DEVELOPMENT OF A COMPOSITIONAL SIMULATOR FOR LIQUID-RICH SHALE RESERVOIRS

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

August 2016
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ABSTRACT

Hydrocarbon production from shales has gained significant momentum in recent years with the advancement in hydraulic fracturing and horizontal drilling technologies, and production from shales (and unconventional sources in general) is beginning to garner greater share in US energy portfolio. However, storage and production mechanisms in these ultra-tight reservoirs is not well understood. It is widely believed that adsorption accounts for a significant portion of stored gas in shale gas reservoirs. However, whether this mechanism is important in liquid-rich systems is not well established. In addition to this, due to the matrix permeabilities existing in nano-darcy ranges, it is hard to establish physics of flow on Darcy’s law alone.

In this work, we have developed a new thermodynamically consistent adsorption model that is made applicable to liquid-rich shale systems. Standalone calculations reveal that neglecting this storage mechanism could result in under-estimation of reserves by about 5-15%. The model is based on the ideal adsorbate solution theory (IAST), which has been successfully applied to coalbed methane and dry-gas shale systems earlier.

Additionally, a new approach for multi-mechanistic flow formulation is applied in this study. Previously, multi-mechanistic studies include modeling diffusional flow based on the difference in concentration or molar density. However, this approach becomes handicapped when we have a single phase condition (gas/oil) in the matrix and the other single phase condition (oil/gas) in fractures, since it is not possible to consistently define concentration gradient across discontinuous phases. Such a condition is frequently expected to take place in shale systems, where pressure in fractures would be significantly different from that in the matrix, and therefore fractures may have two hydrocarbon phases, while matrix will still be in single phase condition. In our work, we have defined diffusive flux based on gradient in chemical potential, with the resulting equation being mathematically equivalent to the one defined based on concentration
gradient. This approach is consistent across all the thermodynamic conditions (single and/or two phasic conditions).

Finally, flow modeling in near-wellbore region is of utmost importance, especially in shale systems where early production phase is characterized by depletion through the hydraulically fractured region. It is established in literature that flow in near-wellbore region of horizontal well is of ellipsoidal nature. This is more emphasized when we consider that micro-seismic studies state that the fracturing process forms an ellipsoidal region. Thus, in order to model the flow pattern correctly, we have modeled the reservoir in ellipsoidal coordinates. A comparison of our model’s performance is made with analytical models presented for horizontal wells in homogenous regions.

In addition, we also generated pressure-transient and pressure-derivative type curves using the ellipsoidal model. These type curves were validated using type-curve matching process, with satisfactory results. At the end, an in-depth sensitivity analysis was performed on certain important parameters and presented. Also, a case study is shown, using reservoir parameters from Utica and Marcellus shales. Sensitivity analysis is performed on drainage area and SRV volume, with some recommendations provided on economically-feasible drainage area per well.

In summary, we have developed a three-phase, 3D, dual-porosity, dual-permeability compositional reservoir simulator in this study. The features presented above are incorporated in this model. Case studies illustrating the effect of important parameters in each of the above phenomenon are carried out and results are reported.
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ACKNOWLEDGEMENTS

I would like to thank my advisor Dr. Turgay Ertekin, not only for being such a wonderful mentor, but also for his care and friendship during my stay here at Penn State. Without him, this work would not have been brought to its completion. I would also like to thank Dr. Luis Ayala, Dr. Eugene Morgan, and Dr. Terry Engelder for their interest in serving as committee members and insightful suggestions.

I thank the EME department for letting me use their resources to complete my study. I also thank them for all the financial help during the course of this work.

Numerous friends have made my journey memorable. Without their support, it is hard to imagine life in State College.

Finally, I would like to thank my parents for all the support and sacrifices that they have made. I appreciate their guidance at every step of my learning curve and thank them for being such wonderful parents.
Chapter 1

Introduction

As the world energy demand continues to rise, oil and gas exploration and production (E&P) companies are exploiting various unconventional energy sources such as shale gas, shale oil, oil sands, coalbed methane, methane hydrates, etc. in order to cover the energy deficit. The production from each of these sources varies depending upon the geographic location. For example, U.S. is world leader in production and technological development related to shale oil, gas and coalbed methane resources, while Canada is exploiting oil sands. According to U.S. EIA (EIA, 2014), the technically recoverable shale oil resources in U.S. are 58 billion barrels, while that of shale gas is 665 TCF. The same figures worldwide are 345 billion barrels and 7,299 TCF respectively. With the current rate of production, these resources are estimated to last for the next 40 – 50 years in U.S. (EIA, 2015). Elsewhere, China, Argentina and Canada are evaluating their respective shale resources, and have recently started production from these sources.

Shale gas and oil resources are classified as unconventional reservoirs. This is due to the fact that they were considered unrecoverable as lately as 1990’s with the then available technology. However, with advances in drilling and stimulation technologies, this class of reservoirs became accessible. Nevertheless, these reservoirs still present themselves as one of the most challenging reservoirs to produce, due to their complex geology, fluid storage and flow characteristics.
Shale formations exhibit dual porosity characters due to the presence of natural fractures within the matrix domain. When these formations are hydraulically fractured, they still essentially exhibit dual porosity character, as majority of fluid flow takes place in natural and hydraulic fracture network, while a significant amount of fluid is stored in matrix. The fractures act as fast moving highways, transporting fluid from inside of matrix to the producing wellbore. The storage mechanism in shales is also different from conventional reservoirs, since a portion of the total fluid is stored in the form of adsorbed phase on organic shale surface (Schettler et. al, 1989; Xiao-Chun Lu et. al, 1995). Coalbed methane (CBM) also exhibits a similar storage mechanism, although the percentage of adsorbed gas is markedly higher in CBM. Fluid storage by adsorption also reduces the storage space drastically, since a given volume of organic shale could hold about six to seven times as much fluid as the same volume of rock in a conventional reservoirs (Seidle, 2011).

To achieve economic production rates, hydraulic fracturing is one of the most critical processes required, along with drilling of horizontal wells. It has been stated in various literature that fluid flow path (streamlines) in near-wellbore horizontal well is hyperbolic, with the equi-potentials following ellipsoidal curvature (Joshi, 1988). In addition, the process of hydraulic fracturing forms a ‘rubble’ zone, whose shape can be approximated to be elliptical (2D) or ellipsoidal (3D) (Lin and Ma, 2015). Thus, in order to properly model the near-wellbore fluid flow, it is essential that a coordinate system that would correctly represent this flow geometry should be used. Furthermore, majority of fluid production in shale formations takes place from this rubble zone, at the best during the initial production phase. Accordingly, a numerical simulator is developed with
ellipsoidal coordinates such as to mimic the actual flow geometry in a better way, and to reduce the numerical dispersion effects arising from use of the traditional cartesian coordinates.

Current numerical models studying shale formations do not take into account the thermodynamics of adsorption in shales. The thermodynamically-inconsistent, extended Langmuir adsorption model is predominantly used in most commercial simulators (CMG, 2014), partly due to the simple nature of resulting isotherm equation. In addition, these numerical models completely ignore the adsorption phenomenon in liquid-rich systems, and there is no consistent way of representing adsorbed volume in such reservoirs available in petroleum engineering literature. In this work, we have extended the application of ideal adsorbed solution theory (IAST) to liquid-rich systems, and have incorporated the adsorption model into our numerical simulator.

Previously, the studies employing multi-mechanistic formulation used either an effective value for diffusion coefficients for the entire hydrocarbon phase, or used an alternative form of Fick’s law based on concentration gradients (Remner et al., 1986; Ayala et al., 2006; Ghorayeb and Firoozabadi, 2000). However, this approach is not consistent when there is phase discontinuity, either between two adjacent gridblocks or between matrix and fracture domains within the same gridblock, since Fick’s law is defined within a single phase alone. Such scenarios are likely to occur in shale reservoirs during primary depletion phase or during enhanced oil/gas recovery processes. An alternative mathematically-equivalent form of Fick’s law for multi-component mixtures is therefore employed in this work for modeling the diffusion process, and a case study is
shown that illustrates the usefulness of this approach as against the concentration-gradient based approach.

In order to properly model the above processes, it is best to use a compositional reservoir simulator for studying the production performance behavior of shale formations. In this study, we have developed a three-phase, 3D, dual-porosity, dual-permeability compositional simulator that takes the aforementioned developments into account. The model was validated against a commercial simulator, and subsequently a parametric analysis was carried out. In addition, a geo-chemical based model was developed and incorporated into the simulator as a precursor. This model correlates fluid composition and Langmuir adsorption parameters based on geochemical information collected during evaluation phase of any given shale formation.

This report is organized as follows. Chapter 1 provides the introduction to the research topic. Critical literature review is presented in Chapter 2, with the problem statement mentioned in Chapter 3. Chapter 4 covers the development of numerical model, presenting the equations derived in cartesian and ellipsoidal coordinates. The theory behind the adsorption and diffusion processes in shales is covered in Chapter 5. Results are presented in Chapter 6, in which validation against commercial models and analytical well testing solutions are shown. Chapter 7 introduces a case study for Utica shale formation. Finally, conclusions and future work are presented in Chapter 8.
Shale formations are naturally fractured reservoirs, consisting of two porosity domains, namely matrix and natural fracture. Fractures have high permeability and low porosity, while matrix has low (nano-darcy) permeabilities and high porosity. In essence, fractures act as the freeways for the fluid flow, while matrix act as the storage units. These freeways connect the inner portions of matrix to the producing wellbore. Hydrocarbon fluids are stored in free, porous space under compression, as well as due to adsorption on the organic shale surface. The nature of fluid storage in shales is similar to that of CBM, however, unlike the shale reservoirs, almost 100% of the gas is stored in the form of adsorbed phase in CBM.

In order to achieve economically feasible production rates from shale formations, it is necessary to hydraulically fracture the near-wellbore region. Depending upon the stress regime, these fractures form a densely connected network. After the fracturing fluid flow-back period, the free gas present in the fracture domain will be produced first. As the reservoir pressure decreases further, the adsorbed gas from organic matrix will be released. A significantly larger portion of gas is released at lower values of pressure, however, it is not until the late production phase that the reservoir pressure will fall to those level of values. Fluid transport in both domains is governed by two parallel fields: pressure field (convective flow) and concentration field (diffusive flow). The transport...
equation for fluid flowing under pressure field can be explained by Darcy’s law, while that under concentration field can be explained by Fick’s law.

This chapter is broadly divided into five sections. First, it will discuss the various approaches taken by different researchers regarding modeling of shale reservoirs. Next, we will discuss grid orientation effects in reservoir simulators, and how these effects can be minimized using grids that align with the actual flow geometry. The concept of stimulated reservoir volume will also be reviewed. Modeling of adsorption and diffusion phenomenon in shales will be discussed next. Finally, other research topic prominent among shale researchers such as nano-pore confinement effects on phase behavior will be discussed.

2.1 Numerical Modeling of Shale Reservoirs

Various approaches have been used by researchers for modeling of shale reservoirs. The modeling approaches can be sub-divided into single porosity, dual porosity, triple porosity, and even quad porosity. The difference between these models basically lies in how the fractures and organic/inorganic matter is accounted for. Further division can be made depending upon whether fluid transfer within the same porosity domain is considered (i.e. concepts related to single permeability, dual permeability, etc.). Inherently, the more detailed model would seem to be desirable, however, extensive information is required to build a realistic model. Also, the transfer function (defined as the flow transfer term between two porosity domains) needs to be defined before any of the aforementioned models can be used. On the other hand, single porosity models
require the explicit definition of natural/hydraulic fractures. The number of grid blocks
required to accurately represent the fractured system is also large. Thus, there are
advantages and disadvantages related to each approach, and all of these need to be
evaluated in a careful manner before selecting any particular modeling approach.

**Single porosity (SP) models**

As stated earlier, this approach requires fractures to be represented explicitly in the
numerical grid system. Cipolla et. al (2010) performed simulations using a detailed grid
that represented the complex fracture network, primary fracture and tight shale matrix.
The authors also acknowledged that use of single porosity models increases
computational time, while stating that use of dual porosity/dual permeability
approximations may not sufficiently capture the very long transient behavior in shale
matrix blocks. Cheng (2010) evaluated the dynamics of loaded slick water during
fracturing treatment using a generic, single porosity model of hydraulically fractured
horizontal well in gas shales. Karimi-Fard and Firoozabadi (2003) explained that large
number of grid blocks are required in single porosity models due to the different length
scales associated with matrix size and fracture thickness. They also stated that
disconnected fracture media can be modeled in single porosity simulators since there is
only one continuum.
Dual porosity (DP) models

To date, dual porosity modeling has been the preferred way of modeling naturally fractured reservoirs to date. Warren and Root (1963) were the first to use the concept of dual porosity, with the use of their sugar-cube model. This model is shown in Fig. 2.1 below.

![Figure 2.1. The sugar-cube model (Reproduced after Warren and Root, 1963)](image)

The reservoir grid block consists of both matrix and fracture porosities in the same location. Thus, this is an extension of the overlapping continuum theory. As a result, each grid block in the reservoir would have a fracture pressure and a matrix pressure, along with their respective porosities. In these models, permeability is only assigned to fractures. No flow takes place between two matrix blocks, and thus these models can also be called dual porosity single permeability (DPSK).
Du et. al (2010) modeled the hydraulic fracture network in shale reservoirs as dual porosity systems. They incorporated important physical and engineering parameters such as frac fluid mass conservation, interpreted hydraulic fracturing treatments main fractures and fracture network intensity in their model. Samandarli et al. (2011) used dual porosity concept for history matching and forecasting shale gas reservoir production performance.

Dual porosity, dual permeability (DPDK) models have also found their way into modeling for naturally fractured reservoirs. Studies conducted at Penn State (Manik, 1999; Thararoop, 2010) have focused on modeling of coalbed methane reservoirs. This had resulted into development of in-house research simulator, PSU-COALCOMP. Recently, Kulga (2014) applied a modified version of the simulator, named PSU-SHALECOMP, to study the effectiveness of carbon dioxide sequestration in depleted shale gas reservoirs. In this study, DPDK approach is followed, as it allows a reasonable balance between accuracy and computational time.

**Triple porosity (TP) and Quad porosity (QP) models**

Certain researchers have felt the need to account for different mineral content and/or porous space in order to better capture the real flow/storage physics. Haghshenas et. al. (2013) have defined three distinct porosities, each for organic matter, inorganic matter and natural fractures. Sorption process is set to be activated only in organic matter. Their model also has three different permeability values, classifying their model as triple porosity triple permeability (TPTK). They studied three different configurations, depending upon how the organic/inorganic are interconnected and how do these feed the natural fracture system. Li et. al. (2013) proposed a triple porosity model, where the shale
rock is composed of globally connected natural fractures, micro fractures connecting matrix to global fractures, and low permeability matrix rock. Sun et. al. (2015) used a triple porosity dual permeability (TPDK) model, with organic matter, inorganic matter, and natural/hydraulic fractures representing the porosity domains, while permeability is defined for inorganic material and fractures. Multi-mechanistic formulation is used in their model. The authors also concluded that DPDK models are sufficient to model shale reservoirs, after a comparison was made with TPDK and single porosity, single permeability (SPSK) models, and that more complex models such as TP or even quad porosity may not be needed for modeling of real shales.

Few researchers have proposed quad porosity models for shales. Hudson et. al. (2012) have proposed one such model. The four porosities are comprised of inorganic matrix, organic matrix, natural fracture, and hydraulic fractures. All the four porosities are able to hydro-dynamically communicate with each other. Sorption effects are only considered in organic matter, while gas/water dissolution/evolution effects are accounted for in inorganic matter, natural fractures, and hydraulic fractures. Hinkley et. al. (2013) compared the performance of one, two, three, and four porosity models. They concluded that no significant impact on the production performance was observed when increasing the porosity types from three to four. One paper (Lopez and Aguilera, 2013) even discusses quintuple (or five) porosity model, where the additional porosity is accounting for the adsorbed volume.

Although active research is going on regarding the proper modeling approach for shale reservoirs, the use of multiple porosity models seems to have certain problems
associated with them. Firstly, the reservoir characteristics such as porosity, permeability, wettability, diffusion coefficients needs to be known *apriori* for all the porosity types defined. Furthermore, while performing numerical simulation studies, inter-porosity transfer terms need to be formulated as well. The performance of a particular model varies drastically depending upon the definition of this transfer function. Even today, the formulation of inter-porosity term for dual porosity models attracts a considerable debate and discussion, and no exact formulation exist in the literature. Therefore, definition of transfer terms for multiple porosity models seems to be extremely difficult, and further research should be carried out in this area. As a result, the use of multiple porosity (i.e. more than dual porosity) models looks less attractive at this point, and was therefore one of the motivations in selecting DPDK approach for this current study.

**Compositional modeling of shale reservoirs**

Compositional modeling has been traditionally used for modeling depletion behavior of retrograde gas condensates and volatile oil reservoirs, as well as for chemical and miscible flooding processes of reservoir fluids. This type of modeling, as against the black-oil simulation, is used when compositional variations are large, or when fluid properties are a strong function of phase compositions. Computationally speaking, these models take considerable amount of time to execute in comparison to black-oil models.

In shale reservoirs, compositional models are used to properly account for sorption processes of certain components, as well as modeling the diffusion process. These are also the models of choice when studying enhanced recovery processes. Alharthy et. al. (2013) used a DPDK compositional model to study phase behavior
changes associated with nanoporous shale materials. Wan et. al. (2014) evaluated the enhanced oil recovery process in shale reservoirs through cyclic gas injection using a compositional model, while Wan and Sheng (2015) analyzed the diffusion effects in gasflooding process in shale oil reservoirs.

**2.2 Grid Orientation Effects in Reservoir Simulation**

In this study, we have implemented ellipsoidal grids in order to properly model the flow geometry in the near-wellbore region. In essence, we are trying to reduce the numerical errors introduced when a particular grid is superimposed on the model, and when the grid axis are not aligned in the direction of flow. It is therefore essential to review the literature regarding different methods used to reduce this effect.

A grid is superimposed on the reservoir so that the fluid flow equations can be solved on them. Most commonly used approach of dividing the reservoir is to use block-centered grids, due to the fact that reservoir engineers find it easier to think of dividing the reservoir into discrete blocks (Aziz, 1993). However, Settari and Aziz (1972) had demonstrated that point-distributed grids would provide superior accuracy. The result of using different types of grids is more important where saturation/pressure changes are large. These changes are typically large near wellbore, where flow does not remain linear (or laminar), and the assumptions used in deriving fluid flow equations are violated. Thus, it would be logical to use different grid geometry as compared to that used in rest of the reservoir.
Further research in this area has resulted in use of local grid refinement, hybrid grids, voronoi grids, dynamic grids, etc. Each of these have their own advantages and disadvantages. Early research work in this aimed at providing solution to simple, homogenous problems. In such scenarios, the flow near the wellbore is radial-cylindrical (for vertical wells). The use of radial cylindrical grids alone partially solves the problem for single well systems. Due to reservoir heterogeneity, the flow does not always remain radial cylindrical. Nevertheless, these single well models are useful in numerical comparison against analytical solutions.

Next improvement in gridding technology came in the form of local grid refinement in Cartesian grids. Since the improvement in gridding solution is predominantly required in near-wellbore region, some authors (Quandalle and Besset, 1983; Heinemann et. al., 1983) have used Cartesian grid refinement within Cartesian grids. However, other studies (Nacul and Aziz, 1991) reveal that this method does not always improve solution, due to the requirement of accurate calculation of inter-block flow. To reduce these inaccuracies, hydrid grids are suggested, where radial-cylindrical grids are used for near-wellbore region, while Cartesian grids are used in far away reservoir region (Pedrosa and Aziz, 1986). This approach creates irregular grids at the intersection of the two regions, which requires special methods for calculating inter-block transmissibility terms. In addition, this approach reduces the grid block and consequently computational runtime requirements to achieve desired numerical accuracy. The authors compared the performance of their method with analytical solution with satisfactory accuracy.
Other authors have used voronoi grids to reduce grid orientation effects. A voronoi block is defined as the region of space closer to its gridpoint than to any other gridpoint (Aziz, 1993). Heinemann and his colleagues (Heinemann et. al., 1983) were the pioneers of this method, with Palagi and Aziz (Palagi and Aziz, 1991) later resolving some of the problems associated with heterogeneous reservoirs. Use of voronoi grids is particularly useful in modeling coning phenomenon in vertical horizontal wells (Aziz, 1993). Other advantages of these grids are that they can provide accurate computations for simulations of well tests in complex reservoirs, and also reduce the grid orientation effects. An example of voronoi grids is shown in Figure 2.2 below.

![Figure 2-2. Example of application of voronoi grids [Reproduced from Palagi and Aziz, 1994]](image)

Dynamic gridding is proposed to track the saturation and pressure changes along the sharp saturation front encountered during waterflooding or gasflooding operations. This technique relies on sub-dividing the gridblocks along a saturation front based on a
switching algorithm, while the rest of the reservoir still has the original, coarse grid system. Once the front moves forward, the fine gridblocks revert back to their original size, while new grid-blocks around saturation front are sub-divided. Ertekin and co-workers (Biterge and Ertekin, 1992; Shree and Ertekin, 1996; Kilic and Ertekin, 2003) applied this technique to study performance of horizontal wells and highly faulted reservoir architectures. They concluded that dynamic grids reduce the computational runtime by 100-200 folds as compared to finely refined grid system, and is comparable to conventional refined grid models. Recently, the application of this technique to field IOR/EOR problems was presented (Batenburg et. al., 2011, Hoteit and Chawathe, 2014). Such an example of dynamic gridding is presented in Figure 2.3.

![Figure 2-3. Example of dynamic gridding showcasing oil saturation contours with different pore volume injected [Reproduced from Hoteit and Chawathe, 2014]](image)

Orthogonal curvilinear grids are also used to reduce grid orientation effects. These grids are defined based on the streamlines and equipotential lines, which are mutually
orthogonal. Basically, when radial-cylindrical grids are used in near-wellbore region, we are essentially using curvilinear grids in order to properly match the fluid flow and potential geometry. In this case, the flow is radially inward, while the potentials are circular. Robertson and Woo (1978) studied the application of curvilinear grids to estimate the pattern flood performance, and concluded that curvilinear grid modeling can be easily implemented in available simulator codes with minimal modifications. When the reservoir geometry conforms with a particular curvilinear system, this forms another motivation for using curvilinear grids. Hirasaki and O’Dell (1970) investigated one such application where the coordinates are made to conform to the reservoir shape by specifying the coordinate surfaces to coincide with the reservoir boundaries. However, one limitation with their formulation was that the coordinate system presented was not orthogonal. If the orthogonality condition is satisfied, no additional terms are required beyond those defined for Cartesian grids (Aziz, 1993). In addition to reducing/eliminating grid orientation effects and improved modeling of reservoir geometries, a significant reduction in computational runtime was reported.

2.3 Modeling of Stimulated Reservoir Volume (SRV)

Hydraulic fracture modeling, and it’s incorporation in reservoir simulation, is a complex task. Figure 2.4 shows the fracture growth process. No single workflow exists for this process, and a lot of research is currently going on in this area in academia as well as industry. Earlier models utilized the concept of planar fractures to model the fracture network. However, Mayerhofer (2010) concluded that this approach is insufficient to
describe the stimulation performance in tight gas sand reservoirs. Current commercial simulators (CMG, 2014) also use planar fracture models, with locally refined grid systems in fractured zones. Various geo-mechanical models are also developed based on stress analysis of the fracturing region (Kresse et al., 2012; Al-Ajmi et al., 2011). However, these models need to be coupled with reservoir simulators in order to perform production analysis/forecasts, and this in itself is an arduous task.

