the flow model CBM simulator were running out of the memory quickly. Following sub-chapters will discuss different matrix storage schemes utilized in this study for sparse matrix systems.

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Coefficient Matrix

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Figure 6 - 4 Sample Reservoir with its Coefficient Matrix and CSR Storage Scheme
6.2.1 Compressed Sparse Row (CSR) / Column (CSC)

In these matrix storage techniques, $M \times M$ sparse matrix is converted to three vectors. In the case of compressed sparse row method, first vector stores the list of the indexes where each row starts, second vector holds the J coordinate indexes for the each stored value and finally the third vector holds the value of the non-zero entries of the coefficient matrix $A$. Figure 6-4 demonstrates an example how a single layer 3 by 3 reservoir model with a single phase fluid system will be stored with a CSR storage scheme.

In the case of CSC storage scheme, the only difference is column indexes are stored in a compressed form instead of the row indexes. Both schemes have the same memory usage and equal random memory access times.

6.2.2 Coordinate List (COO)

Similar to the CSR and CSC, coordinate list matrix storage scheme stores the coefficient matrix $A$ under three vectors. Different than CSR or CSC schemes, with COO scheme there will be no compression in the row or column vectors (Figure 6-5). Therefore the memory usage is somewhat more as compared to those schemes. However, implementation of COO scheme to the complex reservoir models is much easier with respect to other schemes. Moreover, due to easy access of its elements, applying parallel processing algorithms are much easier in the case of COO schemes. Because of its flexibility on parallel processing and implementation, in this research project COO matrix storage scheme has been implemented to the CBM simulator.
Reservoir simulation is a large mathematical undertaking, incorporating large systems of linear equations. Large problems correspond to a large system of equations and large matrices. The greater the number of grid blocks in a reservoir model, the larger the matrices that must be reckoned with. Today, tens of millions of cells may be present in a single model and solution of these models is a challenge for reservoir simulators. In this section, the linear equation solvers which are tested in the model will be discussed.
6.3.1 Direct Solver (Gaussian Elimination)

The previous CBM simulator used direct solver (Gaussian Elimination), which is developed by K. Aziz and A. Settari (1979) and it was implemented to the CBM simulator by J. Manik (1999). The process of Gaussian elimination has two parts. The first part (Forward Elimination) reduces a given system to either triangular or echelon form. This is accomplished through the use of elementary row operations. The second step uses back substitution to find the solution of the system.

Even though direct solvers are guaranteed to find the solution of a given linear system of equations, the time spent on finding the solution increases exponentially as the size of the coefficient matrix increases. This was one of the main concerns of this research project since the local grid refinement technique requires the usage of large number of grid blocks. The following sections will discuss about the different iterative solvers that were tested for the CBM simulator.

6.3.2 Bi-Conjugate Gradient Stabilized Method

One of the more common iterative solvers is the conjugate gradient solver. In numerical linear algebra, the bi-conjugate gradient stabilized method, often abbreviated as BICGSTAB, is an iterative method developed by H. A. van der Vorst. The difference between the conjugate gradient and the bi-conjugate gradient method is that the bi-conjugate gradient method can solve the non-symmetric linear equations. Its difference from regular bi-conjugate gradient method is that after each bi-conjugate iteration a generalized minimum residual (GMRES) technique is performed to ensure the
stabilization and to eliminate the irregular convergence behavior of the bi-conjugate gradient method. Even though, the bi-conjugate gradient method is an advanced iterative solver and widely used in numerical analysis, it is proven (Sifuentes, 2006; Saad, 2003) that it fails to converge in cases where the coefficient matrix is not diagonally dominant. In those cases, bi-conjugate gradient stabilized method stagnates or prematurely terminates without achieving convergence.

In this research program, three different bi-conjugate methods, (1) Bi-CG, (2) BICGSTAB, and (3) BICGSTAB(l) were tested. None of the Bi-CG methods were stable enough. Since the CBM simulator is designed to handle ten different gas components in the gas phase in a dual porosity system, its coefficient matrix does not necessarily generate a diagonally dominant matrix. In order to solve this non-diagonally dominant matrix, the generalized minimum residual method was implemented in the CBM simulator.

### 6.3.3 The Generalized Minimum Residual Method

In numerical computations, the generalized minimum residual method, GMRES, is an iterative method for the solution of non-symmetric system of linear equations. Yousef Saad and Marthin H. Shultz (1986) developed the GMRES method on the basis of the minimum residual (MINRES) method which is developed by Chris Page in 1975. The generalized minimum residual method uses the Arnoldi iteration to find the minimum residual vector in the Krylov subspace. After that, this vector is used for
approximating the solution of the linear system. The generalized minimum residual method can be described as follows;

- Denote the Euclidean norm of any vector $\mathbf{v}$ by $\|\mathbf{v}\|$. Denote the system of linear equations to be solved by

$$Ax = b \quad (6-2)$$

- The matrix $A$ is assumed to be invertible of size $m$-by-$m$ Furthermore, it is assumed that $b$ is normalized, i.e., that $\|b\| = 1$.
- The $n$th Krylov subspace for this problem is

$$K_n = \text{span}\{r, Ar, A^2r, ..., A^{n-1}r\} \quad (6-3)$$

GMRES approximates the exact solution of $Ax = b$ by the vector $x_n \in K_n$ that minimizes the Euclidean norm of the residual $Ax_n - b$.

The vectors $r, Ar, A^2r, ..., A^{n-1}r$ might be almost linearly dependent, so instead of this basis, the Arnoldi iteration is used to find orthonormal vectors $q_1, q_2, ..., q_1$ which form a basis for $K_n$. Hence, the vector $x_n \in K_n$ can be written as $x_n = Q_n y_n$ with $y_n \in R_n$, where $Q_n$ is the $m$-by-$n$ matrix formed by $q_1, q_2, ..., q_1$.

The Arnoldi process also produces an $(n+1)$-by-$n$ upper Hessenberg matrix $\bar{H}_n$ with

$$AQ_n = Q_{n+1} \bar{H}_n \quad (6-4)$$

Because $Q_n$ is orthogonal, we have
\[ \|Ax_n - b\| = \|\bar{H}_n y_n - \beta e_1\|. \] (6-5)

where

\[ e_1 = (1,0,0,...,0) \] (6-6)

is the first vector in the standard basis of \( R_{n+1} \), and

\[ \beta = \|b - Ax_0\|. \] (6-7)

\( x_0 \) being the first trial vector (usually zero). Hence, \( x_n \) can be found by minimizing the Euclidean norm of the residual

\[ r_n = \bar{H}_n y_n - \beta e_1 \] (6-8)

This is a linear least squares problem of size \( n \).

This yields the GMRES method. At every step of the iteration:

1. do one step of the Arnoldi method;
2. find the \( y_n \) which minimizes \( \|r_n\| \);
3. compute \( x_n = Q_n y_n \);
4. repeat if the residual is not yet small enough.

At every iteration a matrix-vector product \( Aq_n \) must be computed. This costs about \( 2m^2 \) floating-point operations for general dense matrices of size \( m \), but the cost can decrease to \( O(m) \) for sparse matrices. In addition to the matrix-vector product, \( O(n,m) \)
floating-point operations must be computed at the nth iteration. A sample code for GMRES method with restart option can be found in Appendix-C.

In order to compare the performance of the generalized minimum method, the numerical test was performed on a sample reservoir model between direct solver, and GMRES. As it can be seen from Table 6-1, for small systems direct solver outperforms the GMRES method. As the dimension of the linear system increases, direct solver loses its advantage and GMRES gets faster convergence. Even though, GMRES outperforms Direct Solver method and BiCGSTAB method had some problem with converging, it does not mean that GMRES is the best solver for the solution of every non-symmetric linear equation. Each problem has its unique coefficient matrix therefore, multiple solvers should be tried to see which performs best and generates more stable results.

<table>
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<th>Number of Grid Blocks/Unknowns</th>
<th>Direct solver</th>
<th>GMRES</th>
<th>Parallel and Preconditioned GMRES</th>
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</table>

Similar to the conclusions achieved in this study, A. Farschtschi and T. Richter performed a study using gauss elimination method, GMRES and PGMRES on the calculation of induction and proximity effects of electric machines in an intermediate frequency range (Table 6-2).
Table 6 - 2 Study on Linear Solver Performances on Inductance Phenomena

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<td>4.07</td>
<td>2.22</td>
<td>0.72</td>
</tr>
<tr>
<td>12</td>
<td>287</td>
<td>7.18</td>
<td>3.56</td>
<td>0.84</td>
</tr>
<tr>
<td>13</td>
<td>337</td>
<td>10.13</td>
<td>6.34</td>
<td>1.10</td>
</tr>
<tr>
<td>14</td>
<td>391</td>
<td>18.11</td>
<td>9.41</td>
<td>1.34</td>
</tr>
<tr>
<td>15</td>
<td>449</td>
<td>26.2</td>
<td>15.09</td>
<td>1.89</td>
</tr>
</tbody>
</table>

### 6.4 Matrix Preconditioners

Preconditioning is a procedure of an application of a transformation that conditions a given problem into a form that is more suitable for numerical solution. Preconditioning is typically related to reducing a condition number of the problem. The preconditioned problem is then usually solved by an iterative method. In this segment of the study three different preconditioners were tested, first one is the \( LU \) decomposition, the second one is the Parasails iterative preconditioner, and the third one is the Fast Auxiliary Space Preconditioner (FASP). Even though \( LU \) decomposition generates better conditioned matrix, the time spend on and the memory used during the process is excessive compared to ParaSails and FASP preconditioners. Since the proposed CBM simulator demands excessive matrix operations over and over again, it is proven that using advance preconditioners is a better choice rather than \( LU \) decomposition. The following two subchapters discuss about the \( LU \), the ParaSails preconditioner and the FASP preconditioner in detail.
6.4.1 LU Decomposition

LU decomposition (also called LU factorization) is a matrix decomposition which writes a matrix as the product of a lower triangular matrix and an upper triangular matrix. The product sometimes includes a permutation matrix as well. This decomposition is used in numerical analysis to solve systems of linear equations or calculate the determinant of a matrix. LU decomposition can be viewed as a matrix form of Gaussian elimination. LU decomposition was introduced by mathematician Alan Mathison Turing (1948).

Definition:

Let A be a square matrix. An LU decomposition is a decomposition of the form

\[ A = LU \]  \quad (6-9)\

where L and U are lower and upper triangular matrices (of the same size), respectively. This means that L has only zeros above the diagonal and U has only zeros below the diagonal. For a 3x3 matrix, this becomes:

\[
\begin{bmatrix}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{bmatrix} =
\begin{bmatrix}
l_{11} & 0 & 0 \\
l_{21} & l_{22} & 0 \\
l_{31} & l_{32} & l_{33}
\end{bmatrix}
\begin{bmatrix}
u_{11} & u_{12} & u_{13} \\
u_{22} & u_{22} & u_{23} \\
u_{33} & 0 & 0
\end{bmatrix}
\]

Application of any of the upper or the lower triangular matrixes as a preconditioner will increase the efficacy of the linear equation solver.
6.4.2 Iterative Preconditioner – ParaSails

ParaSails is a parallel sparse approximate inverse preconditioner for the iterative solution of large, sparse systems of linear equations. It is a kind of parallel implementation of a SAI preconditioner. It is a self-contained module in the HYPRE preconditioner library currently being developed at the Center for Applied Scientific Computing. It uses least-squares (Frobenius norm) minimization to compute a sparse approximate inverse. The sparsity pattern used is the pattern of a power of a sparsified matrix. ParaSails also uses a post-filtering technique to reduce the cost of applying the preconditioner. The pattern of the preconditioner can be reused to generate preconditioners for different matrices in a sequence of linear solvers. ParaSails can solve general (nonsymmetric and/or indefinite) problems with a nonfactorized preconditioner.

A sparse approximate inverse \( M \) of the matrix \( A \) may be computed by minimizing the Frobenius norm of \( I - AM \) where \( M \) has a fixed sparsity pattern. In parallel, this is equivalent to a least squares minimization of \( e_j - A m_j \) for each column \( j \), where \( e_j \) is the \( j \)th column of the matrix \( I \), and \( m_j \) is the \( j \)th column of the sparse matrix \( M \). Similar expressions can be written to approximate the inverse of the factors of \( A \), i.e., an approximate inverse in factorized form.
6.4.3 Fast Auxiliary Space Preconditioner

Fast auxiliary space preconditioner (FASP) (Xu – 2013) is developed by the Department of Mathematics at The Pennsylvania State University. The driving force behind the FASP preconditioner is that there is no one-size-for-all method for discrete linear systems and the bottle necks can be overcome by utilizing the preconditioners for the given problem. The FASP preconditioner separates the Jacobian entries of the different type of equations, in this case hyperbolic equations for saturation terms and parabolic equations for pressure terms, and creates separate preconditioning matrixes and then combine all the individual matrixes to generate the resultant preconditioner matrix. The implementation of FASP preconditioner increased the efficacy of the CBM simulator significantly. By providing faster and more accurate solution, the time spent on the simulations cut significantly. The table 6-3 shows some of the comparisons between the FASP preconditioner and the ParaSails preconditioner. The first of the seven cases, which has 153228 grid blocks and 612912 unknowns, represents the case where both preconditioners are having problems to find the solutions. Even for these cases, the FASP preconditioner spends at least half of the time and iterations to find the solutions. Case eight is a case where both preconditioners are performing well; in this case, FASP preconditioner performs almost six times faster than the ParaSails preconditioner.¹

¹ Platform: Intel Xeon E31125 @3.10 GHZ
Table 6-3 Comparisons between ParaSails and FASP Preconditioners

<table>
<thead>
<tr>
<th>Case</th>
<th>ParaSails</th>
<th></th>
<th>FASP</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td># of Iterations</td>
<td>Time (secs)</td>
<td># of Iterations</td>
<td>Time (secs)</td>
</tr>
<tr>
<td>1</td>
<td>73</td>
<td>21.867</td>
<td>38</td>
<td>11.537</td>
</tr>
<tr>
<td>2</td>
<td>86</td>
<td>25.640</td>
<td>40</td>
<td>12.098</td>
</tr>
<tr>
<td>3</td>
<td>95</td>
<td>28.214</td>
<td>45</td>
<td>13.338</td>
</tr>
<tr>
<td>4</td>
<td>104</td>
<td>30.680</td>
<td>49</td>
<td>18.561</td>
</tr>
<tr>
<td>5</td>
<td>113</td>
<td>33.297</td>
<td>47</td>
<td>15.026</td>
</tr>
<tr>
<td>6</td>
<td>130</td>
<td>38.075</td>
<td>53</td>
<td>18.601</td>
</tr>
<tr>
<td>7</td>
<td>145</td>
<td>42.427</td>
<td>50</td>
<td>17.572</td>
</tr>
<tr>
<td>8</td>
<td>31</td>
<td>4.187</td>
<td>4</td>
<td>0.732</td>
</tr>
</tbody>
</table>

6.5 Parallelization of the Matrix Solver and Preconditioner

In this research program, parallel processing option has been implemented into the proposed CBM reservoir simulator for calculating the solution of the coefficient matrix. The ParaSails preconditioner and GMRES linear equation solver are parts of HYPRE library and both developed in parallel programming using message passing interface (MPI). The reason why parallel processing is necessary is not just to reduce the time that is spent on computations, but also to make the problems more solvable. Some problems require large amounts of computation and memory that cannot be handled by a single processor. Parallel computing can save time and memory; making it possible to solve larger problems that could never be accomplished with single processor units.

Unlike serial coding techniques, there are factors to be considered with parallel programming, that include: (Blaise Barney - 2010, Snir - 1998, Gropp - 1999)

- Cost of communication: Inter-task communication and synchronization.
Latency and bandwidth: Latency is the transferring of zero byte from one memory location to another and bandwidth is the amount of data that can be transferred in a unit time.

Visibility: The visibility of how the communications are handled between CPUs and memory (MPI has a good interface for this task).

Synchronous and asynchronous: Synchronous programming needs a "handshaking protocol" between CPUs to continue for the next calculation step, which has a negative effect on performance but eliminates programmer concerns about memory control. Asynchronous programming has a huge speed advantage on communication but the memory overflows can be dangerous for the stability of the process.

Overhead and complexity: Overhead is the time consumed for communication between memory location and CPUs. Complexity refers to how convoluted the communications are between each CPU and memory location.

In theory, speed increase with parallel computing is defined by Amdahl's law (Equation 6-10). Amdahl's law states that the speed-up depends on the fraction of the code parallelized:

$$speed\text{–up} = \frac{1}{1-P} \quad (6-10)$$

where, $P$ is the fraction of the code parallelized.
However, this speed increase only exists in theory. In practice, as it can be seen in Figure 6-7, introducing the number of CPUs changes the speed-up by equation 6-11.

\[
\text{speed - up} = \frac{1}{\frac{P}{N} + S} \quad (6-11)
\]

In this equation, P is the fraction of code that parallelized, N is the number of CPUs, and S is the fraction of the code that is in serial.

One of the main reasons that the speed-up increase has an upper limit is due to communication overhead. Communication overhead is the measure of additional workload incurred in parallel algorithm applications due to communication between the nodes of the parallel system. The proposed CBM code is developed with message passing interface (MPI) so it allows users to get nodes, CPUs, from different computers on the same network. Even though in theory it should increase the overall performance of the
simulation, the simulation runs show that in many cases the communication overhead was taking more time than the actual computation time. For the simulation runs performed in this research study, it was observed that using more than 4 CPUs had a negative effect on the simulation time. It should be noted the overall performance of simulations depends on many parameters and it should not be concluded as no simulations would be run on more than 4 CPUs.

Figure 6 - 7 Actual Speed-Up with respect to Number of Processors (Blaise Barney -2010)
Chapter 7
Model Validation

In this chapter, the proposed CBM model with LGR module was tested and validated against commercial reservoir simulator. The proposed model will be first validated by using the dual-porosity - single-permeability model CMG-GEM reservoir simulator. After that, local grid refinement schemes will be compared with the Peaceman’s wellbore model calculations.

7.1 Validation of CBM simulator against Commercial Simulator

The proposed CBM simulator has a dual-porosity – dual-permeability flow model. The dual-permeability flow mechanism considers flow not only in the fracture domain but also in the matrix domain. Since dual-porosity – single-permeability CMG-GEM reservoir simulator does not have the capabilities of the proposed CBM simulator; the proposed CBM simulator can be modified to behave like single-permeability system by using very small permeability values in the matrix domain.