Figure 2-4. Different levels of fracture complexity [Reproduced from Warpinski et al., 2008]

The other common approach followed in reservoir simulation is to use stimulated reservoir volume (SRV). SRV is a near-wellbore region that can be approximated by modifying the values of fracture permeability, fracture porosity and fracture spacing (Mayerhofer, 2010). The information from microseismic data is sometimes used to define the extent and volume of SRV. Fisher et al. (2002) were the first authors to propose SRV concept, and since then, a number of researchers have used this modeling approach in their simulation studies. The concept is also easy to incorporate in numerical simulators,
since the fracture properties are changed in the SRV zone. These properties are then modified during history matching process.

In this study, we implement ellipsoidal (or more specifically, prolate spheroidal coordinates) for modeling of hydraulically fractured shale reservoirs. Prolate spheroid is the surface formed when an ellipse (2D) is rotated about it’s major axis, with confocal hyperbolas intersecting the ellipsoidal surface. In such a coordinate surface, the ellipsoid represents the equi-potential and/or the outer boundary of SRV region, while the hyperbolas represent the flow streamlines. The underlying hypothesis is that the SRV region would essentially be defined as a rubble ellipsoidal zone. The microseismic data presented in various papers (Fisher et. al., 2004; Warpinski et. al., 2004) support this proposition. Lin and Ma (2015) have used this concept to best-fit an ellipsoid to the available microseismic data, in order to characterize the SRV volume properly. Their ellipsoidal representation of the microseismic data is shown in Figure 2.5 below. Also, microseismic data presented in Fisher et. al. (2004) and an imposed 2D ellipsoidal SRV region is shown in Figure 2.6.
Figure 2-5. Best fit ellipsoid for microseismic data and identified fractures [Reproduced after Lin and Ma, 2015]

Figure 2-6. 2D ellipsoidal fit to SRV region obtained from microseismic events [Reproduced from Fisher et al., 2004]
Numerical modeling of transverse fractures in horizontal wells have also shown that pressure transients essentially follow an elliptical path (Roney et al., 2014). In addition, the depletion profile of a horizontal well is ellipsoidal (Joshi, 1991), which further enhances the ellipsoidal nature of flow. This is shown in Figure 2.7 below. We therefore state that the use of prolate spheroidal coordinates would diminish the numerical dispersion effects associated with the modeling of hydraulically fractured wells in shales in the SRV zone as equipotential (ellipses) and streamlines (hyperbolas) describe the control volume.

![Figure 2-7. Schematic of vertical and horizontal well drainage areas (Joshi, 1991)](image)

**2.4 Modeling of Adsorption in Shales**

Adsorption accounts for close to 45% of the original gas in place, and its modeling is therefore important during development of a reservoir simulator for shale reservoirs. A number of thermodynamically-consistent and inconsistent methods have been used in the
industry to model the effects of adsorption. Majority of these models were developed for coalbed methane reservoirs, and have found their way into modeling of shale reservoirs as well. For multi-component systems, the most commonly used models include the Extended Langmuir (EL), Ideal Adsorbed Solution (IAS) theory, and Modified Vacancy Solution (MVS) (Clarkson and Haghshenas, 2013). The most preferred model for adsorption in commercial simulators is the EL model, which extends the single component Langmuir model to multi-component systems by accounting for their partial pressures and molar composition. Equation 2.1 below presents the EL model for multi-component systems (Arri et al., 1992).

\[
V_i = \frac{V_{Li} \cdot (P_g \cdot y_i)}{P_{Li} + \sum_j \frac{P_{Lj}}{P_{Li}} (y_j \cdot P_g)}
\] (2.1)

where:

- \(V_{Li}\) = Langmuir volume constant for pure component \(i\), (SCF/ton);
- \(P_{Li}\) = Langmuir pressure constant for pure component \(i\), (psia);
- \(y_i\) = Gas phase composition of component \(i\), (fraction);
- \(P_g\) = Gas phase pressure, (psia);
- \(V_i\) = Adsorbed volume of component \(i\), (SCF/ton).

As can be seen from the above equation, the implementation of the EL method is straight-forward, and this is the reason behind its extensive use. Clarkson and Haghshenas (2013) noted that this method is thermodynamically-inconsistent, since thermodynamic consistency states equal sorption limit for all components, which is violated by the EL model. On the other hand, this method works fine when compositional
effects are minimal, such as in coalbed methane reservoirs (where the majority of gas composition is methane). However, the method will be unreliable in shale gas reservoirs where large compositional changes are expected to take place during the primary depletion and enhanced recovery phases.

IAS theory was proposed by Myers and Prausnitz (1965), with the hypothesis that free gas and adsorbed gas phase equilibrium is similar to vapor-liquid equilibrium (VLE) (Manik, 1999). The theory had proposed two models: ideal adsorbed solution and real adsorbed solution. Ideal adsorbed model assumes that the adsorbed phase behaves as ideal solution, while real adsorbed solution introduces non-ideality correction factor through activity coefficients. However, Stevenson et al. (1991) compared the performance of both methods for adsorption on coal samples, and concluded that no significant improvement was obtained when using real adsorbed model over IAS. After derivation (which is neglected at this point), Equation 2.2 describes the thermodynamic equilibrium between adsorbed and free gas phases using the ideal adsorbed phase assumption (Manik, 1999).

\[
P_g \cdot y_i \cdot \phi_i = P_i^0 \cdot \phi_i^0 \cdot x_i^i
\]  

(2.2)

where:

- \( P_g \) = Gas phase pressure, (psia);
- \( y_i \) = Gas phase composition of component \( i \), (fraction);
- \( \phi_i \) = Fugacity coefficient of pure component \( i \) in gas phase, (dimensionless);
- \( P_i^0 \) = Standard state pressure of pure component \( i \) in gas phase, (psia);
\( \phi_i^\theta \) = Fugacity coefficient of pure component \( i \) in gas phase at standard state condition, (dimensionless);

\( x_i^a \) = Molar composition of component \( i \) in adsorbed phase, (fraction);

IAS requires implementation of pure component isotherms, which can be obtained either through Langmuir, Toth or UNILAN isotherms.

Vacancy solution/Potential theory hybrid model was proposed by Clarkson (2003). The model treats the components in the adsorbed solution as mixture of a hypothetical solvent (i.e. vacancy), with adsorbate species. The equilibrium gaseous phase is also thought to be composed of these components. Thus, we treat the two phases as two vacancies, the equilibrium between them is established through multi-component VLE computations. Non-ideality in adsorbed phase is accounted for by defining activity coefficient in adsorbed phase. The model proposed by Clarkson was not the original one, rather it was a modification of the earlier models presented by Cochran and co-workers (1985). Other rigorous adsorption models are 2D-EOS model (Zhou et al., 1994) and Simplified Local Density (SLD) model (Chareonsuppanimit et al., 2012). However, these models have found limited application in commercial models due to their complexity.

Adsorption modeling in case of two hydrocarbon phases (liquid and vapor) has found little attention so far, primarily because of limited field applications. However, due to emergence of hydraulic fracturing and horizontal wellbore drilling, production from liquid-rich shales has become economically possible. It is therefore of utmost importance to model adsorption in a thermodynamically consistent way. Clarkson and Haghshenas (2013) have acknowledged that there have been relatively fewer studies of heavy hydrocarbon sorption in shales. Whitson and Sunjerga (2012) stressed that sorption
modeling in liquid-rich shale formations requires further investigation. Recently, Haghshenas et al. (2014) themselves used extended Langmuir approach to investigate the importance of sorption phenomenon on fluid production and recovery from liquid-rich shales. Other studies (Lei et al., 2014; Xiong et al., 2015) even completely ignore the adsorption effects while performing numerical simulation studies. These deficiencies were, therefore, the driving force behind constructing a thermodynamically-consistent adsorption model for liquid-rich shales, with the aim of keeping the model as simple as possible. In Chapter 5, we present the development of such a model using the IAS theory, which was previously implemented in Penn State’s coalbed and shale gas simulators, PSU-COALCOMP (Aslan, 2013) and PSU-SHALECOMP (Kulga, 2014), respectively.

2.5 Modeling of Diffusion Phenomenon in Shales

Basic fluid flow equations in any physical phenomena are derived by combining continuity equations with some form of momentum equation representing the flow in that particular medium. In porous media, it is Darcy’s law that represents the connection between flow rate and potential gradients, and is combined with continuity equation to then provide flow equations in petroleum reservoir engineering. However, when permeability is in the order of micro- to nano-darcies, potential gradient (i.e. Darcy’s law) alone might not be responsible for flow, and concentration gradient may play an important role in driving fluid movement. Ertekin et al. (1986) proposed that in tight systems (permeability < 0.1 md), fluid flow due to concentration gradient (or Fick’s law) may be representing the primary flow mechanism, ahead of Darcy’s law. This
formulation is known as *Multi-mechanistic*, and the two gradient fields: pressure and concentration act in parallel (such that their flow velocities are additive) (Ertekin et al., 1986).

da Silva and Belery (1989) stated that diffusion can be important recovery mechanism for naturally fractured reservoirs. Their conclusions were supported by single matrix block studies and multi-component experiments. Since then, a number of studies have addressed the effect and importance of diffusion in fractured reservoirs. Lenormand et al. (1998) modeled the diffusion flux between matrix and fracture domain, and found good agreement with experimental results. Darvish et al. (2006) performed experimental and numerical study of CO$_2$ injection into fractured cores, illustrating the importance of diffusion. Ayala et al. (2006) investigated the role of diffusion in hydrocarbon recovery in naturally fractured, gas-condensate reservoirs. They found out that due to condensate dropout, gas flowing capability is impaired at the edges of matrix blocks, and diffusion can be important in recovering the fluid stored deep inside matrix blocks. Hoteit and Firoozabadi (2009) applied multi-mechanistic flow concept for studying gas injection and recycling schemes in fractured media. Ghorayeb et al. (2003) explained the unusual distribution of hydrocarbon fluid in Yufutsu field, Japan, where heavy fluid mixture floated on top of light mixture, on the basis of thermal diffusion effects. Recently, Wan and Sheng (2015) performed compositional modeling studies for gasflooding EOR operation in shale oil reservoirs. The authors concluded that diffusional mass transfer at matrix-matrix and matrix-fracture interfaces would determine the recovery efficiency of such EOR process.
Another important aspect during modeling of diffusion, is the calculation of diffusion coefficients. Sigmund (1976) measured the coefficient values in binary fluid systems, and proposed an equation to predict binary diffusion coefficients. Wilke and Chang (1955) presented correlations for predicting liquid phase diffusion coefficients. Commercial simulators such as CMG (CMG, 2014) use these correlations to calculate gas and liquid phase diffusion coefficients, respectively. Hoteit and Firoozabadi (2009) state that most of the multi-component diffusion coefficient correlations are mainly based on data for binary diffusion coefficients, and may not follow thermodynamic stability considerations. Also, the coefficient values may not hold valid at reservoir pressure and temperature conditions (Ghorayeb and Firoozabadi, 2000). Leahy-Dios and Firoozabadi (2007) presented a unified model for calculating coefficient values for non-ideal gas and liquid multicomponent mixtures. Comparison with experimental data showed that their model predictions were superior to that by Sigmund and Hayduk-Minhas. Others (Ayala et al., 2006) have used an effective value for diffusion coefficient, where the effect of molecular and Knudsen diffusion are lumped together.

In this work, we are using an alternate formulation for calculating the diffusional flux. This formulation is based on the work by Moortgat and Firoozabadi (2013), where the diffusional flux is proportional to gradient in chemical potential rather than gradient in molar concentration (as originally stated by Fick’s law). Although both formulations are mathematically equivalent, the newer approach is consistent in definition of diffusional flux in cases where there is phase discontinuity across grid boundaries and/or matrix-fracture interface. Such conditions are expected to occur in under-saturated shale reservoirs, where fractures may contain two-phasic hydrocarbon fluid while the adjacent
matrix might be under-saturated oil. Details about this method, as well as the equations for calculating diffusion coefficients, are presented in Chapter 5.

2.6 Pore Proximity Effects in Shales

Phase behavior of fluids under pore or wall confinement is different than that in bulk, unconfined conditions. Since shale pores are of the order of few nanometers, the pore confinement effects are expected to change fluid behavior in shale pores, and this topic has attracted lot of interest among shale researchers recently. Here, we briefly review some of the important contributions in this area, however, pore proximity effects are not modeled in our research work.

Studies on pore proximity-affected phase behavior are not new, and have been studied before in chemical engineering fields. Gelb et al. (1999) state that the introduction of wall forces, and enhanced fluid-wall and fluid-fluid interactions lead to surface-driven changes which are responsible for phase behavior modifications. Conventional PVT modeling in oil and gas industry did not have to deal with such effects, since fluid behavior in micro- and meso-pores is similar to the one in bulk, unconfined conditions. However, due to hydrocarbon production from nanoporous shales, modifications to the PVT modeling are therefore necessary and important. It has been shown through a number of theoretical studies (Singh et al., 2009; Firincioglu et al., 2012) that pore sizes in the range of 2 to 50 nm can cause a significant shift in phase behavior of reservoir fluids. Although Wang et al. (2014) presented the results of nanoconfinement on phase behavior, their experiments were conducted for much larger
(100 nm) pores, while the theoretical studies reveal that effect would be observed only for pores less than ~50 nm. Thus, a conclusive experimental and numerical validation is yet to be provided for this effect.

The ongoing research on quantifying the effects of pore proximity seems to be divided into two main methods:

- Modifications of critical properties (temperatures and pressures) as a function of pore size and molecular diameters (Sanaei et al., 2014)
- Inclusion of capillary pressure in vapor-liquid equilibrium calculations (Firincioglu et al., 2012; Nojabaei et al., 2013)

Others (Teklu et al., 2014) have combined the two approaches and presented their results. Figure 2.8 presents the phase envelope shift caused when either critical property method or both methods are applied in PVT equilibrium calculations. Certain other studies (Wang et al., 2013; Sanaei et al., 2014) have implemented either one of the two methods in compositional reservoir simulation models, and have reported their analysis. For commercial simulators, it is possible to include the method of modifying critical properties only. Current research at Penn State involves deployment of the capillary pressure approach to model this effect (Siripatrachai, 2014). Nevertheless, it is critical to validate both models with experimental findings before their deployment in reservoir simulators.
Figure 2-8. Phase envelope shift for different nanopore sizes (From Teklu et al., 2014)
Chapter 3

Problem Statement

The principal objective of this research is to develop a compositional reservoir simulator designed specifically for liquid-rich shale reservoirs. Modeling unconventional resources presents different challenges to reservoir simulator developer. Fluid storage mechanism such as adsorption and flow mechanism such as diffusion are extremely important in very tight shale reservoirs, as explained in literature review in previous chapter. Additionally, the production profile, at the least in the early production period, is dependent heavily on the definition and modeling of hydraulically fractured zone. All of these concepts, therefore, require a detailed attention on the part of modeling scientist.

The following questions were thought to be answered through this particular research study:

i. What is the best possible option to model stimulated reservoir volume zone? How important are grid orientation effects, and how do these effects be minimized?

ii. In view of current status of modeling adsorption in shales, what can be done to account for this important storage mechanism in liquid-rich formations?

iii. Are diffusion processes important in shale reservoirs? If so, what impact do they have on production profiles and ultimate recoveries? Is there a
better approach available to model diffusion coefficients and consequently, the diffusion flux equation itself?

iv. Is there a way to accommodate geochemical data obtained during exploration process into reservoir simulation study?

In order to address the first question, we implemented ellipsoidal grids in the near-wellbore region to properly model the flow geometry in fractured zone. Horizontal wells, when placed in homogenous reservoirs, effectively generate ellipsoidal flow geometry around its wellbore length. Additionally, the fractured zone is thought to create an ellipsoidal structure by itself, as supported from micro-seismic data presented in various literature papers. This will further enhance the ellipsoidal nature of flow around wellbore. It is therefore appropriate to implement ellipsoidal grids in and around the fractured zone, where equi-potentials and streamlines are confocal ellipses and hyperbolas, respectively. Comparison of numerical solution for horizontal well in homogenous, unstimulated reservoir with analytical solution presented in literature results in good agreement between the two solutions. Also, other advantage of using these curvilinear grids is that the number of gridblock requirement decreases substantially, since grid orientation effects are reduced. This is observed when comparing the numerical solutions for ellipsoidal and Cartesian grid systems, where gridblock requirement is lower for ellipsoidal coordinates for similar level of accuracy.

Due to inadequacy of current simulators to model adsorption in liquid-rich formations, a new formulation is developed for adsorption in such cases. The model is thermodynamically consistent, and uses ideal adsorbed solution (IAS) theory in calculation of vapor phase adsorption values from pure component adsorption data.
Standalone examples are shown that present the calculation procedure for a four-component reservoir fluid are shown. The examples also present the parametric analysis with respect to certain important adsorption parameters. Finally, the new algorithm is implemented in simulation code, with parametric analysis shown later.

Current diffusion modeling capability in PSU-SHALECOMP is to use an effective diffusion coefficient value, which is used as a parameter for parametric analysis. However, thermodynamics dictates that diffusion coefficient values are a function of pressure, temperature, and fluid composition, and therefore need to be dynamically calculated during simulation runs. We have implemented the procedure suggested by Ghorayeb and Firoozabadi (2000) to calculate the diffusion coefficient values. Furthermore, the conventional approach of defining diffusional flux based on composition gradient (Fick’s law) fails to provide consistent results in problems where phase discontinuity occurs either in matrix-matrix or matrix-fracture domains. This inconsistency is removed by implementing a mathematically-equivalent formulation for diffusion flux based on chemical potential gradient. Examples are presented that illustrate the advantages of this approach as against the old approach in resolving these issues.

Finally, a geochemical model is prepared based on conventionally used geochemical parameters. This model acts as a precursor for simulation cases, where the user can provide geochemical information such as total organic carbon content (TOC), maximum paleo-temperature reached during deposition, hydrogen index, and transformation potential. These parameters are routinely obtained during any exploration phase of an oil and gas project. The precursor will calculate the overall fluid composition based on transformation ratio of the organic matter, in addition to adjusting the Langmuir
volume and pressure constants (which are found to be varying with TOC content). Once fluid composition and Langmuir parameters are obtained, they are then fed into reservoir simulation dataset. The advantage of using the precursor is to perform an integrated simulation study, taking into account the geochemical information of that particular reservoir/field.

Table 3.1 summarizes the important capabilities of PSU-SHALECOMP (Kulga, 2014) and our proposed model.

**Table 3-1. A comparison of existing and proposed model capabilities**

<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>Dual-porosity, dual-permeability model</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Three-phase modeling</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Adsorption in dry gas shales</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Adsorption in liquid-rich shales</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Multi-mechanistic gas flow mechanism</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Multi-mechanistic liquid flow mechanism</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Curvilinear grids</td>
<td>No</td>
<td>Yes</td>
</tr>
</tbody>
</table>
Chapter 4
Development of Numerical Model

In this chapter, the mathematical equations representing multi-mechanistic flow in shale porous media are presented. The equations are shown for a dual-porosity, dual-permeability, naturally fractured system. Three-phase (oil-gas-water) flow is considered in the presence of viscous, capillary, and gravitational forces. First, flow equations for Cartesian coordinates are presented, followed by the equations for prolate spheroidal coordinates. This is followed by the finite difference approximation, and writing the residual equations. Next, the calculation of transmissibility terms is presented. Equations for explicit (well definitions) and implicit (matrix-fracture transfer function) source/sink terms are shown. Finally, implementation of Generalized Newton-Raphson (GNR) protocol is outlined.
4.1 Governing Equations

4.1.1 Cartesian Coordinates

The generalized form of $m^{th}$ component conservation equation for fracture domain can be written as follows:

$$
\frac{\partial}{\partial x} \left[ x_m \rho_o A_x \frac{k_F^F k_{ro}^F}{\mu_o^F} \partial \phi_o^F + y_m \rho_g A_x \frac{k_F^F k_{rg}^F}{\mu_g^F} \partial \phi_g^F \right] \Delta x
$$

$$
+ \frac{\partial}{\partial y} \left[ x_m \rho_o A_y \frac{k_F^F k_{ro}^F}{\mu_o^F} \partial \phi_o^F + y_m \rho_g A_y \frac{k_F^F k_{rg}^F}{\mu_g^F} \partial \phi_g^F \right] \Delta y
$$

$$
+ \frac{\partial}{\partial z} \left[ x_m \rho_o A_z \frac{k_F^F k_{ro}^F}{\mu_o^F} \partial \phi_o^F + y_m \rho_g A_z \frac{k_F^F k_{rg}^F}{\mu_g^F} \partial \phi_g^F \right] \Delta z
$$

$$
+ M_m + \left( 379.6 \times 5.615 \right) = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left[ \phi^F \left( S_o x_m \rho_o^F + S_g y_m \rho_g^F \right) \right];
$$

$$
m = 1, 2, 3, ..., n_c
$$

(4.1)
Similarly, we can write the $m^{th}$ component conservation equation for matrix domain as follows:

$$
\begin{align*}
\frac{\partial}{\partial x}
&= \left[ x_m \frac{\rho_o^M}{\rho_o^M} A_x \frac{k^M_{x} k^M_{ro}}{\mu_o^M} \frac{\partial \Phi^M_{o}}{\partial x} + y_m \frac{\rho_g^M}{\rho_g^M} A_x \frac{k^M_{x} k^M_{rg}}{\mu_g^M} \frac{\partial \Phi^M_{g}}{\partial x} \right] \\
&+ \phi^M S_o^M \frac{\rho_o^M}{\rho_o^M} A_x \frac{5.615}{5.615} \left( \sum_{i,j=1}^{n_c} \beta_{o,i,comp} \cdot x_{m,comp} \cdot \frac{\partial \mu_{comp}}{\partial x} \right) \Delta x \\
&+ \phi^M S_g^M \frac{\rho_g^M}{\rho_g^M} A_x \frac{5.615}{5.615} \left( \sum_{i,j=1}^{n_c} \beta_{g,i,comp} \cdot y_{m,comp} \cdot \frac{\partial \mu_{comp}}{\partial x} \right) \Delta y \\
&+ \phi^M S_o^M \frac{\rho_o^M}{\rho_o^M} A_y \frac{5.615}{5.615} \left( \sum_{i,j=1}^{n_c} \beta_{o,i,comp} \cdot x_{m,comp} \cdot \frac{\partial \mu_{comp}}{\partial y} \right) \\
&+ \phi^M S_g^M \frac{\rho_g^M}{\rho_g^M} A_y \frac{5.615}{5.615} \left( \sum_{i,j=1}^{n_c} \beta_{g,i,comp} \cdot y_{m,comp} \cdot \frac{\partial \mu_{comp}}{\partial y} \right) \\
&+ \phi^M S_o^M \frac{\rho_o^M}{\rho_o^M} A_z \frac{5.615}{5.615} \left( \sum_{i,j=1}^{n_c} \beta_{o,i,comp} \cdot x_{m,comp} \cdot \frac{\partial \mu_{comp}}{\partial z} \right) \\
&+ \phi^M S_g^M \frac{\rho_g^M}{\rho_g^M} A_z \frac{5.615}{5.615} \left( \sum_{i,j=1}^{n_c} \beta_{g,i,comp} \cdot y_{m,comp} \cdot \frac{\partial \mu_{comp}}{\partial z} \right) \\
&+ M_{ads,m} + \frac{\Gamma_m^M}{(379.6 \times 5.615)} \\
&= \frac{V_b}{5.615} \frac{\partial}{\partial t} \left[ \phi^M \left( S_o^M x_m^M \rho_o^M + S_g^M y_m^M \rho_g^M \right) \right]; \quad m = 1, 2, 3..., n_c \\
\end{align*}
$$

(4.2)

Equations (4.1) and (4.2) differ quite markedly from each other. Even though each domain has their own permeability values, matrix equations have to account for diffusive flux as well as source/sink terms due to sorption process. We are taking into
account multi-mechanistic formulation for both, oil and gas phases. The flow between matrix and fracture domain is modeled through the definition of transfer function ($\Gamma$).