The data sets in Table 7-1 and 7-2 are prepared for the proposed CBM simulator and CMG-GEM simulator to compare the performances of the model under similar conditions. As it can be seen from Figures 7-1 and 7-2, the commercial reservoir simulator (CMG-GEM) and the proposed CBM simulator are in good agreement in both water and gas flow responses.
### Table 7 - 1 Reservoir Data for Validation of Vertical Well

<table>
<thead>
<tr>
<th></th>
<th>Proposed CBM Model</th>
<th>CMG-GEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir Model</td>
<td>7-7-1</td>
<td>7-7-1</td>
</tr>
<tr>
<td>Well Location</td>
<td>4-4-1</td>
<td>4-4-1</td>
</tr>
<tr>
<td>Reservoir Size</td>
<td>1400 ft - 1400 ft</td>
<td>1400 ft - 1400 ft</td>
</tr>
<tr>
<td>Thickness (ft)</td>
<td>40</td>
<td>40</td>
</tr>
<tr>
<td>Fracture Porosity</td>
<td>0.50%</td>
<td>0.50%</td>
</tr>
<tr>
<td>Matrix Porosity</td>
<td>3%</td>
<td>3%</td>
</tr>
<tr>
<td>Fracture Permeability (md)</td>
<td>8</td>
<td>8</td>
</tr>
<tr>
<td>Matrix Permeability (md)</td>
<td>0.001</td>
<td>-</td>
</tr>
<tr>
<td>Fracture Spacing (ft)</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>Diffusivity</td>
<td>0.00000001</td>
<td>-</td>
</tr>
<tr>
<td>Coal Density (lb/ft³)</td>
<td>89.5841</td>
<td>89.5841</td>
</tr>
<tr>
<td>Initial Pressure (psia)</td>
<td>1100</td>
<td>1100</td>
</tr>
<tr>
<td>Water Saturation (Fracture)</td>
<td>0.95</td>
<td>0.95</td>
</tr>
<tr>
<td>Water Saturation (Matrix)</td>
<td>0.01</td>
<td>0.01</td>
</tr>
<tr>
<td>Formation Temperature (˚F)</td>
<td>80</td>
<td>80</td>
</tr>
<tr>
<td>Langmuir Pressure (psia)</td>
<td>625</td>
<td>625</td>
</tr>
<tr>
<td>Langmuir Volume (scf/ton)</td>
<td>825</td>
<td>825</td>
</tr>
<tr>
<td>Sorption Time (days)</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

### Table 7 - 2 Relative Permeability Data for Validation Test

<table>
<thead>
<tr>
<th>$S_w$</th>
<th>$K_{rw}$</th>
<th>$K_{rg}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>0.050</td>
<td>0.0006</td>
<td>0.8350</td>
</tr>
<tr>
<td>0.100</td>
<td>0.0013</td>
<td>0.7200</td>
</tr>
<tr>
<td>0.150</td>
<td>0.0020</td>
<td>0.6270</td>
</tr>
<tr>
<td>0.200</td>
<td>0.0070</td>
<td>0.5370</td>
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<td>0.300</td>
<td>0.0240</td>
<td>0.4010</td>
</tr>
<tr>
<td>0.400</td>
<td>0.0490</td>
<td>0.2950</td>
</tr>
<tr>
<td>0.500</td>
<td>0.0880</td>
<td>0.2160</td>
</tr>
<tr>
<td>0.600</td>
<td>0.1540</td>
<td>0.1470</td>
</tr>
<tr>
<td>0.700</td>
<td>0.2510</td>
<td>0.0900</td>
</tr>
<tr>
<td>0.750</td>
<td>0.3120</td>
<td>0.0700</td>
</tr>
<tr>
<td>0.800</td>
<td>0.3920</td>
<td>0.0510</td>
</tr>
<tr>
<td>0.850</td>
<td>0.4900</td>
<td>0.0330</td>
</tr>
<tr>
<td>0.900</td>
<td>0.6010</td>
<td>0.0180</td>
</tr>
<tr>
<td>0.950</td>
<td>0.7310</td>
<td>0.0070</td>
</tr>
<tr>
<td>1.000</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>
The small difference between the responses of the two reservoir simulators is a product of different flow mechanistic. Even though, the proposed CBM simulator was forced to act like a dual-porosity – single-permeability model, it is not possible to achieve the exact same conditions with the commercial model without violating some assumptions in the CBM simulator. Moreover, the commercial model and the proposed model use different correlations for water and gas property calculations.

Figure 7 - 1 Gas Production Rate Comparison between the Proposed CBM Model and CMG-GEM
Figure 7 - 2 Water Production Rate Comparison between the Proposed CBM Model and CMG-GEM

Figure 7 - 3 Well Block Pressure Comparison between the Proposed CBM model and CMG-GEM
Similar to the sandface pressure, $P_{sf}$, specification, CBM simulator tested for flowrate specification case. Once again, table 1 and 2 are used for both CBM and CMG-GEM simulator but this time gas flowrate is specified as 60000 $SCF/D$. Figure 7.4 and figure 7.5 show the comparison for the gas flowrate and water flowrate responses for both systems, respectively. As it can be seen from the graph, they are in good agreement.

![Figure 7.4: Gas Production Rate Comparison between the Proposed CBM Model and CMG-GEM](image)

Figure 7.4 Gas Production Rate Comparison between the Proposed CBM Model and CMG-GEM
Figure 7 - 5 Water Production Rate Comparison between the Proposed CBM Model and CMG-GEM

Figure 7 - 6 Well Block Pressure Comparison between the Proposed CBM model and CMG-GEM
In Figure 7.6, the bottomhole pressure prediction of both systems can be seen. As it was discussed in pressure specification case; the proposed CBM model can be restricted up to a certain level to act like dual-porosity and single-permeability system. Moreover, the formulas used by CMG to calculate the fluid properties are different than the ones in PSU-CoalComp simulator. These differences in property calculations and basic reservoir model calculations yield the differences in the well performances. Even though there are some differences, it can be seen that both models predict very similar pressure responses in the well block, especially during the later times of the simulation.

### 7.2 Validation of Local Grid Refinement Model

As it is proven by the above examples, the proposed CBM reservoir simulator and the commercial reservoir simulator have similar flow responses and pressure distribution in the reservoir using Peaceman’s wellbore model. In this section, the local grid refinement technique will be applied to the same reservoir. Before comparing the differences of local grid refinement technique and Peaceman’s wellbore model, first a sensitivity test will be performed on local grid refinement technique.

As stated earlier, the resolution of the window blocks is determined by $\alpha$ and $\beta$ values. Table 7-3 shows the values of $\alpha$ and $\beta$ parameters, and the additional number of grid blocks introduced in the window block. For these simulations, Table 7-4 and Table 7-5 are used for the reservoir and fluid properties of the system.
As it is discussed in Chapter 2, the accuracy of the reservoir simulator is directly proportional to the size of grid blocks. In window blocks, smaller $\alpha$ and $\beta$ parameters yield higher resolution in the window block.

<table>
<thead>
<tr>
<th>Table 7 - 3 Reservoir Data for Validation of Local Grid Refinement Comparison</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir Model</td>
</tr>
<tr>
<td>Well Location</td>
</tr>
<tr>
<td>Reservoir Size</td>
</tr>
<tr>
<td>Thickness (ft)</td>
</tr>
<tr>
<td>Fracture Porosity</td>
</tr>
<tr>
<td>Matrix Porosity</td>
</tr>
<tr>
<td>Fracture Permeability (md)</td>
</tr>
<tr>
<td>Matrix Permeability (md)</td>
</tr>
<tr>
<td>Fracture Spacing (ft)</td>
</tr>
<tr>
<td>Diffusivity</td>
</tr>
<tr>
<td>Coal Density (lb/ft$^3$)</td>
</tr>
<tr>
<td>Initial Pressure (psia)</td>
</tr>
<tr>
<td>Water Saturation (Fracture)</td>
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<tr>
<td>Water Saturation (Matrix)</td>
</tr>
<tr>
<td>Formation Temperature (°F)</td>
</tr>
<tr>
<td>Langmuir Pressure (psia)</td>
</tr>
<tr>
<td>Langmuir Volume (scf/ton)</td>
</tr>
<tr>
<td>Sorption Time (days)</td>
</tr>
</tbody>
</table>
Table 7 - 4 Relative Permeability Data for Validation Test

<table>
<thead>
<tr>
<th>$S_w$</th>
<th>$K_{rw}$</th>
<th>$K_{rg}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.000</td>
<td>0.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>0.050</td>
<td>0.0006</td>
<td>0.8350</td>
</tr>
<tr>
<td>0.100</td>
<td>0.0013</td>
<td>0.7200</td>
</tr>
<tr>
<td>0.150</td>
<td>0.0020</td>
<td>0.6270</td>
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<tr>
<td>0.200</td>
<td>0.0070</td>
<td>0.5370</td>
</tr>
<tr>
<td>0.300</td>
<td>0.0240</td>
<td>0.4010</td>
</tr>
<tr>
<td>0.400</td>
<td>0.0490</td>
<td>0.2950</td>
</tr>
<tr>
<td>0.500</td>
<td>0.0880</td>
<td>0.2160</td>
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<tr>
<td>0.600</td>
<td>0.1540</td>
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<td>0.700</td>
<td>0.2510</td>
<td>0.0900</td>
</tr>
<tr>
<td>0.750</td>
<td>0.3120</td>
<td>0.0700</td>
</tr>
<tr>
<td>0.800</td>
<td>0.3920</td>
<td>0.0510</td>
</tr>
<tr>
<td>0.850</td>
<td>0.4900</td>
<td>0.0330</td>
</tr>
<tr>
<td>0.900</td>
<td>0.6010</td>
<td>0.0180</td>
</tr>
<tr>
<td>0.950</td>
<td>0.7310</td>
<td>0.0070</td>
</tr>
<tr>
<td>1.000</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>

Table 7 - 5 Local Grid Refinement Window Block Schemes

<table>
<thead>
<tr>
<th>Case</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>Number of Grid Blocks</th>
</tr>
</thead>
<tbody>
<tr>
<td>LGR-1.1</td>
<td>1.1</td>
<td>1.1</td>
<td>77x77x3</td>
</tr>
<tr>
<td>LGR-1.5</td>
<td>1.5</td>
<td>1.5</td>
<td>35x35x3</td>
</tr>
<tr>
<td>LGR-2.0</td>
<td>2.0</td>
<td>2.0</td>
<td>13x13x3</td>
</tr>
<tr>
<td>LGR-2.5</td>
<td>2.5</td>
<td>2.5</td>
<td>11x11x3</td>
</tr>
</tbody>
</table>

As it can be seen in Figures 7-7 and 7-8, high resolution LGR schemes, LGR-1.1 and LGR-1.5, converge to the same flow rate responses even for the early simulation times. For the cases of LGR-2.0 and LGR-2.5 the grid block sizes increase rapidly around the wellbore which yields low precision in the pressure and saturation distributions. Due
to this error, the expected flow rate predictions for both phases have relatively large error margin.