The mass conservation equation for water in fracture domain can be written as:

$$
\frac{\partial}{\partial x} \left[ \frac{A_x k_x^F k_{rw}^F}{\mu_w B_w^F} \frac{\partial \Phi_w^F}{\partial x} \right] \Delta x + \frac{\partial}{\partial y} \left[ \frac{A_y k_y^F k_{rw}^F}{\mu_w B_w^F} \frac{\partial \Phi_w^F}{\partial y} \right] \Delta y + \frac{\partial}{\partial z} \left[ \frac{A_z k_z^F k_{rw}^F}{\mu_w B_w^F} \frac{\partial \Phi_w^F}{\partial z} \right] \Delta z 
+ q_{w,STB/day} + \Gamma_w^F = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left[ \frac{\phi^F S_w^F}{B_w^F} \right];
$$

(4.3)

and similarly, we can write the water conservation equation in matrix domain as:

$$
\frac{\partial}{\partial x} \left[ \frac{A_x k_x^M k_{rw}^M}{\mu_w B_w^M} \frac{\partial \Phi_w^M}{\partial x} \right] \Delta x + \frac{\partial}{\partial y} \left[ \frac{A_y k_y^M k_{rw}^M}{\mu_w B_w^M} \frac{\partial \Phi_w^M}{\partial y} \right] \Delta y + \frac{\partial}{\partial z} \left[ \frac{A_z k_z^M k_{rw}^M}{\mu_w B_w^M} \frac{\partial \Phi_w^M}{\partial z} \right] \Delta z 
+ \Gamma_w^M = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left[ \frac{\phi^M S_w^M}{B_w^M} \right];
$$

(4.4)

The fluid flow potentials can be related to the phase pressures as follows:

$$
\Phi^\alpha = P^\alpha - \frac{1}{144} \frac{g}{g_c} \rho^\alpha G; \quad \alpha = matrix, fracture, \quad \lambda = oil, gas, water
$$

(4.5)

While deriving these equations, we invoke the following assumptions:

- The naturally-fractured shale system is represented by the idealized sugar-cube model,
- The reservoir in its entirety is modeled using ellipsoidal coordinates. The inner rubble zone as well as the outer original reservoir are modeled in these
coordinates. This assumption is considered to be valid based on the fact that there will be negligible flow from original reservoir during the production life of a well, and the pressure transients will not reach the outer boundaries of the reservoir. Thus, a hybrid grid system is not considered here,

- Flow to wellbore only takes place through fracture system, with matrix blocks acting as implicit source/sink terms,
- Inter-porosity transfer term accounts for flow between matrix and fractures,
- Hydrodynamic communication exists between two matrix blocks (i.e. DPDK model),
- Isothermal conditions exist in reservoir,
- Flow of water is governed by Darcy’s law, while hydrocarbon fluid phases follow Darcy’s as well as Fick’s law,
- Water is always present in reservoir, with single- or two-phase conditions existing in hydrocarbon fluids,
- There is no solution gas in water phase, and water does not exist in any of the hydrocarbon phases. Water also does not interfere with thermodynamics of hydrocarbon fluids,
- No-flow outer boundary is considered,
- Pressure dependency of permeability is neglected,
- Pore compressibility effects are not taken into consideration.
4.1.2 Prolate Spheroidal Coordinates

As stated in Chapter 2 earlier, ellipsoidal coordinates are used in near-wellbore region, in order to properly model the flow geometry. Flow geometry is predominantly ellipsoidal, due to production profile generated by horizontal wells, as well as due to the physical ellipsoidal region generated in SRV. In addition to writing the conservation equations in ellipsoidal coordinates, permeability transformation is also required to generate accurate results. In this sub-section, we present the equations derived for this coordinate system. However, before the generalized forms for conservation equations are presented, a basic review of prolate spheroidal coordinates is given here.

Figure 4.1 shows a three-dimensional view of a prolate spheroid. According to Moon and Spencer (1961), prolate spheroidal coordinates are generated by rotating an orthogonal family of confocal ellipses and hyperbolas about the major axis of the ellipses. Alternatively, when confocal ellipses and hyperbolas are rotated about the minor axis of the ellipse, we form oblate spheroidal coordinates. Since the nature of flow geometry around the horizontal well as well as the physical shape of the rubble zone is such that the use of prolate spheroid is more appropriate. The 2D mapping in y-z plane is shown in Figure 4.2.
Figure 4-1. 3D view of a prolate spheroid (Reproduced from Wolfram Mathematica, 2015)

Figure 4-2. 2D view of the prolate spheroid in y-z plane (Reproduced from Wolfram Mathematica, 2015)

Prolate spheroidal coordinates \((\xi, \eta, \psi)\) are related to Cartesian coordinates as follows:
\[
\begin{align*}
\begin{cases}
x &= d \cdot \sinh \xi \cdot \sin \eta \cdot \cos \psi, \\
y &= d \cdot \sinh \xi \cdot \sin \eta \cdot \sin \psi, \\
z &= d \cdot \cosh \xi \cdot \cos \eta
\end{cases}
\end{align*}
\] (4.6)

The variable \(\xi\) has a range from 0 to \(+\infty\). A constant value for this variable forms an ellipsoid. In equations 4.6 above, \(d\) represents the focal length of this ellipse. To relate this to our physical problem, \(d\) would represent the half-wellbore length of the horizontal well. When \(\xi\) is 0, the ellipse would collapse into a straight line. On the other hand, as \(\xi\) increases, the ellipse approximates into a sphere. While modeling this coordinate, the values of \(\xi\) would be limited by the physical location of horizontal well as the inner limit, while the extent of SRV would justify the outer limit. At the inner limit, the innermost equipotential ellipse represents the horizontal well, since we are ignoring the pressure drop inside the horizontal wellbore.

The surfaces of constant \(\eta\) are hyperboloids of two sheets (Moon and Spencer, 1961). Basically, \(\eta\) is the angle between the asymptotic cone of the hyperboloid and the \(z\)-axis. This variable can take values between 0 to \(\pi\). For \(\eta = 0\), the cone of hyperbolas degenerate into the portion of \(z\)-axis from \(+d\) to \(+\infty\). Similarly, when \(\eta = \pi\), we get \(z\)-axis from \(-d\) to \(-\infty\). \(\eta = \pi/2\) reduces the hyperbolas into \(xy\)-plane.

\(\psi\) is the angle measured about the \(z\)-axis. Constant values of \(\psi\) are half-planes containing the \(z\)-axis. This variable ranges from 0 to \(2\pi\).

We now present the conservation equations in prolate spheroidal coordinates, starting with the generalized form of \(m^{th}\) component conservation equation for fracture domain:
\[
\frac{\partial}{\partial \xi} \left\{ \frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left[ x_m^F \rho_o^F A \frac{k^F}{\mu_o^F} \frac{\partial \Phi^F}{\partial \xi} + y_m^F \rho_g^F A \frac{k^F}{\mu_g^F} \frac{\partial \Phi^F}{\partial \xi} \right] \right\} \Delta \xi
\]
\[
+ \frac{\partial}{\partial \eta} \left\{ \frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left[ x_m^F \rho_o^F A \frac{k^F}{\mu_o^F} \frac{\partial \Phi^F}{\partial \eta} + y_m^F \rho_g^F A \frac{k^F}{\mu_g^F} \frac{\partial \Phi^F}{\partial \eta} \right] \right\} \Delta \eta
\]
\[
+ \frac{\partial}{\partial \psi} \left\{ \frac{1}{d \cdot \sinh \xi \cdot \sin \eta} \left[ x_m^F \rho_o^F A \frac{k^F}{\mu_o^F} \frac{\partial \Phi^F}{\partial \psi} + y_m^F \rho_g^F A \frac{k^F}{\mu_g^F} \frac{\partial \Phi^F}{\partial \psi} \right] \right\} \Delta \psi
\]
\[
+ \frac{\Gamma_m^F}{(379.6 \times 5.615)} = \frac{V_b}{5.615} \frac{\partial}{\partial t} \left[ \phi^F \left( S_o^F x_m^F \rho_o^F + S_g^F y_m^F \rho_g^F \right) \right];
\]
\[
m = 1, 2, 3, ..., n_c
\]
(4.7)

If we compare Eqs. 4.1 and 4.7, the right hand side terms are the same. The reason behind this development is that, the right hand side terms represent the accumulation (or depletion) taking place in a particular gridblock. The variables inside this term are independent of the shape and size of the gridblock. However, the explicit source/sink term is missing from left hand side of Equation 4.7. Since the coordinate system matches the flow geometry, the production or injection rates will be calculated as inner boundary conditions for this coordinate system. This development is similar to modeling single vertical well performance with radial-cylindrical coordinates, where flow rates are calculated through inner boundary conditions. In essence, we also eliminate the need for defining Peaceman’s equation, which relates flow rate with flowing bottom-hole pressure and well block pressure.

Similarly, we can write the \(m^{th}\) conservation equation for matrix domain as follows:
The mass conservation equation for water in fracture domain for prolate spheroidal coordinates can be written as:

\[
\frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left\{ \begin{align*}
\frac{\partial}{\partial \xi} & \left[ x_m \rho_o A_{\xi} \frac{k_m^M k_{ro}^M}{\mu_o^M} \frac{\partial \Phi_o^M}{\partial \xi} + y_m \rho_g A_{\xi} \frac{k_m^M k_{rg}^M}{\mu_g^M} \frac{\partial \Phi_g^M}{\partial \xi} \right] \\
+ & \phi^M S_o \frac{A_{\xi}}{5.615} \left( \sum_{\text{comp}=1}^{n-1} \beta_{o,\text{comp}} \cdot x_{m,\text{comp}} \cdot \frac{\partial \mu_{\text{comp}}}{\partial \xi} \right) \\
+ & \phi^M S_g \frac{A_{\xi}}{5.615} \left( \sum_{\text{comp}=1}^{n-1} \beta_{g,\text{comp}} \cdot y_{m,\text{comp}} \cdot \frac{\partial \mu_{\text{comp}}}{\partial \xi} \right) \\
\right\} \Delta \xi
\]

\[
\frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left\{ \begin{align*}
\frac{\partial}{\partial \eta} & \left[ x_m \rho_o A_{\eta} \frac{k_m^M k_{ro}^M}{\mu_o^M} \frac{\partial \Phi_o^M}{\partial \eta} + y_m \rho_g A_{\eta} \frac{k_m^M k_{rg}^M}{\mu_g^M} \frac{\partial \Phi_g^M}{\partial \eta} \right] \\
+ & \phi^M S_o \frac{A_{\eta}}{5.615} \left( \sum_{\text{comp}=1}^{n-1} \beta_{o,\text{comp}} \cdot x_{m,\text{comp}} \cdot \frac{\partial \mu_{\text{comp}}}{\partial \eta} \right) \\
+ & \phi^M S_g \frac{A_{\eta}}{5.615} \left( \sum_{\text{comp}=1}^{n-1} \beta_{g,\text{comp}} \cdot y_{m,\text{comp}} \cdot \frac{\partial \mu_{\text{comp}}}{\partial \eta} \right) \\
\right\} \Delta \eta
\]

\[
\frac{1}{d \cdot \sinh \xi \cdot \sin \eta} \left\{ \begin{align*}
\frac{\partial}{\partial \psi} & \left[ x_m \rho_o A_{\psi} \frac{k_m^M k_{ro}^M}{\mu_o^M} \frac{\partial \Phi_o^M}{\partial \psi} + y_m \rho_g A_{\psi} \frac{k_m^M k_{rg}^M}{\mu_g^M} \frac{\partial \Phi_g^M}{\partial \psi} \right] \\
+ & \phi^M S_o \frac{A_{\psi}}{5.615} \left( \sum_{\text{comp}=1}^{n-1} \beta_{o,\text{comp}} \cdot x_{m,\text{comp}} \cdot \frac{\partial \mu_{\text{comp}}}{\partial \psi} \right) \\
+ & \phi^M S_g \frac{A_{\psi}}{5.615} \left( \sum_{\text{comp}=1}^{n-1} \beta_{g,\text{comp}} \cdot y_{m,\text{comp}} \cdot \frac{\partial \mu_{\text{comp}}}{\partial \psi} \right) \\
\right\} \Delta \psi
\]

\[
+ M_{\text{ads,m}} + \frac{\Gamma^M_m}{(379.6 \times 5.615)}
\]

\[
= \frac{V_o}{5.615} \frac{\partial}{\partial t} \left[ \phi^M \left( S_o x_m \rho_o^M + S_g y_m \rho_g^M \right) \right] ; \quad m = 1, 2, 3, ..., n_c
\]

(4.8)
\[
\begin{align*}
\frac{\partial}{\partial \xi} \left\{ \frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left[ A_{\xi} k^F_{\xi} k^F_{rw} \frac{\partial \Phi^F_w}{\partial \xi} \right] \right\} & \Delta \xi \\
+ \frac{\partial}{\partial \eta} \left\{ \frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left[ A_{\eta} k^F_{\eta} k^F_{rw} \frac{\partial \Phi^F_w}{\partial \eta} \right] \right\} & \Delta \eta \\
+ \frac{\partial}{\partial \psi} \left\{ \frac{1}{d \cdot \sinh \xi \cdot \sin \eta} \left[ A_{\psi} k^F_{\psi} k^F_{rw} \frac{\partial \Phi^F_w}{\partial \psi} \right] \right\} & \Delta \psi \\
+ \Gamma^F_w & = \frac{V_b}{5.615 \frac{\partial}{\partial t}} \left[ \frac{\phi^F S^F_w}{B^F_w} \right];
\end{align*}
\]

(4.9)

And finally, we can write the water conservation equation in matrix domain for prolate spheroidal coordinates as:

\[
\begin{align*}
\frac{\partial}{\partial \xi} \left\{ \frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left[ A_{\xi}^M k^M_{\xi} k^M_{rw} \frac{\partial \Phi^M_w}{\partial \xi} \right] \right\} & \Delta \xi \\
+ \frac{\partial}{\partial \eta} \left\{ \frac{1}{d \cdot \sqrt{\cosh^2 \xi - \cos^2 \eta}} \left[ A_{\eta}^M k^M_{\eta} k^M_{rw} \frac{\partial \Phi^M_w}{\partial \eta} \right] \right\} & \Delta \eta \\
+ \frac{\partial}{\partial \psi} \left\{ \frac{1}{d \cdot \sinh \xi \cdot \sin \eta} \left[ A_{\psi}^M k^M_{\psi} k^M_{rw} \frac{\partial \Phi^M_w}{\partial \psi} \right] \right\} & \Delta \psi \\
+ \Gamma^M_w & = \frac{V_b}{5.615 \frac{\partial}{\partial t}} \left[ \frac{\phi^M S^M_w}{B^M_w} \right];
\end{align*}
\]

(4.10)
4.2 Auxiliary Equations

In defining the conservation equations (Eqs. 4.1 to 4.4 for Cartesian coordinates, or Eqs. 4.7 to 4.10 for prolate spheroidal coordinates), a total of \((2n_c + 12)\) unknowns are also defined. These include

\[ P_o^F, P_o^M, P_g^F, P_g^M, P_w^F, P_w^M, S_o^F, S_o^M, S_g^F, S_g^M, S_w^F, S_w^M, z_1^F, z_2^F, \ldots, z_{nc}^F, z_1^M, z_2^M, \ldots, z_{nc}^M. \]

However, out of these, we select a set of primary unknowns that will be solved using the linearized form of conservation equations. In this work, we have selected the following primary set of variables (Ayala, 2004):

- Gas phase pressure in fracture and matrix, \( P_g^F, P_g^M \);
- Water saturation in fracture and matrix, \( S_g^F, S_g^M \);
- Overall molar composition of \((n_c-1)\) components in fracture and matrix,

\[ z_1^F, z_2^F, \ldots, z_{nc-1}^F, z_1^M, z_2^M, \ldots, z_{nc-1}^M. \]

The remaining unknowns are calculated using auxiliary equations, which are a set of fixed equations and whose functional values are dependent on the above primary unknowns. We therefore define 10 such equations using thermodynamic relationships, capillary pressure relationships, saturation constraints, and mole fraction constraints for fracture and matrix domains as follows:

i) \[ \text{Mole fraction constraints} \]

\[ z_{n_c}^F = 1 - \sum_{i=1}^{n_c-1} z_i^F; \]

\[ z_{n_c}^M = 1 - \sum_{i=1}^{n_c-1} z_i^M. \]

(4.11)
ii) Thermodynamic relationships

Using the Peng-Robinson equation-of-state (PR-EOS), one can calculate the equilibrium molar vapor fraction \( f_{ng} \). This molar vapor fraction, along with water saturation, can be used to determine the oil phase saturation as:

\[
\begin{align*}
S_a^F &= \frac{\rho_g^F (1 - f_{ng}^F)}{\rho_o^F f_{ng}^F + \rho_g^F (1 - f_{ng}^F)} \cdot (1 - S_w^F); \\
S_a^M &= \frac{\rho_g^M (1 - f_{ng}^M)}{\rho_o^M f_{ng}^M + \rho_g^M (1 - f_{ng}^M)} \cdot (1 - S_w^M);
\end{align*}
\]

\[ (4.12) \]

iii) Saturation constraints

\[
\begin{align*}
S_o^F &= 1 - S_o^F - S_w^F; \\
S_o^M &= 1 - S_o^M - S_w^M.
\end{align*}
\]

\[ (4.13) \]

iv) Capillary pressure constraints

\[
\begin{align*}
P_{cgo}^F &= P_g^F - P_o^F; \\
P_{cgo}^M &= P_g^M - P_o^M; \\
P_{cog}^F &= P_o^F - P_w^F; \\
P_{cog}^M &= P_o^M - P_w^M.
\end{align*}
\]

\[ (4.14) \]

4.3 Finite Difference Approximations

Analytical solution for solving the complex, non-linear continuity equations described above are not available. Therefore, these equations must be approximated using finite
difference (FD) techniques. Once these FD approximations are formulated, we can solve them at discrete points in the reservoir, known as grid points. Spatial derivatives are discretized using central Euler’s approximation, while time derivatives are discretized using backward Euler’s approximation. The fact that a backward time approximation is used states that we are attempting to solve the problem in an implicit manner.

At this point, we just present the residual equation for hydrocarbon component in matrix domain in prolate spheroidal coordinates (which is shown in Eqn. 4.8). This equation is the most complex one, and it’s residual equation is presented for illustration purposes (Other residual equations are calculated similarly).

In general, the residual equation has the following form:

\[ R_{HC,m}^{M} i,j,k = Q_{\text{east}} + Q_{\text{west}} + Q_{\text{north}} + Q_{\text{south}} + Q_{\text{above}} + Q_{\text{below}} + M_{\text{source/sink}} - \text{Accumulation}; \]

\[ (4.15) \]

\( Q_{\text{east}}, Q_{\text{west}}, Q_{\text{north}}, Q_{\text{south}}, Q_{\text{above}}, \) and \( Q_{\text{below}} \) are the inter-block flow terms, while \( M_{\text{source/sink}} \) are the implicit and explicit source/sink terms in continuity equation. The right hand side of continuity equation is the accumulation term. Next, we present the definitions of each of these terms.
\[ Q_{east} = \left( \Delta \eta_j \cdot \Delta \psi_k \right)_{i+\frac{1}{2},j,k} \cdot \left( d \cdot \cos \eta \right)_{i+\frac{1}{2},j,k} \]

\[
\begin{aligned}
&k_{ro} x_m^{M+1}_{i+\frac{1}{2},j,k} - \frac{\rho_o^M}{\mu_o^M}_{i+\frac{1}{2},j,k} \cdot \left( \Phi_{o,i+1,j,k}^M - \Phi_{o,i,j,k}^M \right) \\
&+ k_{rg} y_m^{M+1}_{i+\frac{1}{2},j,k} - \frac{\rho_g^M}{\mu_g^M}_{i+\frac{1}{2},j,k} \cdot \left( \Phi_{g,i+1,j,k}^M - \Phi_{g,i,j,k}^M \right)
\end{aligned}
\]

\[
\begin{aligned}
&+ \left( \phi^M \cdot S_o^M \cdot \rho_o^M \right)_{i+\frac{1}{2},j,k} \cdot \sum_{\text{comp}=1}^{n_i} \beta_{o,i,j,k} \cdot x_{m,\text{comp}}^{M,\text{upstream}} \cdot \left( \mu_{i+1,j,k,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \\
&+ \left( \phi^M \cdot S_g^M \cdot \rho_g^M \right)_{i+\frac{1}{2},j,k} \cdot \sum_{\text{comp}=1}^{n_i} \beta_{g,i,j,k} \cdot y_{m,\text{comp}}^{M,\text{upstream}} \cdot \left( \mu_{i+1,j,k,\text{comp}} - \mu_{i,j,k,\text{comp}} \right)
\end{aligned}
\]

\[
\begin{aligned}
&+ 5.615 \cdot \frac{\xi_{i+\frac{1}{2},j,k} - \xi_{i,j,k}}{\sinh \xi_{i,j,k}} \cdot \frac{\xi_{i+1,j,k} - \xi_{i+\frac{1}{2},j,k}}{\sinh \xi_{i+1,j,k}} \\
&+ 5.615 \cdot \frac{\xi_{i+\frac{1}{2},j,k} - \xi_{i,j,k}}{\sinh \xi_{i,j,k}} \cdot \frac{\xi_{i+1,j,k} - \xi_{i+\frac{1}{2},j,k}}{\sinh \xi_{i+1,j,k}}
\end{aligned}
\]

\[ (4.16a) \]
\[ Q_{\text{west}} = \left( \Delta \eta \cdot \Delta \psi_k \right)_{i \frac{1}{2} j \frac{1}{2}, k} \cdot (d \cdot \cos \eta)_{i \frac{1}{2} j \frac{1}{2}, k} \]

\[
\begin{aligned}
&\left\{ k_{ro} x^M_{m,i \frac{1}{2} j \frac{1}{2}, k} \frac{\rho^M_{o,i \frac{1}{2} j \frac{1}{2}, k}}{\mu^M_{o,i \frac{1}{2} j \frac{1}{2}, k}} \right\}^{n+1} + \left( \Phi^M_{o,i-1, j \frac{1}{2}, k} - \Phi^M_{o,i, j \frac{1}{2}, k} \right) \\
&\quad \cdot \left( \frac{\xi_{i,j,k} - \xi_{i-1,j,k}}{k_{z}^M \cdot \sinh \xi_{i,j,k}} \right)^{n+1} + \left( \Phi^M_{o,i \frac{1}{2}, j \frac{1}{2}, k} - \Phi^M_{o,i-1, j \frac{1}{2}, k} \right) \\
&\quad \cdot \left( \frac{\xi_{i-1,j,k} - \xi_{i,j,k}}{k_{z}^M \cdot \sinh \xi_{i-1,j,k}} \right)^{n+1}
\end{aligned}
\]

\[
\begin{aligned}
&\left\{ k_{rg} y^M_{m,i \frac{1}{2} j \frac{1}{2}, k} \frac{\rho^M_{g,i \frac{1}{2} j \frac{1}{2}, k}}{\mu^M_{g,i \frac{1}{2} j \frac{1}{2}, k}} \right\}^{n+1} + \left( \Phi^M_{g,i-1, j \frac{1}{2}, k} - \Phi^M_{g,i, j \frac{1}{2}, k} \right) \\
&\quad \cdot \left( \frac{\xi_{i,j,k} - \xi_{i-1,j,k}}{k_{z}^M \cdot \sinh \xi_{i,j,k}} \right)^{n+1} + \left( \Phi^M_{g,i \frac{1}{2}, j \frac{1}{2}, k} - \Phi^M_{g,i-1, j \frac{1}{2}, k} \right) \\
&\quad \cdot \left( \frac{\xi_{i-1,j,k} - \xi_{i,j,k}}{k_{z}^M \cdot \sinh \xi_{i-1,j,k}} \right)^{n+1}
\end{aligned}
\]