The conclusion from the above is that in order to get better flow rate predictions, small values of $\alpha$ and $\beta$ parameters should be used. According to the multiple simulation runs performed on the sensitivity of these parameters, it is concluded that $\alpha = 1.5$ and $\beta = 1.5$ are optimum for calculations. These values not only create enough resolution in the vicinity of the well but also have better transition between locally refined grids and pseudo grid blocks, while keeping the number of grid blocks in the window block suitable for simulation purposes.

![Figure 7](image.png)

*Figure 7 - Comparison of Gas Production Rate for Different LGR Schemes*
Figure 7-8 Comparison of Water Production Rate for Different LGR Schemes

There are no analytical solutions that exist for dual-porosity-dual-permeability two phase flow system. Therefore, the only validation for Peaceman’s model and local grid refinement technique can be made by performing simulations using local grid refinement technique with $\alpha = 1.5$ and $\beta = 1.5$ and the Peaceman’s model with smaller grid block size.

As it is shown in the above example, using smaller grid blocks in the window block yield better pressure and saturation distribution. In Peaceman’s wellbore model, the flow in the well block is assumed to be steady state. However, using large grid blocks violates this assumption for early times, since the pressure transients will not be able to reach the boundaries of the well block. Therefore, similar to local grid refinement technique, using smaller the grid blocks should yield more accurate result for Peaceman’s
model. In order to test this theory, numerous reservoir models were prepared using different grid block sizes. Table 7-6 shows some of the coarse grid block systems that were tested using Peaceman’s wellbore model. The only differences between the coarse grid systems are the grid block sizes. The overall reservoir size, wellbore diameter and all other properties kept constant for the simulations.

<table>
<thead>
<tr>
<th>Case</th>
<th>DX</th>
<th>DY</th>
<th>Reservoir Grid Blocks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case-1</td>
<td>Uniform – 425 ft</td>
<td>Uniform – 425 ft</td>
<td>11x11x1</td>
</tr>
<tr>
<td>Case-2</td>
<td>Uniform – 187 ft</td>
<td>Uniform – 187 ft</td>
<td>25x25x1</td>
</tr>
<tr>
<td>Case-3</td>
<td>Uniform – 50.3 ft</td>
<td>Uniform – 50.3 ft</td>
<td>93x93x1</td>
</tr>
<tr>
<td>Case-4</td>
<td>Non-uniform, well block is 25 ft</td>
<td>Non-uniform, well block is 25 ft</td>
<td>17x17x1</td>
</tr>
</tbody>
</table>

Figure 7-9 and Figure 7-10 show the gas flow rate and water flow rate predictions and Figure 7-11 shows the cumulative gas production of the conventionally upscaled coarse grid models and the local grid refinement technique. As it was expected, the flow rate responses of the coarse grid models are affected by the grid block size. It can easily be seen from the figures that when the grid block sizes are decreased in the conventionally upscaled systems, the flow rate predictions, hence the cumulative production predictions, are getting closer and closer to the prediction of local grid refinement method for both water and gas phases. This is a crucial observation for this
study. First of all, these results show that rectangular grid blocks can be used to approximate a radial-cylindrical wellbore. Secondly, high resolution local grid refinement system can be used as a replacement of Peaceman’s model. These findings allow us to extend this study on irregular shaped wells and predict the well performances of complex well structures which cannot be simulated by using Peaceman’s equations.

It should be noted that decreasing the grid block size increases the number of grid blocks drastically, hence the simulation time increases. For example, in the above simulation study a reservoir model with 11 by 11 coarse grid dimensions took about one minute to complete the simulations. However, 93 by 93 reservoir model took almost an hour to finish the same simulation. In the meantime, the local grid refinement technique with $\alpha = 1.5$ and $\beta = 1.5$ took around 35 minutes to simulate the given system. Moreover, in the figures it can be seen that reservoir model with 17 by 17 grid dimensions has the closest prediction to the local grid refinement system. In the 17 by 17 system, an approach similar to local grid refinement technique is followed. The well block grid dimensions were set to 25 ft by 25 ft and then they are gradually increased when ones moves away from the well block. Even though this system gave more accurate predictions than the other conventional methods, it will be really difficult to implement in the presence of second or third well.

As it was proven by the studies of Li-Wei Hu (2012) and Baris Goktas (1999), LGR approach is more reliable than Peaceman’s model since it eliminates the assumption of radial flow regime even in the early times.
Figure 7 - 9 Comparison of Water Production Rates between LGR and Peaceman’s Model

Figure 7 - 10 Gas Production Rate Comparison between LGR and Peaceman’s Model
One of the main assumptions of the Peaceman’s model is that the flow regime around the wellbore is radial. The effect of the anisotropy on the development of the radial flow can be analyzed easily by using vertical well in an anisotropic reservoir. Vertical well in an anisotropic medium will lack to develop radial flow in the well block and it will violate one the basic assumption of Peaceman’s model. Tables 7-7 through 7-8 demonstrate the reservoir properties of the sample case.

Figure 7 - 11 Cumulative Gas Production Comparison between LGR and Peaceman’s Model
Table 7 - 7 Reservoir Data for Effects of Anisotropy Test

<table>
<thead>
<tr>
<th>Reservoir Model</th>
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<tr>
<td>Well Location</td>
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<tr>
<td>Well Direction</td>
<td>Vertical Well</td>
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<td>Thickness (ft)</td>
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<tr>
<td>Fracture Porosity</td>
<td>0.50%</td>
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<tr>
<td>Matrix Porosity</td>
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</tr>
<tr>
<td>Fracture Permeability in X and Z (md)</td>
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<td>Matrix Permeability (md)</td>
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<td>Coal Density (lb/ft³)</td>
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<tr>
<td>Initial Pressure (psia)</td>
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<tr>
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<td>Formation Temperature (°F)</td>
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<td>Langmuir Pressure (psia)</td>
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<tr>
<td>Langmuir Volume (scf/ton)</td>
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<td>Sorption Time (days)</td>
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</table>

Table 7 - 8 Relative Permeability Data for Effects of Anisotropy Test

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<th>$S_w$</th>
<th>$K_{rw}$</th>
<th>$K_{rg}$</th>
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</thead>
<tbody>
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<tr>
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<td>0.0006</td>
<td>0.8350</td>
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<tr>
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<td>0.0013</td>
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<td>0.0020</td>
<td>0.6270</td>
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<tr>
<td>0.200</td>
<td>0.0070</td>
<td>0.5370</td>
</tr>
<tr>
<td>0.300</td>
<td>0.0240</td>
<td>0.4010</td>
</tr>
<tr>
<td>0.400</td>
<td>0.0490</td>
<td>0.2950</td>
</tr>
<tr>
<td>0.500</td>
<td>0.0880</td>
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<td>0.600</td>
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</tr>
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<td>0.700</td>
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<td>0.850</td>
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<tr>
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<td>0.6010</td>
<td>0.0180</td>
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<td>0.950</td>
<td>0.7310</td>
<td>0.0070</td>
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<tr>
<td>1.000</td>
<td>1.0000</td>
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</table>
Table 7 - 9 Local Grid Refinement Window Block Schemes

<table>
<thead>
<tr>
<th>Case</th>
<th>$\alpha$</th>
<th>$\beta$</th>
<th>Number of Grid Blocks in the Window Block</th>
</tr>
</thead>
<tbody>
<tr>
<td>LGR-1.1</td>
<td>1.1</td>
<td>1.1</td>
<td>39x39x2</td>
</tr>
<tr>
<td>LGR-1.5</td>
<td>1.5</td>
<td>1.5</td>
<td>29x29x2</td>
</tr>
</tbody>
</table>

Figures 7-12 and 7-13 show the gas and water flowrate comparison, respectively, of Peaceman’s model and local grid refinement technique. In order to be sure that LGR module has reliable solutions, multiple LGR schemes were run and they all have a good agreement. Even though, LGR technique with larger $\alpha$ and $\beta$ creates almost half of the high resolution model, where $\alpha$ and $\beta$ parameters set to 1.1, it is still able to predict exactly the same flow behavior. In this case, the main reason the Peaceman’s model predicts depressed flow rates is due to the calculation of average permeability term in the Equation 5.1.33 and 5.1.34. As mentioned earlier, the average permeabilities in the matrix and fracture domains for the grid block are calculated by using the geometric mean of the permeabilities. In the case of anisotropic reservoir model, the smaller permeability value dominates the average permeability calculations. The calculated average permeability value comes closer to the smaller permeability value, which effects the flow rate prediction for both water and gas phases. In the case of LGR module, there is no need for this kind of average permeability calculations; therefore, the production rates are more accurate and representative.
Figure 7 - 12 Gas Production Rate using Peaceman’s Model and LGR Approach

Figure 7 - 13 Water Production Rate using Peaceman’s Model and LGR Approach
7.3 Summary of CBM Model Validation

As it was discussed in the Chapters 7-1 and 7-2, the proposed CBM model with local grid refinement technique is capable of providing accurate prediction of gas and water production rates, as well as better pressure and saturation distributions in the well blocks, when simulating vertical wells and horizontal wells. Even though the accuracy of the local grid refinement technique is affected by the selection of $\alpha$ and $\beta$ parameters, it is proven that the local grid refinement technique converges to similar flow rates and pressure distribution values for higher resolution systems. Furthermore, it is concluded that, choosing $\alpha = 1.5$ and $\beta = 1.5$ generates accurate simulation results while having optimum number of local grid blocks for simulation time and stability.

The proposed model also proves that the Peaceman’s model generates erroneous results under the conditions where it is not possible to develop radial flow regime in the well block. Also, it is proven that flow rate predictions of Peaceman’s model converge to the local grid refinement technique if the grid block sizes are reduced to decrease truncation errors.
Chapter 8

Effects of Wellbore Geometry on Well Production Performances

In the previous chapter, the model has been verified for the wells on the center of the well block in the vertical plane or the horizontal plane. In other words, prior to this study the only well structures considered were regular wells which can be simulated by using the Peaceman’s wellbore model.

Horizontal, muti-lateral and slanted wells have become more popular with the enhancement in drilling operations. Major oil companies started investing on these technologies to increase the contact surface of the wells with the minimum surface facilities and foot print. However, the numerical solution for these types of the wells is not easy to accommodate with the current wellbore models. Researcher, such as Joshi, 1988a, Ozkan et al., 1987, Goode and Wilkinson 1990, tried to developed new set of equations to accommodate these new well structures, however, they all had the limitations with the complexity of the reservoir and the wellbore geometry. As the was shown in the previous chapter, local grid refinement technique can be extended for better understanding of the effects of well structure on the reservoir depletion and the flow rate predictions. In order to handle complex well geometries, new subroutine was implemented to read the well path in the reservoir and create locally refined grids accordingly.
With this chapter, first, horizontal well will be compared with different complex well structures and then there will be numerous comparison between the complex wells structures to find out the best development strategy for the given reservoir conditions.

**8.1 Comparison of Horizontal Well and Dual-Lateral Wells**

In this section, the performance of horizontal well is considered with respect to different types of dual-lateral wells. Recent developments in the drilling technology enable companies to drill horizontal wells with multiple completions and different angles between the laterals. By changing the angle and completing multiple wells from the same location, the oil and gas companies not only decrease their expenditure on the field development but also decrease the foot print of the well in the surface.

As it can be seen from the Figures 8-2, 8-3, 8-4 and 8-5, the tested models in this section are single lateral horizontal well, dual-lateral well with 90 degrees between the wings, dual-lateral well with 120 degrees between the wings and dual-lateral well with 180 degrees between the wings. For the consistency and better comparison between different well configurations, Table 8-1 and Table 8-2 are used throughout the examples in Chapter 8. In addition, Figure 8-1 represents the computational domain which is used throughout all the simulations in this study. Once again, by doing this, it will be easier to compare all different scenarios.
Table 8 - 1 Reservoir Properties for Chapter 8 Simulation Studies

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir Model</td>
<td>11-11-1</td>
</tr>
<tr>
<td>Well Location</td>
<td>6-6-1</td>
</tr>
<tr>
<td>Reservoir Size</td>
<td>100 ft – 100 ft</td>
</tr>
<tr>
<td>Thickness (ft)</td>
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<tr>
<td>Fracture Porosity</td>
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<td>Matrix Porosity</td>
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<td>Fracture Permeability in X and Z (md)</td>
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<td>Fracture Permeability in Y (md)</td>
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<td>Matrix Permeability (md)</td>
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<td>Diffusivity</td>
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<td>Water Saturation (Fracture and Matrix)</td>
<td>0.70</td>
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<td>Formation Temperature (˚F)</td>
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<td>Langmuir Volume (scf/ton)</td>
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<td>Sorption Time (days)</td>
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</tbody>
</table>

Table 8 - 2 Fluid Properties for Chapter 8 Simulation Studies

<table>
<thead>
<tr>
<th>$S_w$</th>
<th>$K_{rw}$</th>
<th>$K_{rg}$</th>
</tr>
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<tbody>
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<td>0.000</td>
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<td>0.0070</td>
</tr>
<tr>
<td>1.000</td>
<td>1.0000</td>
<td>0.0000</td>
</tr>
</tbody>
</table>
Figure 8 - 1 Computational Domain

Figure 8 - 2 Initial Pressure Distribution of the Horizontal Well (Case 1-a)
Figure 8 - 3 Initial Pressure Distribution of Dual-Lateral Well with 90 Degrees

Figure 8 - 4 Initial Pressure Distribution of Dual-Lateral Well with 120 Degrees
Figure 8-5 Initial Pressure Distribution of Dual-Lateral Well with 180 Degrees

Figure 8-6 and 8-7 show the gas and water production profiles for Case 1 wells. As it can be seen from the figures that wells with 90 degrees and 120 degrees between the wings almost produces the same amount of gas for each ft of well. Both Case 1-b and Case 1-c has the highest production compared to other two cases due to their effectiveness on decreasing the pressure around the well path.

For better understanding of the pressure distribution around the well, Figures 8-8 and 8-9 were prepared for the comparison between pressure distributions of Case 1-a and Case 1-b at 10 days. The calculated average pressure at 10 days for Case-1-b is approximately 540.6 psia whereas the average pressure for Case 1-a is approximately 554.9 psia. The 15 psia difference within 10 days of production is mainly due to effective
dewaterization of the field with dual-lateral completion. Similarly, Figures 8-10 and 8-11 show the pressure distribution of the well block at the end of 1000 days. Once again, dual-lateral well (Case 1-b) is more effective on depleting the reservoir as it can be seen from the graphs. The average pressure for 1000th day is 470 psia for the Case 1-a and 449 psia for the Case 1-b.

![Gas Production Rate for each ft of Well for Case 1 Wells](image)

*Figure 8 - 6 Gas Production Rate for each ft of Well for Case 1 Wells*
Figure 8 - 7 Water Production Rate for Each ft of Well for Case 1 Wells

Figure 8 - 8 Pressure Distribution around the Well; Case 1-a at 10 Days
Figure 8 - 9 Pressure Distribution around the Well; Case 1-b at 10 Days

Figure 8 - 10 Pressure Distribution around the Well; Case 1-a at 1000 Days
As it can be seen from Case 1 simulation results, the wellbore geometry affects the production profile of the well significantly. With this section and the next sections, further investigations will be performed on the using the same reservoir and fluid properties. Once again, the results will be compared per ft of well basis in order to identify the optimum well geometry for the given formation. In this multiple lateral well completion schemes is investigated. The main purpose is to find out the optimum ratio between the wing length and number of wings for the lateral wells. As it can be seen from Figures 8-12 through 8-15, 4 different well geometries are tested.
Figure 8 - 12 Initial Pressure Distribution of the Multilateral Well, Case 2-a

Figure 8 - 13 Initial Pressure Distribution of the Multilateral Well, Case 2-b
Figure 8 - 14 Initial Pressure Distribution of the Multilateral Well, Case 2-c

Figure 8 - 15 Initial Pressure Distribution of the Multilateral Well, Case 2-d
The gas and water production profiles for the Case 2 wells can be seen in Figures 8-16 and 8-17, respectively. As expected, the design of the multilateral wells is very crucial for the development of the reservoirs. Even though the well Case 2-a penetrates deeper into the reservoir with its three long wings, it is production rate per ft of well performance not as high as the Case 2-c. In the Case 2-c, the well has 5 mid-range wings and this setup performs the best among the all Case-2 wells. In the Case 2-d, the well has more wings with shorter length. Even though, the early production rates from the well 2-d has similar values with the other wells, because of the high interference with its wings, its production rates decreases rapidly.

Figure 8 - 16 Gas Production Rate for each ft of Well for Case 2 Wells
Figures 8-18 through 8-21 show the pressure distribution around the wells for Case 2-c and Case 2-d after 10 days and 1000 days of production. It should be noted that even after 10 days of production the average pressure at the well block for Case 2-c drops to 490 psia, in the meantime, case 2-d managed to drop approximately to 550 psia. Similar pressure difference can be observed at the end of 1000 days of simulation. These results show that the design of the wing length and spacing is one of the more critical aspects of the reservoir development process.
Figure 8 - 18 Pressure Distribution around the Well; Case 2-c at 10 Days

Figure 8 - 19 Pressure Distribution around the Well; Case 2-d at 10 Days
Figure 8 - 20 Pressure Distribution around the Well; Case 2-c at 1000 Days

Figure 8 - 21 Pressure Distribution around the Well; Case 2-d at 1000 Days
8.3 Comparison of Undulating Well and Multilateral Well

One of the main applications of complex well geometries involves undulating wells. The main purpose of the undulating wells is to extend the reach of the reservoir without having any trip-in and trip-out operations. The undulating well can be completed in a single drilling operation unlike dual-lateral or multilateral wells. In this section, a multilateral well will be compared with respect to an undulating well. The basic structures of a multilateral well and an undulating well can be seen in Figure 8-22 and Figure 8-23, respectively.