\[
\begin{aligned}
&\left( \phi^M_k S^M_{o} \frac{\rho^M_{o}}{\mu^M_{o}} \right)_{\text{upstream}} + \left\{ \sum_{\text{comp}=1}^{n-1} \beta_{o,j,\text{comp}} \cdot x^M_{m,\text{comp}} \cdot \left( \mu_{i-1, j\frac{1}{2}, k, \text{comp}} - \mu_{i, j\frac{1}{2}, k, \text{comp}} \right) \right\}^{n+1} \\
&\quad \cdot \left( \frac{\xi_{i,j,k} - \xi_{i-1,j,k}}{\sinh \xi_{i,j,k}} \right)^{n+1} + \left( \frac{\xi_{i-1,j,k} - \xi_{i,j,k}}{\sinh \xi_{i-1,j,k}} \right)^{n+1}
\end{aligned}
\]

\[
\begin{aligned}
&\left( \phi^M_k S^M_{g} \frac{\rho^M_{g}}{\mu^M_{g}} \right)_{\text{upstream}} + \left\{ \sum_{\text{comp}=1}^{n-1} \beta_{g,j,\text{comp}} \cdot y^M_{m,\text{comp}} \cdot \left( \mu_{i-1, j\frac{1}{2}, k, \text{comp}} - \mu_{i, j\frac{1}{2}, k, \text{comp}} \right) \right\}^{n+1} \\
&\quad \cdot \left( \frac{\xi_{i,j,k} - \xi_{i-1,j,k}}{\sinh \xi_{i,j,k}} \right)^{n+1} + \left( \frac{\xi_{i-1,j,k} - \xi_{i,j,k}}{\sinh \xi_{i-1,j,k}} \right)^{n+1}
\end{aligned}
\]

\[ (4.16b) \]
\[ Q_{north} = \left( \Delta \xi \cdot \Delta \psi_k \right)_{i,j+\frac{1}{2}k} \cdot \left( d \cdot \cosh \xi \right)_{i,j+\frac{1}{2}k} \]

\[
\begin{align*}
&k_{ro}^M x_{M\text{, }i,j+\frac{1}{2}k}^{n+1} - \rho_{o\text{, }i,j+\frac{1}{2}k}^{n+1} \left( \Phi_{o,i,j+1,k}^M - \Phi_{o,i,j,k}^M \right) \\
&+ k_{rg}^M y_{M\text{, }i,j+\frac{1}{2}k}^{n+1} - \rho_{g\text{, }i,j+\frac{1}{2}k}^{n+1} \left( \Phi_{g,i,j+1,k}^M - \Phi_{g,i,j,k}^M \right) \\
&\left( \phi_{o\text{, }i,j+\frac{1}{2}k}^M - \rho_{o\text{, }i,j+\frac{1}{2}k}^{n+1} \sum_{\text{comp}=1}^{\eta-1} \beta_{o,i,\text{comp},\text{upstream}} x_{m,\text{comp}} \cdot \left( \mu_{i,j+1,k,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \right) \\
&+ \left( \phi_{g\text{, }i,j+\frac{1}{2}k}^M - \rho_{g\text{, }i,j+\frac{1}{2}k}^{n+1} \sum_{\text{comp}=1}^{\eta-1} \beta_{g,i,\text{comp},\text{upstream}} y_{m,\text{comp}} \cdot \left( \mu_{i,j+1,k,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \right) \\
&5.615 \left( \eta_{i,j,\frac{1}{2}k} - \eta_{i,j,k} \right) + \left( \eta_{i,j+1,k} - \eta_{i,j+\frac{1}{2}k} \right) \left( \sin \eta_{i,j,k}^{n+1} \right) + \left( \sin \eta_{i,j+1,k}^{n+1} \right) \\
&5.615 \left( \eta_{i,j,\frac{1}{2}k} - \eta_{i,j,k} \right) + \left( \eta_{i,j+1,k} - \eta_{i,j+\frac{1}{2}k} \right) \left( \sin \eta_{i,j,k}^{n+1} \right) + \left( \sin \eta_{i,j+1,k}^{n+1} \right) \\
\right) \]

(4.16c)
\[ Q_{south} = \left( (\Delta \xi \cdot \Delta \psi_k)_{i,j-k-\frac{1}{2}} \cdot (d \cdot \cosh \xi)_{i,j-\frac{1}{2}} \right) \]

\[ k_{ro}^M x_{m}^{M+1} \frac{\rho_{o}^{M+1}}{\mu_{o}^{M+1}} \left( \Phi_{o,i-j-1,k}^{M} - \Phi_{o,i,j,k}^{M} \right) \]

\[ + k_{rg}^M y_{m}^{M+1} \frac{\rho_{g}^{M+1}}{\mu_{g}^{M+1}} \left( \Phi_{g,i,j-1,k}^{M} - \Phi_{g,i,j,k}^{M} \right) \]

\[ + \left( \phi_{s}^{M} \frac{\rho_{o}^{M}}{\mu_{o}^{M}} \right)_{i,j-k-\frac{1}{2}} \sum_{\text{comp}=1}^{n_{comp}-1} \beta_{o,i\text{ comp}} \cdot x_{m,\text{comp}}^{M} \cdot \left( \mu_{i,j-1,k,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \]

\[ + \left( \phi_{s}^{M} \frac{\rho_{g}^{M}}{\mu_{g}^{M}} \right)_{i,j-k-\frac{1}{2}} \sum_{\text{comp}=1}^{n_{comp}-1} \beta_{g,i\text{ comp}} \cdot y_{m,\text{comp}}^{M} \cdot \left( \mu_{i,j-1,k,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \]

\[ 5.615 \]

\[ \left( \eta_{i,j,k} - \eta_{i,j-\frac{1}{2}} \right) \text{ (sin} \eta_{i,j,k}^{n+1} \text{)} + \left( \eta_{i,j-\frac{1}{2}} - \eta_{i,j-1,k} \right) \text{ (sin} \eta_{i,j-1,k}^{n+1} \text{)} \]

\[ 5.615 \]

\[ \left( \eta_{i,j,k} - \eta_{i,j-\frac{1}{2}} \right) \text{ (sin} \eta_{i,j,k}^{n+1} \text{)} + \left( \eta_{i,j-\frac{1}{2}} - \eta_{i,j-1,k} \right) \text{ (sin} \eta_{i,j-1,k}^{n+1} \text{)} \]

(4.16d)
\[ Q_{\text{above}} = \left( \left( d \cdot \text{term} k \right)_{i,j,k+\frac{1}{2}} \right) \]

\[
\begin{aligned}
k_r^M x_m^{M \left| i,j,k+\frac{1}{2} \right.} \cdot \rho_o^M \mu_o^M \left| i,j,k+\frac{1}{2} \right. & \quad \frac{1}{\psi_{i,j,k+\frac{1}{2}} - \psi_{i,j,k}} \frac{1}{\psi_{i,j,k+1} - \psi_{i,j,k+\frac{1}{2}}} \\
+ k_r^M y_m^{M \left| i,j,k+\frac{1}{2} \right.} \cdot \rho_g^M \mu_g^M \left| i,j,k+\frac{1}{2} \right. & \quad \frac{1}{\psi_{i,j,k+\frac{1}{2}} - \psi_{i,j,k}} \frac{1}{\psi_{i,j,k+1} - \psi_{i,j,k+\frac{1}{2}}} \\
\left( \phi^M S_o^M \rho_o^M \right)_{i,j,k+\frac{1}{2}} \left( \psi_{i,j,k+1} - \psi_{i,j,k} \right) & \quad \left( \psi_{i,j,k+1} - \psi_{i,j,k} \right) \\
\left( \phi^M S_g^M \rho_g^M \right)_{i,j,k+\frac{1}{2}} \left( \psi_{i,j,k+1} - \psi_{i,j,k} \right) & \quad \left( \psi_{i,j,k+1} - \psi_{i,j,k} \right)
\end{aligned}
\]

(4.16e)
\[ Q_{\text{below}} = \left( (d \cdot \text{term}_k)_{i,j,k} \right) \]

\[
\begin{aligned}
&k_{ro}^M x_m^{M+1}_{i,j,k} \cdot \frac{\rho_o^M}{\mu_o^M} 
\cdot \left( \Phi^M_{o,i,j,k-\frac{1}{2}} - \Phi^M_{o,i,j,k} \right) \\
&+ k_{rg}^M y_m^{M+1}_{i,j,k} \cdot \frac{\rho_g^M}{\mu_g^M} 
\cdot \left( \Phi^M_{g,i,j,k-\frac{1}{2}} - \Phi^M_{g,i,j,k} \right) \\
&+ \left( \phi^S_o \rho_o^M \right)_{i,j,k} \cdot \left( \nabla \nabla \right)_{i,j,k} 
\cdot \left( \sum_{\text{comp}=1}^{n-1} \beta_{o,i,\text{comp}} \cdot x_{m,\text{comp}}^{M,\text{upstream}} \cdot \left( \mu_{i,j,k-1,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \right) \\
&+ \left( \phi^S_g \rho_g^M \right)_{i,j,k} \cdot \left( \nabla \nabla \right)_{i,j,k} 
\cdot \left( \sum_{\text{comp}=1}^{n-1} \beta_{g,i,\text{comp}} \cdot y_{m,\text{comp}}^{M,\text{upstream}} \cdot \left( \mu_{i,j,k-1,\text{comp}} - \mu_{i,j,k,\text{comp}} \right) \right) \\
&= \left( \Delta \xi_i \cdot \Delta \eta_j \right)_{i,j,k}^{1,1} \\
&\cdot \left( -\coth \xi_i \cdot \left[ \ln | \csc \eta + \cot \eta \right] - \cos \eta \cdot \left[ \ln | \cosh \xi + \coth \xi \right] \right)_{i,j,k}^{1,1}
\end{aligned}
\]
In general, in the inter-block flow terms’ definition, the first term represents $m^{th}$ component transfer through oil phase due to viscous flow, second term represents $m^{th}$ component transfer through gas phase due to viscous flow, third term represents $m^{th}$ component transfer through oil phase due to fickian (diffusive) flow, while fourth term represents $m^{th}$ component transfer through gas phase due to fickian flow.

And the accumulation term is defined as follows:

\[
\begin{align*}
\text{(Accumulation)}^{n+1}_{i,j,k} &= \frac{V_{h_{i,j,k}} \cdot \phi^M_{i,j,k}}{5.615 \Delta t} \\
&\left[ \left( S^M_o x^M_m \rho^M_o + (1 - S^M_o - S^M_w) y^M_m \rho^M_g \right)_{i,j,k}^{n+1} - \left( S^M_o x^M_m \rho^M_o + (1 - S^M_o - S^M_w) y^M_m \rho^M_g \right)_{i,j,k}^n \right]
\end{align*}
\]

(4.16h)

### 4.4 Source/Sink Terms

In dual-porosity simulators, the source/sink terms ($M_{\text{source/sink}}$) are classified into two groups as follows:

#### 4.4.1 Implicit Source/Sink Terms

Implicit source/sink terms are defined to account for fluid transfer between matrix and fracture domains. The pressure as well as chemical potential gradient between the two domains governs the rate of transfer. In this work, the definition proposed by Chawathe et al. (1996) and modified by Thararoop (2010) is used:
Thararoop (2010) had suggested calculating phase viscosities and compressibility factors using a mean pressure calculated at the matrix-fracture interface. However, in this study, we calculate these properties using the upstream condition. In addition, the diffusional flux is calculated based on the chemical potential gradient rather than concentration gradient. This approach is thermodynamically consistent, and would provide an accurate approach of modeling diffusion in case of phase discontinuities across matrix and fracture interfaces. The derivation of this approach is presented in Chapter 5. Note that the units of each of the terms in Eq. 4.15 is \((RB.lbmol)/(RCF.day)\).

It is important to note here that we have used \(P^2\) approach for calculating flux terms for both, oil as well as gas phases. This approach is valid for low pressure system. Also, we would like to state that our formulation of inter-porosity function may underpredict the flux during transient phase of the production. The above formulation is more applicable to pseudo-steady state condition (i.e. when the boundary effects have

\[
(\Gamma)_{m,i,j,k}^F = \left( \frac{1}{5.615 \times 379.6} \right) \left\{ \gamma_m^{up} \sigma_{i,j,k} V_{b,i,j,k} \frac{T_{sc}}{TP_{sc}} \cdot \left[ \frac{k_{ro}^{up} k_{mean}^{M}}{\mu_o^{up} Z_{o}^{up}} \right] \left( \frac{P_{o,i,j,k}^M}{2} - \frac{(P_{o,i,j,k}^F)^2}{2} \right) \right. \\
+ \left( \gamma_m^{up} \sigma V_{b,i,j,k} \frac{T_{sc}}{TP_{sc}} \cdot \left[ \frac{k_{ro}^{up} k_{mean}^{M}}{\mu_g^{up} Z_{g}^{up}} \right] \left( \frac{P_{g,i,j,k}^M}{2} - \frac{(P_{g,i,j,k}^F)^2}{2} \right) \right) \\
+ \left( \frac{\phi_{o} S_o \rho_o^{up}}{5.615 \times \sigma_{i,j,k}} \right) \cdot \left[ \sum_{comp=1}^{n-1} \beta_{o,i,j,k}^{up} \cdot \gamma_m^{up} \cdot \left( \mu_{i,j,k,comp}^{M} - \mu_{i,j,k,comp}^{F} \right) \right] \\
+ \left( \frac{\phi_{g} S_g \rho_g^{up}}{5.615 \times \sigma_{i,j,k}} \right) \cdot \left[ \sum_{comp=1}^{n-1} \beta_{g,i,j,k}^{up} \cdot \gamma_m^{up} \cdot \left( \mu_{i,j,k,comp}^{M} - \mu_{i,j,k,comp}^{F} \right) \right]
\]

(4.17)
been felt). As such, a better formulation for this transfer is required, and this should be addressed in the future work.

In any definition of transfer function, the way shape factor ($\sigma$) is defined governs whether the function is applicable for transient regime or not. Earlier works developed $\sigma$ which was only applicable to pseudo-steady state regime. Chang’s (Chang, 1993) original definition was applicable to transient regime, but the definition was too complicated to be incorporated into simulator (Sarma and Aziz, 2006). Thararoop’s (2010) definition is based on Chang’s work, and is expected to be applicable to transient flow, however, unlike Chang’s definition, it does not contain any time-dependent terms. In this work, we employ the definition used by Thararoop (2010), and it is given below:

$$\sigma = \pi^2 \left( \frac{1}{L_x^2} + \frac{1}{L_y^2} + \frac{1}{L_z^2} \right)$$

(4.18)

Here, $L_x$, $L_y$, and $L_z$ are the fracture spacing in $x$, $y$, and $z$ directions, respectively. The matrix block lengths in $x$, $y$, and $z$ directions are also used for specifying these dimensions, however, this definition fails when matrix blocks sizes are larger than fracture spacing.

It might be possible to convert the calculation of shape factor from Cartesian to Prolate spheroidal coordinates. However, we believed that since the calculation of shape factor must be related to physical parameters, the values of fracture spacing must remain in Cartesian coordinates.

Similarly, since there is no accumulation of mass during transport from matrix to fracture, or vice-versa, the transfer function in matrix can be defined as below:
4.4.2 Explicit Source/Sink Terms

In curvilinear coordinate system, well flow rates are calculated as the inner boundary condition for the blocks nearest to the well. In essence, we do not need to use well model, such as Peaceman’s, which provides a relationship between flow rate, well block pressure, and bottomhole pressure. As grid geometry follows the flow geometry perfectly, the flow rate calculations are expected to be accurate (with the inherent assumption of linear flow near wellbore, which may be violated in real scenario).

For Cartesian grid system, the explicit source/sink terms are calculated using the following relationship (Ayala, 2004):

\[
\left( M^F_m \right) = x_m^F \rho_o^F q_o^F + y_m^F \rho_g^F q_g^F
\]

(4.20a)

and

\[
q_{w,STB/day}^F = \frac{q_{w,RB/day}^F}{B_w^F}
\]

(4.20b)

Here \( q_o^F \), \( q_g^F \) and \( q_w^F \) are defined by Peaceman’s well model (Peaceman, 1983). For multiphase flow taking place into the vertical well, Peaceman derived the following relationship between flow rate, bottomhole pressure and well block pressure.
\[ q^F_o = \frac{2\pi k_h^F k_{ro}^F h}{\mu_o B_o^F} \left[ \frac{(P_o^F - P_{wf})}{\ln \left( \frac{r_e}{r_w} \right) + s} \right] \]  

\[ q^F_g = \frac{2\pi k_h^F k_{rg}^F h}{\mu_g B_g^F} \left[ \frac{(P_g^F - P_{wf})}{\ln \left( \frac{r_e}{r_w} \right) + s} \right] \]  

\[ q^F_w = \frac{2\pi k_h^F k_{rw}^F h}{\mu_w B_w^F} \left[ \frac{(P_w^F - P_{wf})}{\ln \left( \frac{r_e}{r_w} \right) + s} \right] \]  

(4.21a)  

(4.21b)  

(4.21c)

\( k_h^F \) is the arithmetic average of fracture permeabilities in x and y direction. Note that the above flow rate equations are written for a vertical well placed in a Cartesian coordinate grid system.

### 4.5 Generalized Newton-Raphson (GNR) Protocol

From the residual equations presented in previous sub-section, a total of \((2N_c+2)\) equations can be formed for each gridblock. These equations need to be linearized before any solution procedure can be implemented in order to solve them. The most stable and accurate way of linearizing these equations is the GNR protocol. This procedure basically creates a Jacobian matrix of derivatives of residual equations with respect to the principal
unknowns. Therefore, a reservoir system consisting of a 1 gridblock and 5 hydrocarbon component fluid will result in creation of a Jacobian matrix of 12×12 dimensions, and will subsequently be used to solve for the 12 primary unknowns. Once the values of primary unknowns are determined, auxiliary equations can then be used to solve for the remaining secondary unknowns.

The use of Newton-Raphson procedure results in the formulation of linearized equations in the form of $AX = B$, where $A$ is the Jacobian matrix, $X$ is the vector of unknown variables, and $B$ is the value of residual equations at previous iteration. Fluid flow problems in engineering fields are formulated in the form of partial differential equations, and their linearization generates a sparse nature of Jacobian matrix. Each entry in the Jacobian matrix is calculated using numerical differentiation. The solution (or in other words, inversion) of matrix $A$ requires the application a sparse linear solver, such as Bi-conjugate gradient stabilized algorithm (BiCGSTAB), generalized minimum residual algorithm (GMRES), among others. In this study, restarted GMRES (mGMRES) solver provided by Department of Scientific Computing at Florida State University is used, which was found to be the most stable and fast solver.
Chapter 5

Adsorption and Diffusion Processes in Shales

Adsorption and diffusion act as important storage and transport mechanisms in tight reservoirs such as shales. Therefore, special efforts must be made in order to accurately model these processes. In this chapter, the methods utilized for modeling and their incorporation in simulators are presented.

5.1 Liquid Phase Adsorption Modeling

Multi-component adsorption at liquid-solid interfaces play a significant role in foams, catalysis, pollution control, and other separation methods (Sircar, 1970). Liquid phase adsorption is the preferred method for removal of organic pollutants from industrial wastewater, with activated carbon, resins, and zeolites acting as the adsorbing surfaces (Ruthven, 1984). However, adsorption from liquid phase is entirely different from gas phase adsorption, since the fundamental principles and methodologies are quite different between the two phenomena (Roque-Malherbe, 2007). Liquid phase adsorption is governed by factors such as type of adsorbent, temperature, as well as adsorptive concentration. This is primarily the reason that this adsorption process is less studied in comparison to gas phase adsorption, although industrial importance of adsorption from liquid phase is evident. The adsorption data has to be experimentally determined, or
needs to be predicted using multi-component adsorption models (Roque-Malherbe, 2007).

In shale gas modeling, the formation of adsorbed phase is considered only if a free gas phase is present with an adsorbent. Current models for liquid-rich shales do not consider the change in bulk liquid composition, or in other words, adsorption from liquid mixtures is neglected. In this research, a new method is being proposed to predict the amount of adsorption from a given multi-component liquid mixture, by using the adsorption data of only the pure unsaturated vapors. Next, we present the theory of thermodynamics of adsorption from liquid mixtures, and show that adsorption from liquid mixtures can be explained entirely in terms of the gas adsorption isotherms of the components present. The numerical examples will be presented in the next chapter.

5.1.1 Theory – The Gibbsian Model of Interface

In this study, the Gibbs model of solid-liquid interface is considered. The actual system consisting of a homogeneous bulk liquid phase and an inhomogeneous adsorbed phase (shown in Figure 5.1a) is replaced by two homogeneous phases (shown in Figure 5.1b). In reality, there is a continuous concentration change from the surface of adsorbate to the bulk liquid.
The assumptions of the Gibbs model of interface are as follows:

- Only physisorption exists
- Adsorbed molecules and bulk liquid molecules can be treated as two separate phases

A fundamental difference that exists between adsorption from vapor mixtures and that from liquid mixtures is that, in case of liquid phase adsorption, the surface of adsorbent always remains covered with molecules. This fact prevails even in absence of adsorption. Previously, it was assumed that adsorption from liquids on solids is restricted to monolayer formation (Kipling and Tester, 1952). The monolayer assumption thus cannot be subjected to experimental verification due to the reason stated above. In addition, this assumption is not thermodynamically consistent and puts strict limitations on the shape of isotherms (Jones and Mill, 1957).
5.1.2 Ideal Adsorbate Solution (IAS) Theory

In this work, the Ideal Adsorbed Solution (IAS) forms the backbone on which the theory of liquid phase adsorption is based. Thus, it will be worthwhile to review the basic concepts of IAS theory first.

Adsorption isotherms such as Langmuir, Toth or UNILAN provide fairly accurate predictions for a single component gas system (Manik, 1999). An example of Langmuir isotherm is given below:

\[ n = n_L \frac{P}{P + P_L} \]  

(5.1)

However, for a multi-component system, an extended version of these equations proves to be unreliable and inaccurate (Yang, 1987). Myers and Prausnitz (1965) first proposed a thermodynamically consistent multi-component sorption model to predict the adsorption capacity of multi-component gases. The model considers the thermodynamic equilibrium between vapor and adsorbed phases to be analogous to that of vapor-liquid equilibria (VLE).

According to the Gibbs law, the free and adsorbed gas phases are in equilibrium when the chemical potentials of the components in both phases are equal to each other:

\[ \mu_i^g(T, P, y_i) = \mu_i^a(T, \pi, x_i) \]  

(5.2)

If a standard state of component \( i \) is pure component \( i \) adsorbed at the same \( \pi \) and \( T \) as the adsorbed gas mixture, then the chemical potential of gas components in adsorbed phase is given by:
\[ \mu_i^a(T, \pi, x_i^i) = \mu_i^{a0}(T, \pi) + RT \ln \left( \gamma_i x_i^i \right) \]  
\hspace{1cm} (5.3)

Since equilibrium also exists at standard state between free gas and adsorbed gas mixtures, the chemical potentials of pure components in both phases are also equal:

\[ \mu_i^{a0} = \mu_i^{g0} = \mu_i^{ref}(T) + RT \ln \left( f_i^0 \right) \]  
\hspace{1cm} (5.4)

Substituting Eq. (5.4) in Eq. (5.3), we get:

\[ \mu_i^a(T, \pi, x_i^i) = \mu_i^{ref}(T) + RT \ln \left( f_i^0 \right) + RT \ln \left( \gamma_i x_i^i \right) \]  
\hspace{1cm} (5.5)

Similarly, by using the same reference state, the chemical potential of gas components in free gas phase can be given by:

\[ \mu_i^g(T, P, y_i^i) = \mu_i^{ref}(T) + RT \ln \left( f_i \right) \]  
\hspace{1cm} (5.6)

Substituting Eqs. (5.5) and (5.6) in Eq. (5.2), we get:

\[ f_i = f_i^0 \gamma_i x_i^i \]  
\hspace{1cm} (5.7)

The above equation can be rewritten in terms of fugacity coefficients as:

\[ P y_i \varphi_i = P_i^0 \varphi_i^0 \gamma_i x_i^i \]  
\hspace{1cm} (5.8)

Eq. (5.8) forms the fundamental relationship for multi-component adsorption equilibria. In IAS model, the correction factor for non-ideality in adsorbed phase (i.e. activity coefficient \( \gamma \)) is relaxed and assumed to be unity. The values of activity coefficients are a function of spreading pressure, temperature and mole fraction of adsorbed phase. These can be determined through experiments, however, there is no direct experimental method that can be used to measure spreading pressure. Theoretical correlations are available, but
provide coefficient values with unacceptable accuracy for coalbed reservoirs (Stevenson et al., 1992) and none have been found for shale gas applications.

With the help of the assumptions of IAS theory, Eq. (5.8) can be written as:

\[ P_y \varphi_i = P_i^0 \varphi_i^0 x_i \]

(5.9)

5.1.3 Liquid Phase Adsorption Theory

Let us now derive the relationship between adsorption from liquids and adsorption from vapors. To simplify the problem, we consider a binary component mixture at under-saturated condition (although the theory and derivation could easily be extended to more than two components by analogy). This binary mixture is brought in contact with an adsorbent and the system temperature is maintained at T. The system pressure is held at sub-atmospheric conditions, and is shown in Figure 5.2 below.
Under these system conditions, the Gibbs equation for the condensed phase is given by (Myers and Sircar, 1972):

\[ n_1 \dot{\mu}_1 + n_2 \dot{\mu}_2 + n_a \dot{\mu}_a = V' dP \]  
(5.10)

The \( V' dP \) term can be neglected as adsorbed volume is small and since the pressure is subatmospheric, the change in pressure is negligible. At thermodynamic equilibrium, we can write \( \mu_1' = \mu_1 \) and \( \mu_2' = \mu_2 \), where \( \mu_1 \) and \( \mu_2 \) are chemical potentials in the gas phase. At low pressure of interest, we have:

\[ d \mu_i = RT d \ln (P_{Y_i}) \]  
(5.11)

Thus, combining Eqs. (5.10) and (5.11), we get:

\[ -\frac{n_a d \mu_a}{RT} = n_1 d \ln (P_{Y_1}) + n_2 d \ln (P_{Y_2}) \]  
(5.12)
Eq. (5.12) is integrated in three steps over a closed path as shown in Figure 5.4. In Step 1, adsorption of pure vapor of component 2 takes place and we can write:

$$\frac{-n_2 d\mu_a}{RT} = \int_{p=0}^{P^s} \frac{n_2}{P} dP$$  \hspace{1cm} (5.13)

Similarly, Step 3 is the desorption of pure vapor of component 1:

$$\frac{-n_1 d\mu_a}{RT} = -\int_{p=0}^{P^s} \frac{n_1}{P} dP$$  \hspace{1cm} (5.14)

In Step 2, the adsorbent is immersed in a liquid mixture of components 1 and 2. This liquid mixture is in equilibrium with its saturated vapor. The vapor phase is now in equilibrium with the liquid phase, and the partial pressure in the vapor is equal to the fugacity in the bulk liquid. Again, the temperature is held constant at T, and the system to be considered in this step is shown schematically in Figure 5.3.

![Figure 5-3. Binary mixture system at saturation condition (adapted from Myers and Sircar, 1972)](image-url)
According to the Gibbs-Duhem equation, the activity coefficients in the bulk liquid are related as:

\[ x_1 d \ln (\gamma_1) + x_2 d \ln (\gamma_2) = 0 \]  

(5.16)

Combination of Eqs. (5.12), (5.15) and (5.16) gives:

\[ -n_a d \mu_a \frac{n_i - (n_i + n_2) x_i}{x_2} d \ln (\gamma_1 x_1) \]  

(5.17)

It is important to introduce the concept of surface excess at this point. To verify the liquid adsorption theory, Sircar and Myers (1970) defined a new term called surface excess as follows:
\[ n^e_i = n^* - \left( n^*_i + n^*_j \right) x_i \]  
\hspace{1cm} (5.18)

The reason for introduction of this variable was that, the amount adsorbed at the liquid-solid interface is rarely a meaningful experimental variable. The important experimental variable in such a case is the surface excess of component \( i \) of liquid mixture \( (n^e_i) \), and in other words, it can also be defined as follows (Roque-Malherbe, 2007):

\[ n^e_i = n^* \cdot \left( x^*_i - x_i \right) \]  
\hspace{1cm} (5.19)

where \( n^* \) is the total number of moles of binary liquid mixture brought into contact with unit mass of adsorbent, and \( x^*_i \) and \( x_i \) are mole fraction of component \( i \) in the bulk liquid before and after contact with the solid adsorbent, respectively.

Thus, the integration of Eq. (5.17) over step 2 gives us:

\[ -\frac{n_a \Delta \mu_a}{RT} = -\int_{x_i=0}^{x_2} \frac{n^e_i}{x_2} d\ln\left( \gamma_i x_i \right) \]  
\hspace{1cm} (5.20)

Finally, combining Eqs. (5.13), (5.14) and (5.20), we get:

\[ \int_{P=0}^{p^s} \frac{n^e_2}{P} dP - \int_{P=0}^{p^s} \frac{n^e_1}{P} dP + \int_{x_i=0}^{x_1} \frac{n^e_i}{\gamma_1 x_i x_2} d(\gamma_i x_i) = 0 \]  
\hspace{1cm} (5.21)

This equation provides the thermodynamic consistency test that relates adsorption from binary, unsaturated vapors to adsorption from their liquid mixtures. The first two integrals relate to the adsorption from vapors, while the last integral refers to the adsorption from liquid mixture.

The surface excess of vapor phase is defined as:
\[ n_i^{ev} = n^* - x_i \left( \sum n_i \right) \]  

(5.22)

At limiting saturation condition, we can define (Myers and Sircar, 1972):

\[ n_i^e = \lim_{p \to p^S} \left( n_i^{ev} \right) \]  

(5.23)

This equation relates adsorption from liquids to adsorption from vapor mixtures. As we approach the saturation pressure (i.e. bubble point pressure in our case), the surface excess of liquid phase becomes equal to that of vapor phase.

Thus, if we have a single-liquid phase mixture, we should take this mixture to its bubble-point pressure and calculate its equilibrium vapor composition. Any equation-of-state (EOS) package can be utilized at this point. We, then, apply the IAS theory to calculate the composition of the equilibrium adsorbed phase present with this two-phase mixture. The amount of adsorbed phase can also be calculated using a simple material balance equation.

An important point should be noted here. The amount of adsorbed phase and its composition is a function of the composition of liquid phase, adsorption constants of pure gas components, and the amount of adsorbent present. For a given liquid-rich shale reservoir, these conditions are expected to remain constant until the reservoir pressure reaches the bubble point pressure. This process of primary depletion is depicted in Figure 5.5. Therefore, the amount of adsorbed phase is also expected to remain constant during this depletion phase. Once the system enters two-phase conditions, only then will the adsorbed phase amount and composition change. While performing numerical simulation of such a system, we have to conduct the calculation procedure only once at the start of
simulation run, until we reach two-phase condition where the calculation procedure of liquid-vapor-adsorbed phase equilibrium will take over.

Figure 5-5. Phase diagram illustrating primary depletion in liquid-rich shale reservoirs

The calculation procedure, along with a standalone numerical example on a four-component fluid case, will be shown in Chapter 6. This will be followed with parametric study for important parameters in implementation of liquid-phase adsorption model in numerical simulator.

5.2 Diffusion Modeling

First, we will derive the diffusional flux equation based on chemical potential approach. After that, the approach used in calculating the diffusion coefficient will be illustrated. Finally, the mathematical form of multi-component flux derived on concentration gradient and on chemical potential gradient will be shown.
Irreversible thermodynamics dictates that processes are driven by generalized forces, \( X \), and are characterized by transport or Onsanger phenomenological coefficients, \( L \) (Onsager, 1931). This can be expressed as below:

\[
J_k = -\sum_{i=1}^{nc} L_{ki} X_i
\]  

(5.24)

where \( k,i \) are the component index, \( L_{ki} \) are the Onsager phenomenological coefficients, and \( X_i \) are the generalized forces. Familiar examples of such relations are Fick’s first law of diffusion, Fourier’s law of heat transfer, Ohm’s law of electricity conduction, among others (Roque-Malherbe, 2007).

Now, the real driving force of mass transport is the gradient of chemical potential (Onsager, 1931), where the generalized forces can be expressed as:

\[
X_i = \nabla \left( \frac{\mu_i}{T} \right)
\]  

(5.25)

Thus, for isothermal systems, substitution of above expression in Eq. (5.24) presents the basic form of diffusional flux:

\[
J = -L \nabla (\mu)
\]  

(5.26)

The experimental evidence that the driving force of diffusive transport is the chemical potential gradient was provided by Haase and Siry (1968). They performed binary mixture experiments at critical points, illustrating the fact that diffusion will be zero at such conditions (due to equality of chemical potentials). However, this cannot be established using the conventional concentration gradient approach.
The next important development is the relation between Onsager and Fickian diffusion coefficients. In this work, we follow the development by Moortgat and Firoozabadi (2013). The diffusion flux for multi-component systems in terms of concentration gradient is given by:

\[
J_i = -\rho \sum_{k=1}^{n_c-1} D_{ik}^{\text{Fick}} \nabla x_k, \quad i = 1, 2, \ldots, n_c - 1
\]  

(5.27)

Here, \(x_k\) is the molar composition of \(k^{th}\) species.

We can write chemical potential gradient as:

\[
\nabla \mu_i = \sum_{k=1}^{n_c-1} \frac{\partial \mu_i}{\partial x_k} \cdot \nabla x_k, \quad i = 1, 2, \ldots, n_c - 1
\]  

(5.28)

Thus, chemical potential gradient, and hence the diffusional flux, incorporate the compositional dependence of the fluid. This dependence also relates to the non-ideality of the fluid.

Let us define \(\Gamma_{ik}\) such that:

\[
\frac{\partial \mu_i}{\partial x_k} = RT \frac{\partial \ln f_i}{\partial x_k} = \frac{RT}{x_k} \Gamma_{ik}
\]  

(5.29)

where

\[
\Gamma_{ik} = \frac{\partial \ln f_i}{\partial \ln x_k}, \quad i, k = 1, 2, \ldots, n_c - 1
\]  

(5.30)

Note that \(\Gamma_{ik}\) defined above is not the same as the transfer function defined earlier, although the symbol used for both is same.
Here, we also define matrix $X$ such that $X_{ii} = x_i$. Therefore, Eqn. (5.28) can be recasted as below:

$$
\nabla \mu = RTX^{-1}\Gamma \nabla x \\
\therefore \nabla x = \frac{\nabla \mu}{RTX^{-1}\Gamma}
$$

(5.31)

Now, the Fickian diffusion coefficients can also be derived from the Stefan-Maxwell’s diffusion coefficients ($\overline{D}_{ij}$) for each pair of components I and j (Leahy-Dios and Firoozabadi, 2007). Here, we define $B^M$ as:

$$
B^M_{ii} = \frac{x_i}{D_{in}} + \sum_{k=1, \neq i}^{n_c} \frac{x_k}{D_{ik}} \quad i = 1, 2, \ldots, n_c - 1 \\
B^M_{ij} = -x_i \left( \frac{1}{D_{ij}} - \frac{1}{D_{in}} \right) \quad i = 1, 2, \ldots, n_c - 1, \; i \neq j
$$

(5.32)

Now, $\beta^M = (B^M)^{-1}$. In terms of $\beta^M$, we can write Fickian coefficients as:

$$
D^{Fick} = \beta^M \cdot \Gamma
$$

(5.33)

Now,

$$
J = \overline{\rho} D^{Fick} \nabla x \\
= \frac{\overline{\rho} \nabla \mu}{RTX^{-1}\Gamma} \quad \text{... From Eqn. 5.31} \\
= \frac{\overline{\rho} \beta^M \Gamma \cdot \nabla \mu}{RTX^{-1}\Gamma} \quad \text{... From Eqn. 5.33} \\
= \frac{\overline{\rho}}{RT} \beta^M \nabla x
$$

(5.34)

For multi-component mixtures in porous media, the conventional form of Fick’s law can be written as:
Similarly, for chemical potential gradient approach, we write:

\[ J_{a,i} = -\phi_a S_a \rho_a \sum_{k=1}^{n_c} \phi_{a,ik}^k \nabla x_{a,k}, \quad i = 1,2,\ldots,n_c - 1 \]  

(5.36)

Eqn. 5.36 represents the final form of the diffusional flux equation used in the multi-mechanistic formulation in this work. In order to cast the above flux equation in proper units \((lbmol.RB/RCF.day)\), we need to formulate it as below for oil and gas phases:

\[ J_{o,i} = -\phi_o S_o \rho_o \frac{A_i}{5.615} \sum_{k=1}^{n_c} \beta_{o,ik} x_{o,k} \frac{\partial \mu_{o,k}}{\partial x}, \quad i = 1,2,\ldots,n_c - 1 \]  

\[ J_{g,i} = -\phi_g S_g \rho_g \frac{A_i}{5.615} \sum_{k=1}^{n_c} \beta_{g,ik} x_{g,k} \frac{\partial \mu_{g,k}}{\partial x}, \quad i = 1,2,\ldots,n_c - 1 \]  

(5.37)

Also note that these equations are written for matrix domain only. The equations developed above are substituted in residual equations developed in Chapter 4 as diffusional flux.
Chapter 6
Results and Discussion

In the previous chapters, we have covered the theoretical development of the numerical model, along with discussing the theory of adsorption and diffusion to be implemented in the compositional simulator. In the current chapter, we will present the validation of Cartesian compositional model with a commercial simulator, followed by validation of ellipsoidal model with an analytical solution. Next, we will present the standalone calculations for a numerical example of liquid phase adsorption model. A case study showcasing the integration of geochemical precursor with the compositional simulator will then be presented. Finally, we will present the parametric analysis on important adsorption and diffusion parameters.

6.1 Validation of Cartesian Compositional Model

The Cartesian model is validated with Computer Modeling Group’s GEM (CMG\(^1\) GEM\(^2\), 2014). Although the model is dual-porosity, dual permeability (DPDK), the validation is performed for the single porosity reservoir. This can be modeled by making the shape factor in matrix-fracture transfer function to be equal to zero. This also validates the fact that there is no unnecessary flow taking place between matrix and fracture, when shape factor is made to be zero. The relevant input data for this validation run are given in

---

\(^1\) CMG: Computer Modeling Group

\(^2\) GEM: Generalized Equation-of-State Model Compositional Reservoir Simulator
Table 6.1. For this case, we are considering a four-component fluid system, and the relevant details are given in Tables 6.2 and 6.3. In addition, the effect of adsorption and diffusion is neglected. As a matter of fact, even if these effects would have been included, they would not affect the overall solution, since these effects take place only in matrix domain (which is not modeled in this validation run). The total production time is 1 year.

Table 6-1. Input data for validation run with single-permeability, single-porosity model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir size</td>
<td>$2200 \times 2200 \times 100$</td>
</tr>
<tr>
<td>Fracture porosity</td>
<td>1%</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>15%</td>
</tr>
<tr>
<td>Fracture permeability (i,j,k)</td>
<td>0.01 md, 0.01 md, 0.001 md</td>
</tr>
<tr>
<td>Matrix permeability (i,j,k)</td>
<td>50 nd, 50 nd, 5 nd</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>2400 psia</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5 ft</td>
</tr>
<tr>
<td>Fracture initial water saturation</td>
<td>10%</td>
</tr>
<tr>
<td>Matrix initial water saturation</td>
<td>10%</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>250 F</td>
</tr>
<tr>
<td>Number of grid blocks (i,j,k)</td>
<td>$11 \times 11 \times 5$</td>
</tr>
<tr>
<td>Well location</td>
<td>6,6,1 to 6,6,5</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>750 psia</td>
</tr>
</tbody>
</table>
Table 6.2: Physical properties of the components.

<table>
<thead>
<tr>
<th>Component</th>
<th>Molecular weight</th>
<th>Critical temperature (F)</th>
<th>Critical pressure (psia)</th>
<th>Pitzer’s eccentric factor</th>
<th>Peng-Robinson attraction parameter</th>
<th>Peng-Robinson co-volume parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>16.043</td>
<td>-116.59</td>
<td>667.17</td>
<td>0.008</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>30.070</td>
<td>90.05</td>
<td>708.36</td>
<td>0.098</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>n-C₄H₁₀</td>
<td>58.124</td>
<td>305.69</td>
<td>551.14</td>
<td>0.296</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>n-C₆H₁₄</td>
<td>86.178</td>
<td>453.65</td>
<td>430.59</td>
<td>0.296</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
</tbody>
</table>

Table 6.3: Binary interaction parameters (BIPs) of the components.

<table>
<thead>
<tr>
<th>Component</th>
<th>P₁</th>
<th>P₂</th>
<th>P₃</th>
<th>P₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>n-C₄H₁₀</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>n-C₆H₁₄</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

The relative permeability data used is the one provided in the third SPE comparative project (Kenyon and Behie, 1987).

Figures 6.1 and 6.2 compare the gas and oil production rates at surface conditions. As can be seen, there is a good match between the proposed model versus the commercial simulator. Gas production rates predicted by our model are within 3-4% of the results given by the commercial model, while the difference is ~2% for oil production rates. A similar level of accuracy is obtained when comparing the molar production rates. This is shown in Figure 6.3, where the average difference between the models is about 2%.

Figure 6.4 shows the incremental material checks for the four components obtained from our simulator. The error in these calculations is consistently less than $10^{-7}\%$, which is
noteworthy. This example shows that the Cartesian model is well validated against the solution provided by commercial model.

Figure 6-1. Gas production rate comparison against commercial model

Figure 6-2. Oil production rate comparison against commercial model
Figure 6-3. Molar production rates comparison for validation run

Figure 6-4. Incremental material balance checks for validation run
6.2 Ellipsoidal (Prolate Spheroidal) Model Validation

In this sub-section, we provide the validation of the ellipsoidal model with an approximate analytical solution, as well as with fine-grid Cartesian model. The computational times are also compared for Cartesian and ellipsoidal models for showing similar accuracy. Next, we present the analytical solution used, along with its assumptions and limitation. This will be followed by input parameter description for ellipsoidal and Cartesian models. Finally, the comparison of the production performance of these models will be compared against analytical solution.

In this validation case, we try to use solutions for infinite-acting or transient state. Analytical solutions for horizontal wells during transient state can be broadly divided into three categories: i) Uniform flux solutions; ii) Infinite-conductivity solutions (i.e. uniform flux solution evaluated at equivalent pressure point); and iii) uniform flux with wellbore pressure averaging solutions (Joshi, 1991). In this study, we use the uniform flux approximation along the wellbore for calculating the analytical solution part of the validation problem.

Another important approximation used in available literature models is that of radial or pseudo-radial flow regime during early, transient phase. Fuchuk (1995) acknowledged that the first flow regime would be elliptic-cylindrical, however, he then proceeded to use to pseudo-radial approximation. Joshi (1988) decomposed the 3D problem into two 2D problems. The mathematical solutions of these 2D problems are then added to calculate horizontal well flow rate. In one of the 2D cases, he considered elliptical flow regime along the horizontal well section. The final 3D solution was
compared against steady-state solution and laboratory experiments with excellent agreement. However, since steady-state approximation cannot be applied perfectly in actual field cases as well as to our simulator, we did not use their solution method.

Instead, the infinite conductivity solution provided by Ozkan et al. (1989) for a horizontal well in an infinite reservoir is used in this work. A schematic of their horizontal well model is presented in Figure 6.5.

![Horizontal Well Model](image)

**Figure 6-5. Schematic of Horizontal Well Model [Reproduced from Ozkan et al., 1989]**

Their proposed analytical solution is shown below:

\[
p_D = \frac{\sqrt{\pi}}{4} \sqrt{k_h} \int_0^L \left[ erf \left( \frac{k_h}{k_v} + \frac{x_D}{2\tau} \right) + erf \left( \frac{k_h}{k_v} - \frac{x_D}{2\tau} \right) \right] \\
\times \left[ \exp \left( -\frac{y_D}{4\tau} \right) \right] \\
\times \left[ 1 + 2 \sum_{n=1}^\infty \exp \left( -n^2\pi^2L_D^2\tau \right) \cos(n\pi z_D) \cos(n\pi z_{wD}) \right] \frac{d\tau}{\sqrt{\tau}}
\]

(6.1)
where:

\[ p_D = \frac{k_h h (p_i - p_{\text{wellbore}})}{141.2 q B \mu}; \]

\[ L_D = \frac{L}{2h} \frac{k_y}{k_h}; \]

\[ x_D = \frac{2x}{L} \frac{k_h}{k_x}; \]

\[ y_D = \frac{2y}{L} \frac{k_h}{k_y}; \]

\[ z_D = \frac{z}{h}; \]

\[ z_{wD} = \frac{z_w}{h}; \]

\[ r_{wD} = \frac{2r_w}{L} \frac{k_h}{k_y}; \]

\[ t_D = \frac{0.001055 k_h t}{\phi \mu c L^2}; \]

\[ k_h = \sqrt{k_x k_y}; \]

Also,

\[ z_w = \text{vertical distance measured from the bottom boundary of the payzone to the well}; \]

\[ k_x = \text{permeability in the x direction in the areal plane, md}; \]

\[ k_y = \text{permeability in the y direction in the areal plane, md}; \]

\[ k_z = \text{permeability in the z direction, md}; \]

However, the above solution is too complex to implement in a practical manner.

Therefore, considering the early time radial flow, the above solution can be simplified to following (Joshi, 1991):
\[ p_i - p_{wf} = \frac{162.6qB\mu}{\sqrt{k_xk_yL}} \log \left( \frac{\sqrt{k_xk_y t}}{\phi \mu c \phi^2 \mu^2} \right) - 3.23 + 0.868s \]  

(6.3)

where \( s \) is the skin factor.

This equation is used to validate the results obtained from numerical simulator. A critical assumption here is the radial flow regime, along with infinite conductivity wellbore approximation. In addition, the rock and fluid properties such as oil viscosity, formation volume factor, total compressibility, absolute permeability, etc. are assumed to remain constant. While performing numerical simulation runs, some of these assumptions will be violated to a certain degree, and this will therefore have an impact on their solution comparison.

The input parameters for the Cartesian model are presented in Table 6.4 below. The same input parameters are used for ellipsoidal model, with the reservoir bulk volume kept the same for both cases. Table 6.5 presents the dimensions used in ellipsoidal model. Also, an isotropic formation is considered, since we wanted to check the performance of the developed ellipsoidal model versus the available analytical and Cartesian solutions. A four-component fluid system is considered, with the majority of fluid composition (~97%) being hexane, and the rest of the three components having a composition of 1% each. This assumption was taken to minimize the variation of fluid properties with pressure. Table 6.6 and 6.7 lists the fluid composition, individual component properties, and binary interaction parameters used in this run. Even though the dual-porosity, dual-permeability (DPDK) model is used, we have made the transfer function to be zero, such
that we only simulate the reservoir from a single-porosity single-permeability perspective.