Figure 8 - 22 Initial Pressure Distribution of the Multilateral Well, Case 3-a
So far, the well length used for the simulations in the previous sections was kept equal for all the cases. This helped us to analyze the pressure distribution data more objectively without worrying about the well length. In this section, the undulating well and multilateral well length was unable to be kept equal; however, the comparisons on the flow rate performances were done on per unit well length. Figures 8-24 and 8-25 show the comparison of the actual gas and water flow rate values. For a comparison, Figures 8-26 and 8-27 were prepared to show the gas and water flow rate responses of the wells per ft of the well length. The results are somewhat interesting, the actual data shows that the multilateral well and undulating well performing similarly with a little favor.
towards multilateral well. However, it is very clear from Figures 8-26 and 8-27 that, the undulating well is performing much better than the multilateral completion.

The main reason that multilateral well completion does not perform as well as undulating well is that the interference between the lateral sections. It can be seen from Figure 8-28 that, the pressure drop between the multilateral sections at day 1000 are close to 200 psia range whereas the sections outside of the laterals are close to 500 psia range. Even though having undulating

![Figure 8 - 24 Actual Gas Production Rate for Case 3 Wells](image-url)
Figure 8 - 25 Actual Water Production Rate for Case 3 Wells

Figure 8 - 26 Gas Production Rate for each ft of Well for Case 3 Wells
Figure 8 - 27 Water Production Rate for each ft of Well for Case 3 Wells

Figure 8 - 28 Pressure Distribution around the Well; Case 3-a at 1000 Days
8.4 Effects of Dual-Lateral Location on the Performance

In this section, dual-lateral well with 90 degrees between its wings is further investigated. As it was discussed in section 8-1, the dual-lateral well has a horizontal section and then two wings at the end of this horizontal section. This section is dedicated on investigating how the aspect ratio between the horizontal section and length of the wings affects the performance of the well. There will be four different scenarios (Figures 8-29 through 8-32). Their actual performances and flow rate per ft of well performances will be studied for better understanding of their impact on the field development.

Figure 8 - 29 Initial Pressure Distribution of the Multilateral Well, Case 4-a
Figure 8 - 30 Initial Pressure Distribution of the Multilateral Well, Case 4-b

Figure 8 - 31 Initial Pressure Distribution of the Multilateral Well, Case 4-c
Figure 8-33 and 8-34 compares the gas flow rate per ft of well and actual gas flow rate of the Case 4 wells. As it can be seen from both graph, the gas production rates for wells 4-a, 4-b and 4-c are very close to each other and 4-d displays the least efficiency. However, for total production, well Case 4-d produces the highest amount of production. Similarly, Figures 8-35 and 8.36 show the flow rate performance per ft of well and actual water flow rate of this system. The main reason for well Case 4-d has the highest gas production is that the well 4-d has the highest penetration into the well block and it can drain the highest amount of water. Therefore, allowing the system desorb more gas from the coal matrix and increases the amount of gas available for production.
Figure 8 - 33 Gas Production Rate for each ft of Well for Case 4 Wells

Figure 8 - 34 Actual Gas Production Rate for Case 4 Wells
Figure 8 - 35 Water Production Rate for each ft of Well for Case 4 Wells

Figure 8 - 36 Actual Water Production Rate for Case 4 Wells
8.5 Comparison between Slanted Well and Undulating Well

Other common complex well structures practiced by the industry include the use of vertical slanted wells and vertically undulating wells. In this section the X-Z cross section of these two well configurations are shown in Figures 8-37 and 8-38, as they are investigated for their production performances.

![Figure 8-37 Initial Pressure Distribution of the Slanted Well, Case 5-a](image-url)
As it can be seen from the Figures 8-39 and 8-40, the actual gas and water production values for the undulating well are higher than the slanted wells. It should be noted that both slanted well and the undulating well outperformed all the previous complex wellbore models. The main reason for this high production rates is due to the use of the prolific reservoir properties. The reservoir in question is very restricted vertical flow and all the horizontal wells had problem producing from the zones below and above the well layer. However, for the vertically undulating and slanted well, it was not a challenge since the wellbores in both cases penetrate through several layers of the formation.
Figure 8 - 39 Actual Gas Production Rate for Case 5 Wells

Figure 8 - 40 Actual Water Production Rate for Case 5 Wells
One thing should be noted that, even though actual production rates for undulating well is more than the slanted well and all the other wells that is studied so far, its production rates per ft of well length is not much better than the slanted well. As it is demonstrated in Figures 8-41 and 8-42, undulating well is performing better than slanted well at the early times of the simulation, however, once the interference between the different wellbore sections of the undulating well begins, its production rates drops sharply below the slanted well. This interference effect can be seen much clearly if the pressure distribution for 1000\textsuperscript{th} days of simulation is compared. Figures 8-43 and 8-44 show the pressure distribution for undulating well and slanted well, respectively, after 1000 days of production.

![Gas Production Rate for each ft of Well for Case 5 Wells](image)

**Figure 8 - 41 Gas Production Rate for each ft of Well for Case 5 Wells**
Figure 8 - 42 Water Production Rate for each ft of Well for Case 5 Wells

Figure 8 - 43 Pressure Distribution at 1028 days for Well 5-a
Now, let us combine the most efficient wells and most productive wells from each of the cases studied. So far, 16 different well configurations are investigated. For comparison, 7 of these configurations picked based on their simulation performances. First, their actual daily gas and water production rates will be compared. Figures 8-45 through 8-48 show the gas and water production rates and cumulative productions, respectively, of the selected wells. As it can be seen, well Case 5-b outperforms all the other configurations in actual gas and water production performances. As it was discussed before, the main reason why Well 5-b outperforms all the other wells is that it penetrates multiple vertical layers in a system where the vertical flow is restricted. With the help of this design, well 5-b is able to produce $2 \times 10^6 SCF$ of gas in 400 days.
whereas it took well 5-a around 600 days and all the other wells at least 2000 days of production. At the end of 2000 days of simulation, well 5-b produces almost 30% more than well 5-a and almost 4 times more than all the other well configurations. To understand why the other wells are not producing that effective, X-Z cross-section pressure distribution of well 2-c is shown in Figure 8-49.

If the production rate per ft of well is compared, Figures 8-50 and 8-51, it can be seen that well 5-a is performing better than well 5-b. At this point, which well should be drilled in such a reservoir is more of an economic issue. Depending on the cost of the well and price of the gas, and facility cost; reservoir engineers and project development personnel should decide which well configuration should be implemented.
Figure 8 - 46 Water Production Rate Comparison between All Cases

Figure 8 - 47 Cumulative Gas Production Comparison between All Cases
Figure 8 - 48 Cumulative Water Production Comparison between All Cases

Figure 8 - 49 X-Z Cross-Section Pressure Distribution of Well 2-b after 10 Days of Production
8.5 Case Study – 2 Reservoir with Increased Vertical Permeability Value

In the previous case study, the vertical permeability of the given reservoir was very low and this was creating problem for the horizontal wells. In this case study, the vertical permeability value will be increased so that it will be as large as 0.1 times of the horizontal permeability values and the similar comparison reservoir study will be performed. The most productive and efficient well configurations from the previous case study will be used to see how the well performances are changing with changing the vertical permeability of the reservoir. Horizontal and vertical well configurations are also added to the graphs to reflect the advantages of complex well geometry completions. See Appendix-D for the actual reservoir rock and fluid properties and well configurations.
Figure 8 - 51 Gas Production Rate Comparison between All Cases

Figure 8 - 52 Water Production Rate Comparison between All Cases
Figures 8-51 and 8-52 show the comparisons for the gas and water flow rates between different well configurations considered. Once again, well 5-b, vertically undulating well, outperforms all the other wells, however, this time the results are not significantly different. Since the reservoir has some vertical connectivity between its layers, horizontal wells started to produce from the other vertical layers and it helped them to produce more. If one compares Figures 8-53 and 8-54 with Figures 8-49 and 8-50, it is obvious that well 2-b started to deplete the reservoir more effectively. The X-Z cross-sectional view shows that unlike the previous case study, the pressure values around the well are distributed more evenly and there are not huge pressure differences between layers.

Figure 8 - 53 X-Z Cross-Section Pressure Distribution of Well 2-b after 10 Days of Production
Figure 8 - 54 X-Z Cross-Section Pressure Distribution of Well 2-b after 1000 Days of Production
Chapter 9

Summary and Conclusions

A local grid refinement (LGR) technique has been developed and implemented to a compositional, dual-porosity, dual-permeability and two-phase flow coalbed methane numerical reservoir simulator. The developed LGR technique uses high resolution window block and residual equation to calculate the performances of the irregular and complex well geometries. The LGR module generates the high resolution grid blocks around the wellbore and reduces the number of grid block for necessary calculations. Even though, an efficient technique is implemented, the number of grid blocks generated in the window block is still excessive in many cases. Moreover, due to the nature of the equations used, a non-symmetric and non-diagonally dominated sparse matrix is created. The generalized minimum residual (GMRES) iterative solver with ParaSails and Fast Auxiliary Space Preconditioner (FASP) preconditioners are also implemented in order to solve this complex system. Additionally, the GMRES and ParaSails modules are parallelized using message passing interface (MPI) method to be able to use multiple computers to speed up the simulation process. Furthermore, two more modules are implemented for more stable and faster Newton-Raphson convergence.

The proposed model predicts the flow performance of complex wells in a significantly different fashion from the current practices. Most of the current reservoir simulators use Peaceman’s wellbore model to predict well performances. With the
proposed model, the assumptions of Peaceman’s model, such as wells at the center of the reservoir or single wellbore geometry for each grid block, are no longer a limitation. The model provides an accurate approximation to the physical structure of the complex well geometries. The flow performances of the complex well completions are determined by using the residual approach. In the window block, fine rectangular grid blocks with the dimensions as small as wellbore diameter is generated. After that, the flow equations are used to calculate the pressure distribution around the wellbore and well performances are calculated using residual equations.

The following conclusions are drawn from this work:

1. Direct solvers are no match to handle large system of equations. For faster and more efficient reservoir simulations one should implement a robust solver, such as the generalized minimum residual method (GMRES), with a better matrix storage scheme.

2. Even more efficient solvers, like GMRES, struggle when encountered with complex linear equations. Using an ideal preconditioner is the way to improve the efficacy of the solvers. In this study, two different preconditioners were tested and even having lack of parallel computing, FASP solver is proved to be faster than ParaSails parallel preconditioner.

3. One of the more important issues with reservoir simulations is to have a stable simulation. The recently implemented modules predicted better initial guesses for the solution and increased the convergence rate.
4. Peaceman’s wellbore model is not suitable for representing the complex wellbore geometries. Peaceman’s model needs small grid blocks to represent complex well configurations and this creates numerical instabilities. Peaceman’s wellbore model for horizontal and vertical wells has even problems if the reservoir system is highly anisotropic, where the radial flow assumption is violated.

5. Using LGR model, even with $\Delta x_{i+1} = \Delta x_i^{1.5}$ and $\Delta y_{j+1} = \Delta y_j^{1.5}$ for local grid block dimensions, is more robust and accurate way to calculate flow performance of the wells rather than using the Peaceman’s wellbore model.

6. Conventional upscaling of the coarse grid system increases the accuracy of the solution; however, it comes with the drastic increase on the simulation times. Using LGR approach optimizes the time spent on the simulations and the accuracy of the solution with a minimum effort.

7. Due to the increased number of fine grid blocks, achieving a stable version of the LGR technique presents a challenge. Modules developed to stabilize and increase the efficacy of the solver cut the oscillations around the solution and also increased the accuracy of the solution. Previously, one in every five iterations of the LGR module had a problem and failed to converge, with the help of the new modules and modifications on the time step size selections; this value is dropped to one in every thirty five iterations.

8. Almost 90% of the CPU time is spent on the finding the solution vector for a given Jacobian matrix and residual vector. This task considered to be one of the biggest challenges in reservoir simulation. Preconditioners help in finding
the solution vector and their performances affects the time spend for each simulation. Even though ParaSails preconditioner and GMRES are parallelized using MPI, tests show that FASP preconditioner and GMRES iterative solver without parallelization performs much better than parallelized code.

9. The proposed LGR module is able to represent complex well geometries in two-phase coalbed methane reservoirs. The performances of the wells are highly depended on formation and fluid properties and there is no single optimum wellbore configuration for the field development. However, using LGR approach helps to identify the strengths of different well configurations and to find the best wellbore design for the given reservoir conditions.

10. For highly anisotropic systems, penetrating multiple layers yields higher production values; however, with decreasing anisotropy, vertical wells start losing their advantages and horizontal multi-lateral wells start outperforming. This kind of behavior can be easily identified by using the proposed LGR technique whereas; Peaceman’s wellbore model lacks to identify this problem.
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Appendix A

Equations and Correlations for Rock and Fluid Properties

In this work, the Peng-Robinson equation of state is used to calculate the necessary compressibility and fugacity coefficient for the given gas components. If the tables for gas formation volume factor, gas viscosity, gas density, water formation volume factor, water density, water viscosity, relative permeability of gas, relative permeability of water, or capillary pressure are not given, the following correlations will be used and a table will be created for a table look-up values for the simulation. If solubility of gas in water ($R_{sw}$) table is not given, then it will be assumed as zero.

Compressibility Factor (Z-Factor)

The Peng-Robinson cubic expression:

$$Z^3 - (1 - B)Z^2 + \left(A - 2B - 3B^2\right)Z - \left(AB - B^2 - B^3\right) = 0$$

(A.1)

where

$$A = \sum_{i}^{n} \sum_{j}^{n} X_i X_j A_{ij}$$

(A.2)

$$A_{ij} = (1 - \delta_{ij}) \sqrt{A_i A_j}$$

(A.3)

$$A_i = \Omega_{ai} \frac{p_{ri}}{T_{ri}^2}$$

(A.4)

$$B = \sum_{i=1}^{n} c_i B_i$$

(A.5)
\[ B_i = 0.077796074 \frac{p_{ri}}{T_{ri}} \]  
(A.6)

\[ p_{ri} = \frac{p}{p_{ci}} \]  
(A.7)

\[ T_{ri} = \frac{T}{T_{ci}} \]  
(A.8)

\[ \Omega_{ai} = 0.457235529 \left[ 1 + m_i (1 - \sqrt{T_{ri}}) \right]^2 \]  
(A.9)

If \( \omega_i \leq 0.49 \) then \( m_i = 0.374640 + 1.54226 \omega_i - 0.26992 \omega_i^2 \)  
(A.10)

If \( \omega_i > 0.49 \) then \( m_i = 0.379642 + 1.48503 \omega_i - 0.164423 \omega_i^2 + 0.01666 \omega_i^3 \)  
(A.11)

\( \delta_{ij} = \) Binary mixture coefficient between the \( i \)-th and \( j \)-th components

Analytical Solution of cubic polynomials:

For the generic polynomial:

\[ x^3 + ax^2 + bx + c = 0 \]  
(A.12)

Calculate

\[ Q = \frac{a^2 - 3b}{9} \]  
(A.13)

\[ R = \frac{2a^3 - 9ab + 27c}{54} \]  
(A.14)

\[ M = R^2 - Q^3 \]  
(A.15)
a) If $M \leq 0$, the polynomial has three real roots.

\[
\begin{align*}
  x_1 &= -\left(2\sqrt{Q}\cos\left(\frac{\theta}{3}\right) - \frac{a}{3}\right) \\
  x_2 &= -\left(2\sqrt{Q}\cos\left(\frac{\theta + 2\pi}{3}\right) - \frac{a}{3}\right) \\
  x_3 &= -\left(2\sqrt{Q}\cos\left(\frac{\theta - 2\pi}{3}\right) - \frac{a}{3}\right)
\end{align*}
\] (A.16)

where

\[
\theta = \arccos\left(\frac{R}{\sqrt{Q^3}}\right)
\] (A.17)

b) If $M > 0$, the polynomial has only one real root equal to

\[
x = S + T - \frac{a}{3}
\] (A.18)

where

\[
\begin{align*}
  S &= \sqrt[3]{-R + \sqrt{M}} \\
  T &= \sqrt[3]{-R - \sqrt{M}}
\end{align*}
\] (A.19)

### Fugacity Coefficients and Fugacity

Fugacity Coefficients and Fugacity can be calculated using Peng-Robinson EOS as follows:

\[
\ln \varphi_i = -\ln(Z - B) + \frac{A}{2.828427125B} \left[ 2\sum_{j=1}^{n} A_{ij} X_j \right] - \frac{B_i}{A} \ln \left[ \frac{Z - 0.414213562B}{Z + 2.414213562B} \right] + \frac{B_i}{B}(Z - 1)
\] (A.21)

\[
f_i = \phi_i X_i p
\] (A.22)
Gas Formation Volume Factor

\[ B_g = \frac{p_{sc} Z(T + 460)}{5.615 p Z_{sc} (T_{sc} + 460)} \]  \hspace{1cm} (A.23)

Gas Density

\[ \rho_g = \frac{p M_g}{Z R (T + 460)} \]  \hspace{1cm} (A.24)

Gas Viscosity (Lee et al., 1966)

\[ \mu_g = 1 \times 10^{-4} k_v \text{EXP} \left( x_v \left( \frac{\rho_g}{62.4} \right)^{y_v} \right) \]  \hspace{1cm} (A.25)

where

\[ k_v = \frac{(9.4 + 0.02M_g)T^{1.5}}{209 + 19M_g + T} \]  \hspace{1cm} (A.26)

\[ y_v = 2.4 - 0.2x_v \]  \hspace{1cm} (A.27)

\[ x_v = 3.5 + \frac{986}{T} + 0.01M_g \]  \hspace{1cm} (A.28)

Water Formation Volume Factor (McCain, 1991)

\[ B_w = (1 + \Delta V_{wt})(1 + \Delta V_{wp}) \]  \hspace{1cm} (A.29)

where

\[ \Delta V_{wt} = -1.00010 \times 10^{-2} + 1.33391 \times 10^{-4} T + 5.506454 \times 10^{-7} T^2 \]  \hspace{1cm} (A.30)

\[ \Delta V_{wp} = 1.95301 \times 10^{-9} p T - 1.72834 \times 10^{-13} p^2 T - 3.58922 \times 10^{-7} p - 2.25341 \times 10^{-10} p^2 \]  \hspace{1cm} (A.31)
Water Density (McCain, 1991)

\[ \rho_w = 62.368 + 0.438603S + 1.60074 \times 10^{-3} S^2 \]  
(A.32)