**Table 6-4. Input parameters for Cartesian model.**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reservoir size</td>
<td>$2800 \times 175 \times 175$</td>
</tr>
<tr>
<td>Fracture porosity</td>
<td>1%</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>15%</td>
</tr>
<tr>
<td>Fracture permeability (i,j,k)</td>
<td>0.01 md, 0.01 md, 0.01 md</td>
</tr>
<tr>
<td>Matrix permeability (i,j,k)</td>
<td>50 nd, 50 nd, 50 nd</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>2400 psia</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5 ft</td>
</tr>
<tr>
<td>Fracture initial water saturation</td>
<td>10%</td>
</tr>
<tr>
<td>Matrix initial water saturation</td>
<td>10%</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>250 F</td>
</tr>
<tr>
<td>Number of grid blocks (i,j,k)</td>
<td>Variable (depends on the number of grid blocks, but is located in the center of reservoir)</td>
</tr>
<tr>
<td>Well location</td>
<td>Variable (depends on the number of grid blocks, but is located in the center of reservoir)</td>
</tr>
<tr>
<td>Oil flow rate</td>
<td>10 STB/day</td>
</tr>
</tbody>
</table>
Table 6-5. Reservoir dimensions for ellipsoidal model.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Focal length of ellipsoid (i.e. length of wellbore)</td>
<td>1000 ft</td>
</tr>
<tr>
<td>Semi-major axis of ellipsoid</td>
<td>1400 ft</td>
</tr>
<tr>
<td>Semi-minor axis of ellipsoid</td>
<td>150 ft</td>
</tr>
<tr>
<td>Number of grid blocks</td>
<td>Variable</td>
</tr>
<tr>
<td>Well location</td>
<td>Variable (depends on the number of grid blocks, but is located in the center of reservoir)</td>
</tr>
<tr>
<td>Oil flow rate</td>
<td>10 STB/day</td>
</tr>
</tbody>
</table>

Table 6-6. Physical properties of the components.

<table>
<thead>
<tr>
<th>Component</th>
<th>Molecular weight</th>
<th>Critical temperature (F)</th>
<th>Critical pressure (psia)</th>
<th>Pitzer’s accentric factor</th>
<th>Peng-Robinson attraction parameter</th>
<th>Peng-Robinson co-volume parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
<td>16.043</td>
<td>-116.59</td>
<td>667.17</td>
<td>0.008</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>30.070</td>
<td>90.05</td>
<td>708.36</td>
<td>0.098</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>44.097</td>
<td>205.97</td>
<td>615.7</td>
<td>0.152</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>n-C₆H₁₄</td>
<td>86.178</td>
<td>453.65</td>
<td>430.59</td>
<td>0.296</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
</tbody>
</table>

Table 6-7. Binary interaction parameters (BIPs) of the components.

<table>
<thead>
<tr>
<th>Component</th>
<th>P1</th>
<th>P2</th>
<th>P3</th>
<th>P4</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₄</td>
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<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>C₂H₆</td>
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<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>n-C₆H₁₀</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>n-C₆H₁₄</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>
We have used uniform flux approximation in numerical solution, while infinite conductivity assumption was used in analytical solution. The two solutions should therefore be evaluated on a common basis. Ozkan et al. (1989) had also stated that the pressure response for the two solutions (i.e. uniform flux and infinite conductivity) is same at $x_D$ value of 0.732. For the example used in this solution, $x_D$ of 0.732 corresponds to $x$ value of 366 ft. Thus, we evaluate the performance of numerical solution at a distance of 366 ft from heel of the wellbore.

Figure 6.6 presents the comparison of sandface pressure, calculated from numerical solutions for Cartesian and prolate spheroidal coordinates, as well as from analytical solution. Firstly, the numerical solution obtained from coarse grids is very far off the analytical solution. As we increase the grid density, or in other words, reduce the grid size, the numerical accuracy increases and the corresponding solution approaches to that from analytical solution. Also, since we reduce the grid orientation effects in prolate spheroidal coordinates, significantly lesser number of grid blocks are required to obtain the similar level of accuracy in comparison to Cartesian grid systems. This translates into lower computational times for obtaining a particular solution, and generally, the computational cost was lowered by about 10 times to that of Cartesian numerical simulation.

Next, the figure can be divided into two regions: Region 1 starting from 0 to about 20 days, and Region 2 at the end of simulation time (i.e. 150th day). It can be seen that the match for analytical solution and numerical solution is close (error less than 2%) in Region 1. While for region 2, the error increases to about 8%. This difference can be attributed to the simplified assumptions used in development of analytical solution. The
main assumption is that a radial flow regime is assumed in the analytical solution, instead of ellipsoidal flow regime. Also, other factors such as oil formation volume factor, total fluid compressibility, and oil viscosity are taken to be constants. However, these parameters vary, with oil viscosity changing the most. All of these contribute to the divergence of numerical solution from the analytical one, particularly towards the end of simulation time.

Nonetheless, it can be said that the numerical model is validated to an extent with the available analytical solution. Therefore, the prolate spheroidal numerical model can therefore be used for further parametric analysis shown in the next sub-sections.
6.3 Numerical Example of Liquid Phase Adsorption Calculations

In this sub-section, a standalone case is taken, where calculations are performed for a four-component fluid system present in single, liquid phase condition. Next, we provide parametric analysis on three important adsorption variables (viz. the overall composition of the fluid, the amount of adsorbent, and the adsorbent affinity towards each component).

6.3.1 Numerical Example

Let us first consider a four-component fluid system with initial pressure and temperature conditions such that the system exists in single liquid phase condition. This system is presented in Tables 6.8 and 6.9 below.

Table 6-8. Fluid composition for numerical example.

<table>
<thead>
<tr>
<th>Components</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.75</td>
</tr>
<tr>
<td>C2</td>
<td>0.15</td>
</tr>
<tr>
<td>C3</td>
<td>0.045</td>
</tr>
<tr>
<td>C4</td>
<td>0.055</td>
</tr>
</tbody>
</table>

Table 6-9. Pressure and temperature conditions.

<table>
<thead>
<tr>
<th>Initial Condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pressure</td>
<td>1400 psia</td>
</tr>
<tr>
<td>Temperature</td>
<td>350 R</td>
</tr>
</tbody>
</table>
Step 1 of the calculation procedure suggests that the given liquid mixture should be taken to its bubble point condition, and a flash calculation should be performed to determine the equilibrium vapor phase composition. In this study, Peng-Robinson EOS has been employed to perform VLE calculations (Peng and Robinson, 1976). The saturation pressure for the given composition and temperature is found out to be 522.9 (PVTSim, 2009) psia. At this pressure and temperature condition, the composition of the equilibrium liquid and vapor phases is given in Table 6.10 below.

Table 6-10. Equilibrium liquid and vapor phase compositions at pressure of 522.9 psia and temperature of 350 R.

<table>
<thead>
<tr>
<th>Components</th>
<th>Liquid phase composition</th>
<th>Vapor phase composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.7499</td>
<td>0.9434</td>
</tr>
<tr>
<td>C2</td>
<td>0.1501</td>
<td>0.0510</td>
</tr>
<tr>
<td>C3</td>
<td>0.0450</td>
<td>0.0044</td>
</tr>
<tr>
<td>C4</td>
<td>0.0550</td>
<td>0.0013</td>
</tr>
</tbody>
</table>

Step 2 then specifies that ideal adsorbed solution (IAS) theory should be used to calculate the adsorption capacity at this pressure condition. Using the procedure illustrated in Manik (1999), the adsorption capacity obtained is given in Table 6.11 below.

Table 6-11. Adsorption capacity obtained for vapor composition using IAS theory.

<table>
<thead>
<tr>
<th>Components</th>
<th>Adsorption capacity (lbmol/ton)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.0448</td>
</tr>
<tr>
<td>C2</td>
<td>0.0157</td>
</tr>
<tr>
<td>C3</td>
<td>0.0005</td>
</tr>
<tr>
<td>C4</td>
<td>0.0001</td>
</tr>
</tbody>
</table>
It should be noted that the adsorption capacity is mentioned in lbmol per ton of adsorbent present. As we will be using this algorithm for a specified grid block of the reservoir, we would know the amount of adsorbent present from the porosity measurements. Pure gas adsorption parameters, such as the Langmuir volume constant and Langmuir pressure constant for these four components are obtained from Ambrose et al. (2011).

The next part in step 2 is to calculate the limiting value of surface excess of vapor phase at bubble point pressure condition. This condition is specified in Eq. (5.22). Let us consider that initially, we had 1000 moles of fluid present. From the typical shale reservoir volumetric calculations, we can consider the adsorbent amount to be 1750 ton. Thus, from Eq. (5.22), the values of surface excess are presented in Table 6.12.

**Table 6-12. Limiting surface excess values of vapor phase.**

<table>
<thead>
<tr>
<th>Components</th>
<th>Surface excess, $n_i^{ve}$ (lbmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>-1.8682</td>
</tr>
<tr>
<td>C2</td>
<td>11.3860</td>
</tr>
<tr>
<td>C3</td>
<td>-3.8635</td>
</tr>
<tr>
<td>C4</td>
<td>-5.6542</td>
</tr>
</tbody>
</table>

The typical units of surface excess are lbmol/kg of adsorbent. However, in Table 6.12, we have calculated the total surface excess for 1750 ton of adsorbent present.

In step 3, we determine the composition of the contacted liquid phase using Eq. (5.19) and the criteria given in Eq. (5.23). After equating the limiting surface excess values of vapor phase with the definition of surface excess of liquid phase, the composition of liquid phase is calculated and presented in Table 6.13.
Table 6-13. Liquid phase composition after contact with adsorbent.

<table>
<thead>
<tr>
<th>Components</th>
<th>Liquid phase composition after contact</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>0.7519</td>
</tr>
<tr>
<td>C2</td>
<td>0.1386</td>
</tr>
<tr>
<td>C3</td>
<td>0.0489</td>
</tr>
<tr>
<td>C4</td>
<td>0.0606</td>
</tr>
</tbody>
</table>

Thus, we have computed the composition of liquid phase after a given amount is brought in contact with adsorbent. The procedure illustrated above is thermodynamically-consistent, and requires minimal changes to the code implementing IAS-based adsorption calculations. It should be noted that the amount of adsorbed phase is a function of the composition of liquid phase, adsorption constants of pure gas components, and amount of absorbent present. For the example shown above, a total of 107.01 lbmol of liquid phase was adsorbed (i.e. 10.70%). Neglecting this adsorbed phase calculations would therefore result in underestimation of reserves-in-place calculation as this additional storage mechanism is neglected in liquid-rich shale simulations.
6.3.2 Parametric Analysis

Sensitivity analysis (or parametric analysis) should be carried out in order to assess the impact of each variable on the output from a system. In this approach, only one variable is changed systematically while keeping other variables constant. In this study, the variables that underwent parametric analysis include the overall composition of the fluid, the amount of adsorbent, and the adsorbent affinity towards each component (i.e. Langmuir adsorption constants for each component). The base case that will be used to compare these cases is the same as presented in the section above.

**Overall fluid composition.** The first parameter to be varied is the overall fluid composition. The amount of adsorbent present and the adsorption affinity of shale organics towards each component are kept constant for these cases. Since our example considers a four-component reservoir fluid, we vary the composition of each component and study its impact on the total number of moles adsorbed as well as the change in liquid
composition being brought about by adsorption. In our analysis, we keep the initial conditions of the reservoir system as constant. By changing the overall composition, the saturation pressure changes, and thus the pressure at which step 2 calculations are performed changes. The cases to be considered in this exercise are listed in Table 6.14.

Table 6-14. Parametric study with overall fluid composition variation.

<table>
<thead>
<tr>
<th>Case #</th>
<th>Component</th>
<th>Amount of adsorbent present (ton)</th>
<th>Langmuir volume constant (SCF/ton)</th>
<th>Overall fluid composition (fraction)</th>
<th>(x^*_i) (fraction)</th>
<th>(y_i) (fraction)</th>
<th>(x_i) (from Eq. 19)</th>
<th>Total moles adsorbed (lbmol)</th>
<th>Total moles adsorbed (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C1</td>
<td>1750</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7519</td>
<td>107.01</td>
<td>10.70</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1386</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0489</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0606</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>C1</td>
<td>1750</td>
<td>56</td>
<td>0.71</td>
<td>0.7100</td>
<td>0.9572</td>
<td>0.7071</td>
<td>103.46</td>
<td>10.34</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1500</td>
<td>0.0381</td>
<td>0.1402</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.085</td>
<td>0.0850</td>
<td>0.0043</td>
<td>0.0923</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0004</td>
<td>0.0605</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>C1</td>
<td>1750</td>
<td>56</td>
<td>0.71</td>
<td>0.7100</td>
<td>0.9387</td>
<td>0.7055</td>
<td>108.04</td>
<td>10.84</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1500</td>
<td>0.0539</td>
<td>0.1405</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0049</td>
<td>0.0491</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.095</td>
<td>0.0950</td>
<td>0.0026</td>
<td>0.1050</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>C1</td>
<td>1750</td>
<td>56</td>
<td>0.72</td>
<td>0.7200</td>
<td>0.9496</td>
<td>0.7223</td>
<td>105.28</td>
<td>10.52</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.18</td>
<td>0.1800</td>
<td>0.0474</td>
<td>0.1682</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0025</td>
<td>0.0489</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0005</td>
<td>0.0606</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

As stated earlier, the amount of adsorbent present and adsorption affinity or Langmuir volume constant \(n_i\) are kept constant for this analysis. The \(x^*_i\) and \(y_i\) terms represent the equilibrium liquid and vapor compositions before the contact of the fluid with adsorbent, respectively. The \(x_i\) term represents the changed equilibrium liquid phase composition after contact with adsorbent.

As can be seen from the values of \(x_i\) calculated above, there is a significant difference in the fluid composition if adsorption from liquid phase is taken into account. The variation does not show a general trend as other factors such as Langmuir adsorption constants and
the total adsorbent present also play a crucial role in determination of this new composition. However, from the total number of moles adsorbed values presented above, we can suggest that around 10% of the fluid mixture gets adsorbed on the shale organics. This proves important in reserve estimation calculations, as well as fluid flow simulations, since this adsorbed phase might act as a source/sink terms in flow equations. To better understand the effect of the changed composition, we compare the phase diagrams of fluids with initial overall fluid composition with the changed liquid composition. These comparisons are presented in Figures 6.8 to 6.10.

Figure 6-8. Comparison of phase envelopes of original and adsorption-altered reservoir fluid for overall composition variation (case #1)
Amount of adsorbent present. In this case, we keep the composition and Langmuir volume parameter as constants and vary the amount of adsorbent present per 1000 lbmol of fluid mixture that we are considering. In our base case, we had estimated that for 1,000
lbmol of fluid mixture, we can consider 1750 ton of adsorbent present. This calculation was based on the general values of reservoir and fluid characterization for shale reservoirs. In this exercise, therefore, we increment and decrement the amount of adsorbent by 200 and 400 tons each, and present the calculations in Table 6.15 below.

Table 6-15. Parametric study with amount of adsorbent variation.

<table>
<thead>
<tr>
<th>Case #</th>
<th>Component</th>
<th>Amount of adsorbent present (ton)</th>
<th>Langmuir volume constant (SCF/ton)</th>
<th>Overall fluid composition (fraction)</th>
<th>( x_i^* ) (fraction)</th>
<th>( y_i ) (fraction)</th>
<th>( x_i ) (from Eq. 19)</th>
<th>Total moles adsorbed (lbmol)</th>
<th>Total moles adsorbed (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C1</td>
<td>1750</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7519</td>
<td>107.01</td>
<td>10.70</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1366</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0489</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0606</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>C1</td>
<td>1950</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7521</td>
<td>119.24</td>
<td>11.92</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1373</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0493</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0613</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>C1</td>
<td>2150</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7523</td>
<td>131.47</td>
<td>13.15</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1360</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0497</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0619</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>C1</td>
<td>1550</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7517</td>
<td>94.78</td>
<td>9.48</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1399</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0484</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0600</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>C1</td>
<td>1350</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7514</td>
<td>82.56</td>
<td>8.25</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td></td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1413</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td></td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0479</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td></td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0594</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Since we are keeping the overall fluid composition constant, the saturation pressure and hence, the equilibrium liquid and vapor composition remain the same for all the cases. The effect of changing the amount of adsorbent comes into play during the calculation of \( x_i \) from Eq. (5.19). Also, the change in adsorbent amount has a linear impact on the total moles adsorbed, as would be expected. For the cases considered in this exercise, the adsorbed amount varies between 8-14%. Thus, this parameter has one of the strongest
influence on the composition and quantity of adsorbed phase. The comparison between different cases in terms of their phase diagrams is shown in Figure 6.11.

Figure 6-11. Comparison of phase envelopes of original and adsorption-altered reservoir fluid for adsorbent amount variation

**Adsorption affinities towards each component.** The Langmuir adsorption parameters used in this paper are obtained from Ambrose et. al (2011). These values are provided for a reservoir temperature of 180 °F or 639.67 °R. However, in our calculations, the reservoir temperature has been fixed at 350 °R. Adsorption amount, typically, decreases with an increase in temperature and vice-a-versa. Thus, this provides a valid reason to perform a parametric study with varying adsorption constants. In this study, we have only varied Langmuir volume constant, and have kept Langmuir pressure constant as uniform. The variation of \( n_L \) for different cases is shown in Table 6.16. Compared to base case, the \( n_L \) values for all the components are increased by 10 and 20% for cases 1 and 2
respectively, while for cases 3 and 4, the values are decreased by a similar amount. Other parameters such as overall composition and the amount of adsorbent are kept constant.

Table 6-16. Parametric study with adsorption affinity parameter variation.

<table>
<thead>
<tr>
<th>Case #</th>
<th>Component</th>
<th>Amount of adsorbent present (ton)</th>
<th>Langmuir volume constant (SCF/ton)</th>
<th>Overall fluid composition (fraction)</th>
<th>$x_i^*$ (fraction)</th>
<th>$y_i$ (fraction)</th>
<th>$x_i$ (from Eq. 19)</th>
<th>Total moles adsorbed (lbmol)</th>
<th>Total moles adsorbed (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>C1</td>
<td>1750</td>
<td>56</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7519</td>
<td>107.01</td>
<td>10.70</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td>91</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1386</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td>179</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0489</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td>200</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0606</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>C1</td>
<td>1750</td>
<td>61.6</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7521</td>
<td>117.72</td>
<td>11.77</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td>100.1</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1375</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td>196.9</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0492</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td>220</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0612</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>C1</td>
<td>1750</td>
<td>67.2</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7522</td>
<td>128.42</td>
<td>12.84</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td>109.2</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1363</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td>214.8</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0496</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td>240</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0618</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>C1</td>
<td>1750</td>
<td>50.4</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7517</td>
<td>96.31</td>
<td>9.63</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td>81.9</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1398</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td>161.1</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0485</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td>180</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0601</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>C1</td>
<td>1750</td>
<td>44.8</td>
<td>0.75</td>
<td>0.7499</td>
<td>0.9434</td>
<td>0.7515</td>
<td>85.61</td>
<td>8.56</td>
</tr>
<tr>
<td></td>
<td>C2</td>
<td>72.8</td>
<td>0.15</td>
<td>0.1501</td>
<td>0.0510</td>
<td>0.1408</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C3</td>
<td>143.2</td>
<td>0.045</td>
<td>0.0450</td>
<td>0.0044</td>
<td>0.0484</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>C4</td>
<td>160</td>
<td>0.055</td>
<td>0.0550</td>
<td>0.0013</td>
<td>0.0593</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Comparing the total number of moles adsorbed for different cases with base case, we can see that the change is linear and matches the change brought about in $n_L$ values, both in direction and quantity. This means that a 10% increase in Langmuir volume constant causes a similar 10% increase in the number of moles adsorbed. This behavior of the model is again as expected since the amount of adsorbed phase is linearly related to $n_L$ as given in Eq. (5.1). Thus, it is extremely important to estimate the Langmuir adsorption parameters at the correct in-situ temperature values due to the linear dependence of
adsorption quantity on these parameters. The comparison of phase diagrams for these cases is shown in Figure 6.12.

![Figure 6-12. Comparison of phase envelopes of original and adsorption-altered reservoir fluid for adsorption affinities variation](image)

### 6.4 Geochemical Precursor Development

A precursor to the actual reservoir simulator is developed that provides information such as initial phase compositions and adsorption isotherm constants based on geochemical data. As geochemical data varies significantly from one basin to another, a case study approach has been used in this section so as to concentrate on a particular field and provide its calculations. For this purpose, the Barnett shale has been used as a model since certain portion of the field lies in the oil generation window while others lie in gas-condensate and dry-gas window. It should be noted that this precursor can be used for any field as long as the required geochemical data is available.
The precursor calculations are provided in following steps:

**Step 1:** Provide the maximum paleo-temperature reached in basin history ($T_{\text{max}}$), present-day hydrogen index ($\text{HI}_{pd}$), present-day total organic carbon content ($\text{TOC}_{pd}$) and present-day remaining potential ($S2_{pd}$).

For Barnett shale, these values are as follows (Jarvie et al., 2004):

$T_{\text{max}} = 454 \, \text{F}$, $\text{HI}_{pd} = 68 \, \text{mg HC/g TOC}$, $\text{TOC}_{pd} = 3.39\%$ and $S2_{pd} = 2.31 \, \text{mg HC/g rock}$

**Step 2:** Calculate original total organic carbon content ($\text{TOC}_{o}$), original hydrogen index ($\text{HI}_{o}$) and transformation ratio ($\text{TR}$).

For Barnett shale, assumption is made that the average value of carbon in hydrocarbons is about 83% while about 36% of TOC has been lost in the form of HC (Jarvie et al., 2004).

\[
\text{TOC}_{o} = \frac{\text{TOC}_{pd}}{0.64} = \frac{3.39}{0.64} = 5.31\% \, \text{g TOC/g rock}
\]  

(6.4)

\[
\text{TOC}_{\text{change}} = \text{TOC}_{o} - \text{TOC}_{pd}
\]  

(6.5)

\[
\text{TOC}_{\text{change}} = 5.31 - 3.39 = 1.91\% \, \text{g TOC/g rock}
\]

\[
S2_{o} = \frac{\text{TOC}_{\text{change}}}{0.083} + S2_{pd}
\]  

(6.6)

\[
S2_{o} = \frac{1.91}{0.083} + 2.31 = 25.35 \, \text{mg HC/g rock}
\]

\[
\text{HI}_{o} = \frac{S2_{o} \times 100}{\text{TOC}_{o}}
\]  

(6.7)

\[
\text{HI}_{o} = \frac{25.35}{5.31} \times 100
\]
\[ TR = \left( \frac{HI_o - HI_{pd}}{HI_o} \right) \times 100 \]  

\[ = \left( \frac{487 - 68}{487} \right) \times 100 \]

\[ = 86\% \]

**Step 3:** From table look-up, find out thermal maturity (\(\%R_o\)) window using transformation ratio. In case \(T_{max}\) is provided in step 1, calculate \(\%R_o\) from equation given below:

\[ \%R_o \text{ (calculated)} = (0.018 \times T_{max}) - 7.16 \]  

\[ = (0.018 \times 454) - 7.16 = 1.01\% \]

**Table 6-17. Thermal maturity versus transformation ratio data.**

<table>
<thead>
<tr>
<th>Transformation Ratio (TR)</th>
<th>Maturity Value ((%R_o))</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>&lt;0.65</td>
</tr>
<tr>
<td>10</td>
<td>0.66</td>
</tr>
<tr>
<td>20</td>
<td>0.67</td>
</tr>
<tr>
<td>30</td>
<td>0.68</td>
</tr>
<tr>
<td>40</td>
<td>0.7</td>
</tr>
<tr>
<td>50</td>
<td>0.76</td>
</tr>
<tr>
<td>60</td>
<td>0.82</td>
</tr>
<tr>
<td>70</td>
<td>0.88</td>
</tr>
<tr>
<td>80</td>
<td>0.95</td>
</tr>
<tr>
<td>85</td>
<td>1.00</td>
</tr>
<tr>
<td>90</td>
<td>1.11</td>
</tr>
<tr>
<td>92</td>
<td>1.29</td>
</tr>
<tr>
<td>94</td>
<td>1.45</td>
</tr>
<tr>
<td>96</td>
<td>1.58</td>
</tr>
<tr>
<td>98</td>
<td>1.8</td>
</tr>
<tr>
<td>100</td>
<td>&gt;2.5</td>
</tr>
</tbody>
</table>
Thus, if table look-up method is used, the thermal maturity value for 86% transformation ratio would be around 1.02%, which is close to what has been calculated in Eq. 6.9. Waples and Marzi (1998) suggest that for a particular type of kerogen, there is a strong correlation between transformation ratio and vitrinite reflectance regardless of burial and thermal history of the basin. This places a lot of confidence in the table look-up method and hence, Table 6.17 should be used whenever kerogen is of type II marine source.

**Step 4:** Based on TR and/or \%R_o values, predict the overall composition using an artificial expert system.

**Table 6-18. Molar compositions for different thermal maturity values.**

<table>
<thead>
<tr>
<th>Components</th>
<th>Molar Composition (%)</th>
<th>%R_o = 0.7</th>
<th>%R_o = 0.75</th>
<th>%R_o = 0.85</th>
<th>%R_o = 1.2</th>
<th>%R_o = 1.4</th>
<th>%R_o = 1.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO_2</td>
<td>1.28</td>
<td>1.82</td>
<td>2.30</td>
<td>2.68</td>
<td>2.88</td>
<td>3.05</td>
<td></td>
</tr>
<tr>
<td>N_2</td>
<td>0.73</td>
<td>0.10</td>
<td>0.13</td>
<td>0.15</td>
<td>0.16</td>
<td>0.18</td>
<td></td>
</tr>
<tr>
<td>C_1</td>
<td>31.23</td>
<td>44.52</td>
<td>56.44</td>
<td>65.88</td>
<td>70.75</td>
<td>74.73</td>
<td></td>
</tr>
<tr>
<td>C_2</td>
<td>4.31</td>
<td>5.88</td>
<td>7.29</td>
<td>8.33</td>
<td>8.94</td>
<td>9.43</td>
<td></td>
</tr>
<tr>
<td>C_3</td>
<td>4.15</td>
<td>4.50</td>
<td>4.83</td>
<td>4.67</td>
<td>4.98</td>
<td>5.24</td>
<td></td>
</tr>
<tr>
<td>i-C_4</td>
<td>1.35</td>
<td>1.30</td>
<td>1.25</td>
<td>1.04</td>
<td>1.10</td>
<td>1.14</td>
<td></td>
</tr>
<tr>
<td>n-C_4</td>
<td>3.38</td>
<td>2.97</td>
<td>2.61</td>
<td>1.82</td>
<td>1.89</td>
<td>1.96</td>
<td></td>
</tr>
<tr>
<td>i-C_5</td>
<td>1.80</td>
<td>1.50</td>
<td>1.24</td>
<td>0.82</td>
<td>0.80</td>
<td>0.79</td>
<td></td>
</tr>
<tr>
<td>n-C_5</td>
<td>2.14</td>
<td>1.71</td>
<td>1.32</td>
<td>0.79</td>
<td>0.73</td>
<td>0.69</td>
<td></td>
</tr>
<tr>
<td>C_6</td>
<td>4.62</td>
<td>3.28</td>
<td>2.07</td>
<td>1.20</td>
<td>0.67</td>
<td>0.24</td>
<td></td>
</tr>
<tr>
<td>C_7+</td>
<td>45.01</td>
<td>32.43</td>
<td>20.58</td>
<td>12.62</td>
<td>7.03</td>
<td>2.55</td>
<td></td>
</tr>
</tbody>
</table>

These six data sets are provided as training sets to an expert system, which can thus predict molar composition for any %R_o values between 0.7 and 1.8. The expert system used contains 2 hidden layers, with tansig, logsig, and purelin used as transfer functions. The number of neurons used were 5 and 10 in these hidden layers. For basic information regarding neural networks, the reader is referred to other works (Rajput, 2012). For the example case, where %R_o was determined to be 1.01%, the phase composition predicted by expert system is:
### Components Molar composition

<table>
<thead>
<tr>
<th>Components</th>
<th>Molar composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>2.49</td>
</tr>
<tr>
<td>N₂</td>
<td>0.12</td>
</tr>
<tr>
<td>C₁</td>
<td>63.70</td>
</tr>
<tr>
<td>C₂</td>
<td>8.09</td>
</tr>
<tr>
<td>C₃</td>
<td>4.53</td>
</tr>
<tr>
<td>i-C₄</td>
<td>1.05</td>
</tr>
<tr>
<td>n-C₄</td>
<td>1.99</td>
</tr>
<tr>
<td>i-C₅</td>
<td>0.96</td>
</tr>
<tr>
<td>n-C₅</td>
<td>0.97</td>
</tr>
<tr>
<td>C₆</td>
<td>1.90</td>
</tr>
<tr>
<td>C₇⁺</td>
<td>14.20</td>
</tr>
</tbody>
</table>

**Step 5**: Next, we generate phase envelopes using Peng-Robinson (PR) equation of state for the molar composition predicted by the expert system.

**Step 6**: The gas molecules adsorb on the surface of the organic matter. Therefore, the Langmuir adsorption constants such as $V_L$ and $P_L$ should be adjusted accordingly as their values would be different in the reservoir condition than those measured in laboratory based on organic matter content. The following adjustment is therefore proposed:

\[
V_{L,\text{corrected}} = V_{L,\text{laboratory}} \times \frac{\text{TOC}_p}{\text{TOC}_l}\]  \hspace{2cm} (6.10)

\[
P_{L,\text{corrected}} = P_{L,\text{laboratory}} \times \frac{\text{TOC}_p}{\text{TOC}_l}\]  \hspace{2cm} (6.11)

This precursor is added to the compositional simulator, and the integration between them is seamless. The user can therefore provide the geochemical parameters, if available, to the precursor, which will then provide overall composition and Langmuir constants as inputs to the actual fluid flow simulator.
6.5 Comparison of Diffusion Coefficient Models and Mapping of Multi-mechanistic Domain

In this sub-section, we aim to provide a comparison between the chemical-potential-driven diffusion coefficient model versus the conventional, concentration-gradient-based diffusion coefficient model. The former is based on irreversible thermodynamics, and is a function of pressure, temperature, and fluid composition, while an effective diffusion coefficient value is used in the latter. Although it is possible to derive and use thermodynamically-based coefficient values for concentration-based model, we choose to implement the effective values since these are the ones traditionally used in earlier studies at Penn State. Also, they provide a comparatively easier way of formulating the flux equations, although there was no significant increase in computational runtime for the two models. In addition, we try to map the important flow regimes (Darcian, Fickian, or Multi-mechanistic) for various matrix permeability values.

For these runs, we provide input parameters to the geochemical precursor, such that it will then provide overall fluid composition as an output to the reservoir simulator. This also served as an example case where we seamlessly integrated the geochemical precursor with simulation model. We employ the same example used in preceding section for Barnett Shale. As presented in Table 6.18, we have overall composition for 11 different pure components for different thermal maturity levels. However, since our simulator can handle four hydrocarbon components, we recombine the fluid into four pseudo components. The defined pseudo-components, and their properties are given in Table 6.19 below.
Table 6-29. Physical properties of the pseudo-components used.

<table>
<thead>
<tr>
<th>Component</th>
<th>Composition</th>
<th>Molecular weight</th>
<th>Critical temperature (°F)</th>
<th>Critical pressure (psia)</th>
<th>Pitzer’s acentric factor</th>
<th>Peng-Robinson attraction parameter</th>
<th>Peng-Robinson co-volume parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>63.70</td>
<td>16.043</td>
<td>-116.59</td>
<td>667.17</td>
<td>0.008</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>P2</td>
<td>12.61</td>
<td>44.103</td>
<td>206.13</td>
<td>616.55</td>
<td>0.198</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>P3</td>
<td>4.98</td>
<td>58.124</td>
<td>305.69</td>
<td>551.14</td>
<td>0.296</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
<tr>
<td>P4</td>
<td>18.70</td>
<td>86.178</td>
<td>453.65</td>
<td>430.59</td>
<td>0.296</td>
<td>0.45724</td>
<td>0.0778</td>
</tr>
</tbody>
</table>

Figures 6.13 to 6.15 present the cumulative gas production comparison of new diffusion model (based on chemical-potential gradient), old diffusion model (based on concentration gradient), and no diffusion case, for thermal maturity levels of 1.2, 1.4, and 1.8%.

![Cumulative gas production](image)

**Figure 6-13. Cumulative gas production under various flow regimes ($R_o = 1.2\%$)**
Figure 6-14. Cumulative gas production under various flow regimes ($R_o = 1.4\%$)

Figure 6-15. Cumulative gas production under various flow regimes ($R_o = 1.8\%$)
In general, we observe that for matrix permeability of 50 nD, diffusion provides much of the fluid recovery, and multi-mechanistic flow regime recovers 50–75% more cumulative gas production as compared to no diffusion case. The early production profiles, where hydraulic and natural fractures are predominantly depleted, typically fall on top of each other. However, once fluid withdrawal from matrix domain comes into the equation, the role of diffusion becomes significant. Here, we have also plotted the production profiles using the *old* diffusion coefficient model. As can be seen from the three figures, the *old* diffusion model was able to match the cumulative gas production data obtained from *new* diffusion model for $D_{eff}$ values of 0.5 to 1.3 ft$^2$/day. Earlier, values of 5, 10, and even 20 ft$^2$/day were used to compare the effect of multi-mechanistic flow regimes. However, based on this analysis, we can state that $D_{eff}$ values should be in the range given above, in order to realistically model the effect of diffusion on overall production performance. We can also state that values of 5, 10, and 20 ft$^2$/day are significantly large, and may not be realistic for tight reservoirs such as shales.

Next, we try to map the permeability range where each flow regime is important. In this case, we keep all the input parameters same, except the matrix permeability, which is varied from 50 nD to 5000 nD. Typical shale matrix permeabilities varies from 10 to 500 nD (Heller and Zoback, 2013). Three cases are considered, with matrix permeability of 50 nD, 500 nD, and 5000 nD. Figures 6.16 to 6.18 compare the cumulative gas production profiles for these three cases. We also plot production profile using *old* diffusion model, with a fixed $D_{eff}$ value of 2 ft$^2$/day.
Figure 6-16. Cumulative gas production for matrix permeability of 50 nD

Figure 6-17. Cumulative gas production for matrix permeability of 500 nD
As can be seen from the above figures, diffusional flux provides an additional 55% of cumulative gas recovery for 50 nD case. Similarly, the increase in recovery is around 45% for 500 nD case. However, for matrix permeability of 5000 nD, all the production profiles fall on almost top of each other. This type of behavior was expected to take place at a much higher matrix permeability (around 0.1 mD) (Ayala, 2004). However, due to smaller values of diffusion coefficients obtained from thermodynamically-consistent approach, this *overlapping* behavior occurs at a much smaller matrix permeability value, which is 0.005 mD in our case.

In essence, the mapping of different flow regimes can be summarized in Table 6.20 below.
Table 6-20. Mapping of multi-mechanistic flow regimes.

<table>
<thead>
<tr>
<th>Matrix permeability</th>
<th>Flow mechanism</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{matrix} &gt; 0.001$ md</td>
<td>Darcian flow</td>
</tr>
<tr>
<td>$0.001$ md &gt; $k_{matrix}$ &gt; $0.0001$ md</td>
<td>Multi-mechanistic flow</td>
</tr>
<tr>
<td>$0.0001$ md &gt; $k_{matrix}$</td>
<td>Fickian flow</td>
</tr>
</tbody>
</table>

Some explanation regarding the use of diffusion coefficients is due at this point. Ertekin et al. (1986) and da Silva and Belery (1989) had explained that there exist three types of diffusion, namely bulk or molecular diffusion, Knudsen diffusion, and surface diffusion. Bulk or molecular diffusion is important when molecule-molecule interaction is significant, while Knudsen diffusion is important in case of small pore sizes, where molecule-wall interaction would dominate over molecule-molecule interaction. Surface diffusion entails transport of absorbed gas molecules along gas/fluid surfaces. In case of nanopores, a combined effect of molecular and Knudsen diffusion is expected to be important. However, in this research so far, we have only modeled molecular diffusion. Therefore, it would be logical to study Knudsen diffusion effects, and this would be considered in the future work of this study. Nevertheless, the basic role of diffusion would be similar to what was explained in this sub-section, and the inclusion of Knudsen diffusion would only vary the amount of diffusional effects on overall fluid recovery. In addition, we did not pursue the role of diffusion on liquid phase recovery, and this should be taken up in future work.
6.6 Implementation of Liquid Phase Adsorption Model in Compositional Simulator

In this sub-section, we present a case study demonstrating the implementation of liquid-phase adsorption model, which was presented in Chapter 5, in the compositional model. The fluid components used are methane, ethane, propane, and butane. The selection of these components is governed by the adsorption data available in literature. Ambrose et al. (2011) have provided Langmuir adsorption constants for these four components on shales. The Langmuir constants and fluid composition are given in Table 6.21. Initial reservoir pressure is taken to be 1600 psia, while reservoir temperature is 500 rankine. Again, this is a hypothetical case, as reservoir temperature can never be less than atmospheric temperature (or 520 rankine). The initial reservoir pressure and temperature are selected such that the reservoir fluid is in single, liquid phase condition. Other physical properties of these four pure components are obtained from literature.

Table 6.21. Pure component adsorption data (Ambrose et al., 2011) and overall fluid composition information.

<table>
<thead>
<tr>
<th>Component</th>
<th>Langmuir volume constant (SCF/ton)</th>
<th>Langmuir pressure constant (psia)</th>
<th>Overall fluid composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>C1</td>
<td>56</td>
<td>1562</td>
<td>0.7</td>
</tr>
<tr>
<td>C2</td>
<td>91</td>
<td>811</td>
<td>0.15</td>
</tr>
<tr>
<td>C3</td>
<td>179</td>
<td>844</td>
<td>0.1</td>
</tr>
<tr>
<td>n-C4</td>
<td>200</td>
<td>500</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 6.22 presents the comparison of original species in place values for matrix and fracture domains, for with- and without liquid phase adsorption considerations.
Table 6-22. Original species in place calculations for with- and without liquid phase adsorption considerations.

<table>
<thead>
<tr>
<th>Component</th>
<th>No liquid phase adsorption</th>
<th>With liquid phase adsorption</th>
<th>Change (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Matrix (lbmol)</td>
<td>Fracture (lbmol)</td>
<td>Total (lbmol)</td>
</tr>
<tr>
<td>C1</td>
<td>4.85E+08</td>
<td>3.23E+05</td>
<td>4.85E+08</td>
</tr>
</tbody>
</table>

As can be seen from the table above, the species present in fracture domain in both considerations is the same. This is as expected, since adsorption will have negligible effect on fluid present in fractures. With adsorption considerations, the original quantity of methane present increased by 3.2%, while that of ethane, propane, and butane increased by more than 25%. This can be attributed to the data given in Table 6.21, which shows that adsorption affinity for higher carbon chain molecules is more (i.e. higher Langmuir volume constants) at any given pressure. This ultimately translates into 11.9% increase in OGIP calculations.

Another effect of liquid phase adsorption is on cumulative production data. Figure 6.18 shows the cumulative gas production comparison for three cases: neglecting liquid phase adsorption and diffusion, with liquid phase adsorption and neglecting diffusion, and with liquid phase adsorption and diffusion.
This figure provides an insight about the importance of diffusion in recovery processes from tight shales. For the cases where diffusion is neglected, the inclusion of liquid phase adsorption will not provide any improvement in fluid recovery. Even in cases where matrix pressure would drop significantly, fluid desorption from organic shale surfaces will take place, however, these fluids will not be transported from matrix to fracture due to absence of diffusion. Hence, we see the overlap of the two cases where diffusion is neglected, and where adsorption is considered in one of the cases. For the case where both phenomenon are considered, about 20% additional fluid recovery is obtained, mainly attributed to mass transport due to diffusion. Thus, it is important to state that, even though adsorption processes are important, they mainly act as storage terms, while the majority of flow is governed due to diffusion. In real field cases, sorption effects come into play significantly during later production times, when reservoir pressures drop substantially enough for the fluids to desorb and contribute to flow.
6.7 Type curve generation

6.7.1 Aim of the studies

Type curve is one of the most powerful tools available to a reservoir engineer. These curves are often used to estimate key reservoir properties, such as reservoir permeability, reservoir porosity, and reservoir boundaries. In general, there are two types of type curves: pressure-transient type curves and rate-transient type curves. As their names suggest, a pressure-transient type curve is generated when a flow-rate specification is specified at the inner boundary condition (i.e. BC at well), while for rate-transient type curve, bottomhole pressure needs to be specified (i.e. needs to be kept constant). These curves are dimensionless, and the dimensionless parameters are obtained through mathematical modification of the flow equations. For pressure-transient type curves, dimensionless pressure drop is plotted against dimensionless time on a log-log scale, while for rate-transient type curves, dimensionless flow rate versus dimensionless time are plotted.

In this chapter, we first present the definitions of dimensionless parameters. Next, with the help of a type-curve, we illustrate the typical characteristics exhibited by a shale reservoir type curve. The type-curve matching process is explained to validate the plots generated. Finally, we explain the effect of important parameters on type curves with the help of some sensitivity analysis.
6.7.2 Dimensionless parameters

The assumptions made while deriving these parameters are as follows:

- Reservoir is assumed to exhibit homogeneous and isotropic properties
- The capillary effect is negligible
- Diffusion term is neglected (The validity of this assumption lies in the fact that the main motivation here is to test the type-curve generation process for a reservoir with ellipsoidal boundary conditions)
- Only two-phase reservoir condition (gas-water) is considered

Here, we follow the development of type-curve formulation presented by Thararoop (2010). The dimensionless time ($t_D$), dimensionless pressure drop ($p_D$), and dimensionless gas and water flow rates ($q_{D,g}$, $q_{D,w}$) are defined as below:

\[
t_D = \frac{2.637 \times 10^{-4} \left( \lambda_g + \lambda_w \right) t}{\left( \phi_F c_F + \phi_M c_M \right) r_w^2}
\]

(6.12)

\[
p_D = \frac{p_i^2 - p_F^2}{p_i^2 - p_{wf}^2} q_D
\]

(6.13)

\[
q_{D,g} = \frac{1.424 q_{g,sc} ZT}{\lambda_g h \left( p_i^2 - p_{wf}^2 \right)}
\]

(6.14)

\[
q_{D,w} = \frac{282.53 q_{w,sc} B_{w,i} p_i}{\lambda_w h \left( p_i^2 - p_{wf}^2 \right)}
\]

(6.15)

where:
\[ \lambda_g = \frac{k_F k_{rg,F}}{\mu_g} \]  
\[ \lambda_w = \frac{k_F k_{rw,F}}{\mu_w} \]  
\[ c_F = \frac{1}{5.615 \phi_F} \left[ \frac{\partial \phi_F}{\partial p_F} - \phi_F \left( \frac{S_{g,F} \partial B_{g,F}}{B_{g,F}} + \frac{S_{w,F} \partial B_{w,F}}{B_{w,F}} \right) \right] \]  
\[ c_M = \frac{1}{5.615 \phi_M} \left[ \frac{5.615 B_{g,M}}{V_b} \frac{\partial V_M}{\partial p_M} + \frac{\partial \phi_M}{\partial p_M} - \phi_M \left( \frac{S_{g,M} \partial B_{g,M}}{B_{g,M}} + \frac{S_{w,M} \partial B_{w,M}}{B_{w,M}} \right) \right] \]

The units of \( t \) is day, \( k \) is md, \( p \) is psia, \( q_g \) is SCF/day, and \( q_w \) is STB/day.

### 6.7.3 Characteristics of type curve for shale reservoirs

A typical type curve for shale reservoirs is shown in Figure 6.19. Different flow regimes can be described based on this figure, as follows:

i) Points A to B represent the infinite acting flow regime, where the production is dominated by flow from fractures (in our case, the hydraulic fracture network). The extent of this straight line is determined by the efficiency of fracturing operation.

ii) Once the pressure transients reach the matrix boundary, the matrix starts depleting, aiding in the fluid production. It is during this phase that matrix-fracture fluid transfer starts taking place. This flow regime is represented by points B to C.
iii) At point C, the pressure transients have reached the outer boundaries of the reservoir. The production profile after this point is represented by points C to D, and is known as pseudo-steady state.

iv) The values of $\lambda$ and $\omega$ (storativity ratio) control the shape of type curve and the occurrence of these points. If $\lambda$ is high, point B will occur at an earlier time due to higher permeability for fluid to flow (and in turn, shorter time for the transients to reach matrix boundary). If $\omega$ is high, the curve will be shifted upwards due to higher fluid flow rate. Thus, $\lambda$ controls the horizontal movement of the type curve, while $\omega$ controls the vertical movement.

![Figure 6-20. Typical shale reservoir type-curve](image)

6.7.4 Validation of type curve

A type curve needs to be validated before it can be used for reservoir property estimation. In this exercise, we used the ellipsoidal numerical model to generate synthetic production
data, and tried to validate the type curve using type curve matching process. The reservoir properties used in this validation run are given in table 6.23. The dimensionless groups are calculated using equations (6.12), (6.14), and (6.15), and plotted on a log-log scale. Here, sandface pressure was specified, thus, we are generating rate-transient type curves. The synthetic production data is then plotted on log-log scale, and is used to match the log-log type curves. The type curve which provides the best match is selected, and used to estimate certain reservoir properties. These properties are then compared with the actual ones used during simulation run.

Table 6-23. Reservoir properties used during validation run.

<table>
<thead>
<tr>
<th>Reservoir parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture porosity</td>
<td>0.0002</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.1</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>0.7 md</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.00005 md</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>1500 psia</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.1</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5 ft</td>
</tr>
<tr>
<td>Reservoir thickness</td>
<td>300 ft</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>550 R</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>750 psia</td>
</tr>
</tbody>
</table>

The gas and water flow rates are plotted on a log-log scale versus time, and type-curve matching is performed on a set of rate-transient type curves with different values of initial water saturation. After overlaying the actual production log-log plot over type curve, a match was obtained for water saturation of 0.1. The type-curve match is shown in Figure 6.21, and the match point had following coordinate values:
The next step involves calculation of fracture permeability using the following equation:

$$k_f = \frac{1.424 q_{gw} Z T \mu_g}{q_d h (p_i^2 - p_{wf}^2) k_{rg}}$$

(6.20)

Here, gas viscosity is calculated using the volumetric average reservoir pressure, while the compressibility factor \((Z)\) is calculated from flash calculations.

Putting in the match point values, as well as other parameter values, we get fracture permeability to be 0.71 md. This is close to our actual value of 0.7 md. Therefore, the percent error is 1.4%.

Afterwards, we calculate fracture porosity using the following equation:
\[
\phi_f = \frac{2.637 \times 10^{-4} (\lambda_s + \lambda_w) \omega t}{t_D c_F r_w^2}
\]  
(6.21)

After putting in the values, fracture porosity is found out to be 0.00022. The actual value used in numerical simulation was 0.0002. Therefore, the percent error is around 10%.

Finally, we calculate matrix porosity as:

\[
\phi_m = \frac{2.637 \times 10^{-4} (\lambda_s + \lambda_w) (1 - \omega) t}{t_D c_M r_w^2}
\]  
(6.22)

From this equation, matrix porosity is calculated as 0.114. The actual value used in simulation was 0.11. Therefore, the percent error is around 3.6%. This shows that the type curve match was successful, and thus the type curves were validated.

Similarly, we perform the validation through the use of water production data.

The reservoir parameters used for this validation is given in table 6.24.