Water Viscosity (McCain, 1991)

\[ \mu_w = AT^B \left( 0.9994 + 4.0295 \times 10^{-5} p + 3.1062 \times 10^{-9} p^2 \right) \]  
(A.33)

where

\[ A = 109.574 - 8.40564S + 0.313314S^2 + 8.72213 \times 10^{-3} S^3 \]  
(A.34)

\[ B = -1.12166 + 2.63951 \times 10^{-3} S - 6.79461 \times 10^{-4} S^2 - 5.47119 \times 10^{-5} S^3 \]  
\[ + 1.55586 \times 10^{-6} S^4 \]  
(A.35)

Relative Permeability to Gas

Corey’s correlation:

\[ k_{rg} = k_{rgc} \left( 1 - (S_{wn})^2 \right) \left( 1 - S_{wn} \right)^2 \]  
(A.36)

where

\[ k_{rgc} = k_{rg} \text{ at } S_g = 1 - S_{wirr} \]  
(A.37)

\[ S_{wn} = \frac{S_w - S_{wirr}}{1 - S_{girr} - S_{wirr}} \]  
(A.38)

Relative Permeability to Water

Corey’s correlation:

\[ k_{rw} = k_{rwc} (S_{wn})^4 \]  
(A.39)

where

\[ k_{rwc} = k_{rw} \text{ at } S_w = 1 - S_{girr} \]  
(A.40)
\[ S_{wn} = \frac{S_w - S_{wirr}}{1 - S_{girr} - S_{wirr}} \]  
(A.41)

**Capillary Pressure**

Corey’s correlation:

\[ p_{cgw} = \frac{1}{\sqrt{1.448(S_w - S_{wirr})}} \]  
(A.42)
Appendix B

Equations for Shrinkage and Swelling Effect

The following equations are used to calculate the effects of shrinkage and swelling in the coalbed methane reservoirs. It is assumed that permeability is related to porosity as described by Reiss (1980):

$$
\frac{k}{k_i} = \left(\frac{\phi}{\phi_i}\right)^3 \left[ e^{c_{\phi}(p-p_i)} + \frac{f_\beta \rho V_i}{\phi_i} \left( \frac{p_i}{p_L + p_i} - \frac{p}{p_L + p} \right) \right]^3 \tag{B.1}
$$

The following equation gives the volume change due to the release/adsorption of gas in the coal matrix during drawdown for undersaturated coalbed reservoirs is given by:

$$
\Delta V_g = 0 \text{ for } p > p_{\text{sat}} \tag{B.2}
$$

$$
\Delta V_g = f_\beta \rho V_i \left( \frac{p_{\text{sat}}}{p_L + p_{\text{sat}}} - \frac{p}{p_L + p} \right) \text{ for } p \leq p_{\text{sat}} \tag{B.3}
$$

For the injection, $\Delta V_g$, is given by:

$$
\Delta V_g = f_\beta \rho V_i \left( \frac{p_{\text{sat}}}{p_L + p_{\text{sat}}} - \frac{p}{p_L + p} \right) \tag{B.4}
$$

The volume change for multi-component systems;

$$
\Delta V_g = \sum_{i=1}^{NC} \tilde{f}_i \beta_i \rho V_i \left( \frac{Y_{i,j} p_i}{p_{L,j} + p_i} - \frac{Y_i p}{p_{L,j} + p} \right) \tag{B.5}
$$

The shrinkage and swelling model for multi-component systems can be written as:

$$
\frac{k}{k_i} = \left(\frac{\phi}{\phi_i}\right)^3 \left[ e^{c_{\phi}(p-p_i)} + \sum_{i=1}^{NC} \frac{\tilde{f}_i \beta_i \rho V_i}{\phi_i} \left( \frac{Y_{i,j} p_i}{p_L + p_i} - \frac{Y_i p}{p_L + p} \right) \right]^3 \tag{B.6}
$$
Appendix C

The Generalized Minimum Residual (GMRES) Algorithm

Following GMRES algorithm is developed and implemented for the current CBM simulator.

for outerloop = 0,1,2......,outerloop_max
{  
  Compute, r = b - A*x , rho = norm(r), v1 = r / rho; g[0] = rho;
  for k= 0,1,2......innerloop_max
  {  
    v_{k+1} = A * v_k;
    av = norm(v_{k+1})
    for j=0,…k
    {  
      h_{jk} = v_j * v_{k+1} ;
      v_{k+1} = v_{k+1} - h_{jk} * v_j;
    }
    h_{k+1} = norm(v_{k+1})
    v_{k+1} = v_{k+1} / h_{k+1};
    if k > 0
    {  
      y = h_k;
      for j=0, …k-1{  
        g_1 = c_j*y_j - s_j*y_{j+1}  
        g_2 = s_j*y_j + c_j * y_{j+1};
        y_j = g_1;
        y_{j+1} = g_2;
      }
      for j=0, …k
      {  
        h_{jk} = y_j;
      }
    }
  }
  mu = sqrt (h_{kk} * h_{kk} + h_{k+1,k} * h_{k+1,k});
  c_k = h_{kk} / mu;
  s_k = -h_{k+1,k} / mu;
  h_{kk} = c_k * h_{kk} - s_k * h_{k+1,k}
\[ g_1 = c_k \cdot g_k - s_k \cdot g_{k+1}; \]
\[ g_2 = s_k \cdot g_k + c_k \cdot g_{k+1}; \]
\[ g_k = g_1; \]
\[ g_{k+1} = g_2; \]
\[ \text{rho} = \text{abs}(g_{k+1}); \]
\[ \text{check for convergence;} \]
\[ \text{if(converged)} \text{ break;} \]
\}

\[ k = k - 1; \]
\[ y_{k+1} = g_{k+1} / h_{k+1,k+1}; \]
\[ \text{for } i=k, \ldots, 0 \]
\[ \quad y_i = (g_i - h_{i,k+1} \cdot y_{i+1}) / h_{ii}; \]
\[ \text{for } i=1, \ldots, N \]
\[ \quad x_i = x_i + v_{i,k+1} \cdot y_{k+1}; \]
\[ \text{if(converged)} \text{ break;} \]
\}
Appendix D

Case Study Data and Well Configurations

For the Case-2, the following reservoir rock and fluid properties are used. Figures D-1 through D-8 demonstrates the well configurations practiced for the simulation studies.

<table>
<thead>
<tr>
<th>Table D - 1 Reservoir Rock Properties for Case - 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir Model</td>
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<tr>
<td>Well Location</td>
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<tr>
<td>Reservoir Size</td>
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<tr>
<td>Thickness (ft)</td>
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<tr>
<td>Fracture Porosity</td>
</tr>
<tr>
<td>Matrix Porosity</td>
</tr>
<tr>
<td>Fracture Permeability (md)</td>
</tr>
<tr>
<td>Matrix Permeability (md)</td>
</tr>
<tr>
<td>Fracture Spacing (ft)</td>
</tr>
<tr>
<td>Diffusivity</td>
</tr>
<tr>
<td>Coal Density (lb/ft$^3$)</td>
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<td>Initial Pressure (psia)</td>
</tr>
<tr>
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</tr>
<tr>
<td>Water Saturation (Matrix)</td>
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<tr>
<td>Formation Temperature (°F)</td>
</tr>
<tr>
<td>Langmuir Pressure (psia)</td>
</tr>
<tr>
<td>Langmuir Volume (scf/ton)</td>
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<td>Sorption Time (days)</td>
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Table D - 2 Reservoir Fluid Properties for Case - 2

<table>
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<tr>
<th></th>
<th>$S_w$</th>
<th>$K_{rw}$</th>
<th>$K_{rg}$</th>
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</table>

Figure D - 1 Initial Pressure Distribution of the Horizontal Well
Figure D - 2 Initial Pressure Distribution of the Vertical Well

Figure D - 3 Initial Pressure Distribution of the Dual-lateral Well, Case 1-c
Figure D - 4 Initial Pressure Distribution of the Multilateral Well, Case 2-c

Figure D - 5 Initial Pressure Distribution of the Multilateral Well, Case 3-a
Figure D - 6 Initial Pressure Distribution of the Dual-lateral Well, Case 4-d

Figure D - 7 Initial Pressure Distribution of the Slanted Well, Case 5-a
Figure D - 8 Initial Pressure Distribution of the Slanted Well, Case 5-b
VITA

Erhan Aslan was born in Aydin, Turkey. He received a Bachelor of Science degree in Petroleum and Natural Gas Engineering and a minor degree in Geographic Information Systems and Remote Sensing from the Middle East Technical University in June 2005.

Upon graduating from the undergraduate program, he worked for a petroleum consultancy company in Abu Dhabi, UAE. He was responsible for reservoir simulation and characterizations studies. In September 2006, he was granted a scholarship to pursue his Master of Science degree at the University of Tulsa, OK. During his studies at the University of Tulsa, he was responsible for assisting undergraduate students with a computer programming class, reservoir engineering class, and production and drilling labs. After graduating from the University of Tulsa, he was granted a scholarship to pursue his doctoral studies at the Pennsylvania State University. During his three and a half year study at the Pennsylvania State University, he was responsible as a teaching assistant for graduate and undergraduate courses, including “Principles of Well Testing and Evaluation”, “Numerical Reservoir Simulation” and “First-Year Seminar” courses along with teaching “PNG-405 Reservoir Rock and Fluid Properties” class as an instructor in Fall 2012 semester. He received Outstanding Graduate Teaching Assistant award in April 2013.

Mr. Aslan is a member of the Society of Petroleum Engineers and American-Turkish Petroleum Professionals.