**Table 6-24. Reservoir properties used during validation run.**

<table>
<thead>
<tr>
<th>Reservoir parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture porosity</td>
<td>0.0001</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.15</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>0.03 md</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.00005 md</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>1500 psia</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.2</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5 ft</td>
</tr>
<tr>
<td>Reservoir thickness</td>
<td>300 ft</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>550 R</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>750 psia</td>
</tr>
</tbody>
</table>

The type curve match is shown in figure 6.21 below:
The match point had following coordinate values:

\[
\begin{align*}
q_{D,w} & = 0.006684 \\
t_D & = 5172.8
\end{align*}
\]

and

\[
\begin{align*}
q_w & = 475425 \\
t & = 0.01
\end{align*}
\]

The equation for calculation of fracture permeability is given as:

\[
k_f = \frac{282.53q_{w,sc}B_{wc}p_f\mu_w}{q_{D,w}h(p_i^2 - p_w^2)k_{rw}}
\]

(6.23)

The equations for calculating fracture and matrix porosities are same as the ones used in previous validation (viz. equations 7.10 and 7.11, respectively). The calculated values of fracture permeability, fracture porosity, and matrix porosity are 0.0313 md, 0.00015 and 0.159. Thus, the values predicted are close to the actual values used, and hence the type curves generated are validated through water production data as well.
6.7.5 Derivative type curves

Pressure derivative type curves were first proposed by Bourdet (1983). This type curve is generally used in association with the normal type curves presented above. The reason for using these type curves is that they are physically very distinct in comparison to pressure-change type curves. The “derivative” refers to the logarithmic derivative of the solution to the radial diffusivity equation. In such type curves, the derivative of pressure change ($p_{D'}$) is plotted against dimensionless time ($\Delta t_D$), again on a log-log plot. In most cases, the pressure-change and pressure derivative curves are plotted on the same graph.

The derivative of $(p_i - p_{wf})$ with respect to $\ln(t)$ is simply expressed as:

$$
p_{D'} = \frac{\partial (p_i - p_{wf})}{\partial \ln(t)} = \frac{t \partial (\Delta p)}{\partial (t)}
$$

(6.24)

We therefore plot the above-defined $q_{D'}$ versus $\Delta t_D$ to get derivative type curve for validation case 1 (i.e. gas production type curve). This plot is shown in Figure 6.23:

![Derivative type curve for gas production validation case](image)

Figure 6-23. Derivative type curve for gas production validation case
We do not aim to get any new information from this curve. Our goal in plotting the derivative type curve was to reinforce the validation case, as in the derivative plot shown above, the match is again obtained for initial water saturation of 0.1. This provides concrete validation for the type-curve generation process.

**6.7.6 Sensitivity Analysis**

The aim of this part of the exercise is to estimate the key sensitivity parameters with respect to the generated type curves. Here, we plot the pressure-change type curves for different initial pressure to sandface pressure ratio, length of ellipsoid major axis to well length ratio, matrix permeability, fracture permeability, matrix porosity and fracture porosity values. Similarly, the derivative plots are also plotted for different matrix and fracture permeabilities and porosities.

![Figure 6-24. Rate transient type curves for different initial pressure – sandface pressure ratios](image)
Figure 6-25. Rate transient type curves for different rubble zone major axis - well length ratios

Figure 6-26. Rate transient type curves for different matrix permeability values
Figure 6-27. Rate transient type curves for different fracture permeability values

Figure 6-28. Rate transient type curves for different matrix porosity values
Figure 6-29. Rate transient type curves for different fracture porosity values

Figure 6-30. Derivative type curves for different matrix permeability values
Figure 6-31. Derivative type curves for different fracture permeability values

Figure 6-32. Derivative type curves for different matrix porosity values
From the figures above, we can see that the type curves are sensitive to all the parameters studied viz. initial pressure-sandface pressure ratio, rubble zone major axis-well length ratio, matrix and fracture permeabilities, and matrix and fracture porosities. Since fracture properties are important during initial production phase of a well (as production is mainly aided by flow from fractures), the type curves are sensitive to these properties at early time (seen in Figure 6.33). The matrix comes into play during late time, and this is shown in variation in type curves during the corresponding late time production data (refer to Figure 6.32).
Chapter 7

A Case Study for Production Analysis: Utica Shale

7.1 Aim of the studies

In the previous chapters, a flow model in ellipsoidal coordinates was generated, and important mechanisms such as liquid-phase desorption and multi-component diffusion were studied. A series of type curves, with the aim of predicting certain key reservoir parameters, were also generated. In this chapter, we intend to integrate all the work that was achieved in terms of case studies. This study is performed on Utica Shale, and a sensitivity analysis is done on reservoir drainage area and hydraulic fracture effectiveness (SRV volume). At the end, we also perform Monte-Carlo simulation study on Utica and Marcellus shale cases.

7.2 Utica Shale Reservoir Parameters

The typical reservoir parameters for Utica shale are obtained from literature. Since Utica shale is relatively undeveloped, a reliable estimate of these parameters is difficult to obtain. Nonetheless, the key reservoir parameters and their ranges are given in Table 7.1 below (Hickman et. al., 2015; Swift et. al., 2014; Carbo Ceramics, 2016).
Here, we plan to use the geochemical precursor for calculating the hydrocarbon composition based on Utica shale geochemical parameters. In Step 1, we provide the the maximum paleo-temperature reached in basin history ($T_{\text{max}}$), present-day hydrogen index ($\text{HI}_{\text{pd}}$), present-day total organic carbon content ($\text{TOC}_{\text{pd}}$) and present-day remaining potential ($S_{2_{\text{pd}}}$). For Utica shale, these values are found to be as follows (Pennsylvania Geological Website, 2011):

$$T_{\text{max}} = 413 \, \text{F}, \quad \text{HI}_{\text{pd}} = 22 \, \text{mg HC/g TOC}, \quad \text{TOC}_{\text{pd}} = 2.38\% \quad \text{and} \quad S_{2_{\text{pd}}} = 0.53 \, \text{mg HC/g rock}$$

In Step 2, we calculate original total organic carbon content ($\text{TOC}_o$), original hydrogen index ($\text{HI}_o$) and transformation ratio (TR). For Utica shale, assumption is made that the average value of carbon in hydrocarbons is about 83% while about 36% of TOC has been lost in the form of HC (Pennsylvania Geological Website, 2011).

$$\text{TOC}_o = \frac{\text{TOC}_{pd}}{0.64} = \frac{2.38}{0.64} = 3.72\% \quad \text{g TOC/g rock}$$

(7.1)

$$\text{TOC}_{\text{change}} = \text{TOC}_o - \text{TOC}_{pd}$$

(7.2)

$$= 3.72 - 2.38 = 1.34\% \quad \text{g TOC/g rock}$$
\[
S2_o = \frac{TOC_{\text{change}}}{0.083} + S2_{pd} \\
= \frac{1.34}{0.083} + 0.53 \\
= 16.67 \text{ mg HC/g rock}
\]

\[
HI_o = \frac{S2_o}{TOC_o} \times 100 \\
= \frac{16.67}{3.72} \times 100 \\
= 448.1 \text{ mg HC/g TOC}
\]

\[
TR = \left( \frac{HI_o - HI_{pd}}{HI_o} \right) \times 100 \\
= \left( \frac{448.1 - 22}{448.1} \right) \times 100 \\
= 95.1\%
\]

In Step 3, from table look-up, we determine the thermal maturity ($%R_o$) window using transformation ratio. We refer to Table 6.17 presented in Chapter 6 for calculating the thermal maturity. The thermal maturity level obtained is around 1.51%, although this could not be verified since no measurement was reported for vitrinite reflectance. However, the kerogen type was reported to be gas, and this correlates well with the obtained thermal maturity above.

Step 4 involves predicting the overall fluid composition based on transformation ratio and/or $%R_o$ values using an artificial neural network. Again, we use the molar
compositions presented for different thermal maturities in table 6.18. For the example case, where %R_o was determined to be 1.51%, the phase composition predicted by expert system is shown in table below:

**Table 7-2. Fluid composition predicted by expert system for thermal maturity of 1.51%**.

<table>
<thead>
<tr>
<th>Components</th>
<th>Molar composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO₂</td>
<td>2.93</td>
</tr>
<tr>
<td>N₂</td>
<td>0.17</td>
</tr>
<tr>
<td>C₁</td>
<td>71.84</td>
</tr>
<tr>
<td>C₂</td>
<td>9.07</td>
</tr>
<tr>
<td>C₃</td>
<td>5.05</td>
</tr>
<tr>
<td>i-C₄</td>
<td>1.11</td>
</tr>
<tr>
<td>n-C₄</td>
<td>1.91</td>
</tr>
<tr>
<td>i-C₅</td>
<td>0.80</td>
</tr>
<tr>
<td>n-C₅</td>
<td>0.72</td>
</tr>
<tr>
<td>C₆</td>
<td>0.55</td>
</tr>
<tr>
<td>C₇⁺</td>
<td>5.85</td>
</tr>
</tbody>
</table>

We use this composition for performing further sensitivity analysis presented in the next sections of our discussion. Our goal here is to access the impact of drainage area and SRV region effectiveness on overall fluid production. In many instances, the drainage area is not optimized, and this may affect the ultimate recoveries obtained from a particular field. It is our motivation here to show that drainage area selection can be optimized via single-well studies as presented below.

Before the sensitivity analysis with respect of drainage area is presented below, there is one important note that should be explained when we consider drainage area in our case. Since we are using prolate spheroidal (or ellipsoidal) model throughout our simulation runs, the concept of drainage area needs to be clarified. The drainage area reported is the half of the surface area of ellipsoid. Basically, we are approximating the top surface area
of ellipsoid to be equivalent to the drainage area of the reservoir. The following figure illustrates our point:

![Diagram](image)

**Figure 7-1. 2-D schematic of the concept of drainage area in prolate spheroidal model**

### 7.3 Sensitivity Analysis – Drainage Area

In this section, we assess the effect of different drainage area on hydrocarbon recovery, and determine whether an optimum drainage area exists for a given Utica shale reservoir field. The outcome of this exercise will be largest economically-possible drainage area to be developed by a single horizontal well, under the given reservoir and design parameters.

The reservoir parameters used in this exercise are derived from Table 7.1, which are field reported minimum and maximum values. Other parameters, such as initial reservoir pressure and temperature, are obtained from synthetic studies reported in literature.
Table 7-3. Parameters used for sensitivity analysis with drainage area.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture porosity</td>
<td>0.045</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.00045</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>0.021 md</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.00005 md</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>2100 psia</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.4</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5 ft</td>
</tr>
<tr>
<td>Reservoir thickness</td>
<td>300 ft</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>550 R</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>750 psia</td>
</tr>
<tr>
<td>Well length</td>
<td>600 ft</td>
</tr>
<tr>
<td>Major axis to well length ratio</td>
<td>1.2</td>
</tr>
</tbody>
</table>

In this analysis, all the parameters are kept constant during various simulation runs, except the drainage area, which is varied from 20 acres to 120 acres. Most importantly, the stimulated reservoir volume is also kept constant during various runs, along with the horizontal well length and operating conditions.

Figure 7.2 shows the comparison of cumulative gas production for various drainage area scenarios. It can be seen from this figure that although cumulative production increases with larger drainage area, the increase is not significant. This is further illustrated in Figure 7.3, which plots the cumulative gas production at the end of 30th year of production versus drainage area. As we can see, the percentage increase in production after about 100 acres is insignificant.

Similar observations can be made via the data displayed in Figures 7.4 and 7.5. Figure 7.4 plots the percent gas recovery versus drainage area. One can note that with increased reservoir volume, the percent gas recovery decreases, even though the cumulative gas production increased (as seen in Figure 7.2). This is to be expected, since after the
depletion of SRV, the well is unable to deplete the matrix and in effect, the original, unstimulated reservoir. Due to extremely low permeability, the pressure transients do not reach farther away from SRV-boundaries. It is therefore necessary to maximize the SRV dimensions in order to achieve large production volumes. However, once SRV is designed optimally, it is also equally important to optimize the drainage area available for a single well. Ideally, the operator would want to place wells very close to each other (say, 10 acres or less), but the cost of drilling and operating a horizontal well also needs to be taken into account. It is, therefore, a trade-off situation between the number of wells to be drilled and the overall capex. Figure 7.5 plots the percentage change in gas recovery and cumulative gas versus drainage area. From this figure we can see that, the drainage area increase from 20 to 40 acres causes the cumulative production to increase by ~57%. However, a further increase of 20 acres to the area is not very efficient, since there is no correspondingly substantial increase in cumulative volumes. For this particular reservoir, with the design conditions implemented, it can be stated that the optimal drainage area is around 65-70 acres. Furthermore, the area should be definitely less than 100 acres, as a further increase in area makes the well performance economically unsound. Table 7.4 below summarizes the values used to plot these various graphs.

Table 7-4. Results for sensitivity analysis with drainage area.

<table>
<thead>
<tr>
<th>Area</th>
<th>Gas recovery (%)</th>
<th>% Change</th>
<th>Cumulative gas (MSCF)</th>
<th>% Change</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.00</td>
<td>56.80</td>
<td>-</td>
<td>9.37E+05</td>
<td>-</td>
</tr>
<tr>
<td>40.00</td>
<td>44.63</td>
<td>21.43</td>
<td>1.47E+06</td>
<td>57.14</td>
</tr>
<tr>
<td>60.00</td>
<td>36.94</td>
<td>17.22</td>
<td>1.83E+06</td>
<td>24.17</td>
</tr>
<tr>
<td>80.00</td>
<td>31.72</td>
<td>14.15</td>
<td>2.09E+06</td>
<td>14.47</td>
</tr>
<tr>
<td>100.00</td>
<td>27.92</td>
<td>11.97</td>
<td>2.30E+06</td>
<td>10.04</td>
</tr>
<tr>
<td>120.00</td>
<td>25.02</td>
<td>10.38</td>
<td>2.48E+06</td>
<td>7.54</td>
</tr>
</tbody>
</table>
Figure 7-2. Comparison of cumulative gas production for various drainage area scenarios

Figure 7-3. 30th year cumulative gas production values versus different drainage area
Figure 7-4. 30\textsuperscript{th} year gas recovery factor versus different drainage area

Figure 7-5. Percent change in gas recovery (decrease) and cumulative gas (increase) for different drainage area values
7.4 Sensitivity Analysis – SRV Volume

Similar to the previous section, we try to access the effect of SRV volume (or in other words, the effectiveness of hydraulic fracturing operation) on hydrocarbon recovery. Here, there can be two possible parameters with which a sensitivity analysis could be performed: SRV volume and hydraulic fracture permeability. However, in this exercise, an analysis is performed only on SRV volume, keeping the hydraulic fracture permeability constant.

The reservoir parameters used in this exercise are presented in Table 7.5 below.

Table 7-5. Parameters used for sensitivity analysis with SRV volume.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fracture porosity</td>
<td>0.039</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.00039</td>
</tr>
<tr>
<td>Fracture permeability</td>
<td>0.01 md</td>
</tr>
<tr>
<td>Matrix permeability</td>
<td>0.00005 md</td>
</tr>
<tr>
<td>Initial reservoir pressure</td>
<td>1800 psia</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.4</td>
</tr>
<tr>
<td>Fracture spacing</td>
<td>5 ft</td>
</tr>
<tr>
<td>Reservoir thickness</td>
<td>300 ft</td>
</tr>
<tr>
<td>Reservoir temperature</td>
<td>550 R</td>
</tr>
<tr>
<td>Sandface pressure</td>
<td>750 psia</td>
</tr>
<tr>
<td>Well length</td>
<td>1200 ft</td>
</tr>
</tbody>
</table>

In this analysis, all the parameters are kept constant during various simulation runs, except the SRV volume, which is varied from 0.19 to 0.30 fraction of the overall drainage volume. Parameters such as horizontal well length and drainage area (70 acres) are also kept constant.

Figure 7.6 shows the comparison of cumulative gas production for various SRV volume scenarios. As expected, the cumulative production increases with larger volumes.
However, the SRV volume fraction will be physically limited by the fracture half-length propagation. Here, we limit this ratio to be 0.3. Another important point that can be deduced from this analysis is that, as SRV volume increases, there is not a linear increase in cumulative production volumes. For SRV volume-drainage volume ratio of about 0.2, the recovery is around 0.180. However, for the volume ratio of about 0.32, the recovery increases to 0.265. Thus, we can state that the volume nearest to the horizontal well is drained more efficiently as compared to far-away region.

The figure also compares the hydraulic fracture cases with the un-stimulated one. As one can see, there is significant increase in cumulative production due to hydraulic fracturing. Recovery for un-stimulated fracture case is around 2.5% after 30 years of production, while those for fractured cases range from 18 to 26%.

The results can be viewed through a different angle by observing Figures 7.7 and 7.8. Figure 7.7 plots the recovery factor versus the SRV-drainage volume ratio, and the data displayed reiterate the above explanation regarding no linear increase for recovery for unit increase in volume ratio. Figure 7.8 shows the percentage change in recovery factor in comparison to the volume ratio. Again, we see that the percent increase in recovery does not match the increase in volume of SRV. However, a definite conclusion should be made only when we take into account the economics of additional SRV volume creation vs. the additional revenue due to higher cumulative production.

Here, we tried to generate the surface map of recoveries due to different drainage area and SRV-drainage volume ratios. This surface map is shown in Figure 7.9. As expected from previous analysis, increase in drainage area causes a net decrease in recovery factor, while increase in volume ratio increases the recovery factor. Therefore,
the surface map shows a maxima at high volume ratio and small drainage area. Nevertheless, it should be noted that this condition would also point towards highest capital expenditure in terms of drilling additional wells and creating increasing larger SRV volumes. Therefore, the optimum values of SRV volume and drainage area should be expected to be somewhere in the middle of surface map, as dictated by NPV calculations.

![Graph showing cumulative gas production for different SRV-Drainage Volume Ratios](image)

**Figure 7-6. Cumulative gas production for different SRV-Drainage Volume Ratios**
Figure 7-7. Gas recovery factor against different SRV-Drainage Volume Ratios

Figure 7-8. Percent change in gas recovery (increase) for different SRV-Drainage Volume Ratios
The aim of this exercise is to perform Monte-Carlo simulation on typical reservoir parameters, in order to reduce the uncertainty in measurement of their values, and to provide a reliable estimate of recovery factors for Utica shale. Since thermal maturity factors vary largely from gas-prone to oil-prone regions, we performed this study separately for gas-rich and oil-rich fields. At the end, we also performed a comparison study between Utica and Marcellus dry gas field recovery factors.

Table 7.5 below presents the ranges for typical reservoir parameters for Utica shale reservoir (Harper, 2011; Hickman et. al., 2015; Swift et. al., 2014). The type of distribution used for a particular parameter is also illustrated in the table.
Here, we are keeping the fluid-type constant (i.e. gas-rich zone). This is achieved by fixing the geochemical parameters to those of gas-type hydrocarbon zone, obtained from Harper (2011).

In these exercises, we are varying drainage area and SRV-drainage volume ratios at fixed intervals, since these parameters are controlled by the operator, and as such are not unknown and do not follow any particular distribution type. For drainage area, the values considered are 20, 40, 60, 80, and 100 acres. For SRV-drainage volume ratio, we considered 0.1, 0.15, 0.2, 0.25, and 0.3. In total, we have therefore considered 25 cases. For each of these cases, we ran about 200 simulation runs, varying the rest of the reservoir parameters presented in Table 7.6. In essence, we are generating P10, P50, and P90 recovery factors for each of these 25 cases, and they are presented here.

Figures 7.10, 7.11 and 7.12 present the P10, P50 and P90 recovery values respectively. In each of these figures, the recoveries are plotted against SRV-drainage volume ratios, and we have five different curves in each figure (representing different drainage areas). The simulation runtime (production time) considered is 30 years.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Min Value</th>
<th>Max Value</th>
<th>Type of distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area</td>
<td>20</td>
<td>100</td>
<td>-</td>
</tr>
<tr>
<td>Thickness</td>
<td>200</td>
<td>1000</td>
<td>Normal</td>
</tr>
<tr>
<td>Natural fracture permeability</td>
<td>0.0001</td>
<td>0.05</td>
<td>Uniform</td>
</tr>
<tr>
<td>Matrix porosity</td>
<td>0.03</td>
<td>0.08</td>
<td>Normal</td>
</tr>
<tr>
<td>Water Saturation</td>
<td>0.2</td>
<td>0.35</td>
<td>Triangular</td>
</tr>
<tr>
<td>SRV-Drainage volume ratio</td>
<td>0.1</td>
<td>0.3</td>
<td>-</td>
</tr>
<tr>
<td>SRV-permeability</td>
<td>0.01</td>
<td>1</td>
<td>Uniform</td>
</tr>
<tr>
<td>SRV-porosity</td>
<td>0.1</td>
<td>0.15</td>
<td>Normal</td>
</tr>
<tr>
<td>Initial Reservoir Pressure</td>
<td>3000</td>
<td>9000</td>
<td>Normal</td>
</tr>
</tbody>
</table>

Table 7-6. Reservoir properties used for Utica shale monte-carlo simulation exercise.
Figure 7-10. P10 recovery factors for dry-gas case in Utica shale

Figure 7-11. P50 recovery factors for dry-gas case in Utica shale
From the figures we can see that, the recovery factors vary from a high of about 61% for a drainage area of 20 acres and a SRV-drainage volume ratio of 0.3, to a low of 8.2% for 100 acres area and 0.1 volume ratio. In general, we can see that the recovery factor and volume ratio do not follow a linear relationship, which is expected. The recovery values seem to taper off after about a volume ratio 0.25, where incremental increase is smaller. These figures can also be viewed from an economical point of view, where the operator can optimize the fracturing process till the point where incremental gains become rather insignificant. Also, the volume ratio of 0.3 for area of 100 acres might be unrealistic in physical terms, but we are nonetheless presenting it here for comparison purposes.

Next, we perform a similar exercise on oil-prone reservoirs conditions. Again, the geochemical parameters for such a case are taken from Harper (2011). Figures 7.13, 7.14 and 7.15 represent P10, P50 and P90 recovery factors. As compared to the gas-rich region, the oil recovery factors vary between 6.7 to 55.8%.
Figure 7-13. P10 recovery factors for oil-rich case in Utica shale

Figure 7-14. P50 recovery factors for oil-rich case in Utica shale
Finally, we compare the recoveries from a typical Marcellus shale gas field to that from Utica shale. The reservoir parameters used for Marcellus shale case study are provided in Table 7.7 below.

Table 7-7. Reservoir properties used for Marcellus shale monte-carlo simulation exercise.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Min Value</th>
<th>Max Value</th>
<th>Type of distribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area (acres)</td>
<td>20</td>
<td>100</td>
<td>-</td>
</tr>
<tr>
<td>Thickness (ft)</td>
<td>300</td>
<td>1400</td>
<td>Normal</td>
</tr>
<tr>
<td>Natural fracture permeability (md)</td>
<td>0.001</td>
<td>0.1</td>
<td>Uniform</td>
</tr>
<tr>
<td>Matrix permeability (md)</td>
<td>0.000001</td>
<td>0.01</td>
<td>Uniform</td>
</tr>
<tr>
<td>Matrix porosity (fraction)</td>
<td>0.005</td>
<td>0.07</td>
<td>Normal</td>
</tr>
<tr>
<td>Water Saturation (fraction)</td>
<td>0.1</td>
<td>0.4</td>
<td>Triangular</td>
</tr>
<tr>
<td>SRV-Drainage volume ratio</td>
<td>0.1</td>
<td>0.3</td>
<td>-</td>
</tr>
<tr>
<td>SRV-permeability (md)</td>
<td>0.01</td>
<td>1</td>
<td>Uniform</td>
</tr>
<tr>
<td>SRV-porosity (fraction)</td>
<td>0.1</td>
<td>0.15</td>
<td>Normal</td>
</tr>
<tr>
<td>Initial Reservoir Pressure (psia)</td>
<td>1900</td>
<td>3900</td>
<td>Normal</td>
</tr>
</tbody>
</table>
Similar to the previous exercise, the P10, P50 and P90 recoveries are presented in Figures 7.16, 7.17 and 7.18 respectively below.

**Figure 7-16. P10 recovery factors for gas-rich case in Marcellus shale**

**Figure 7-17. P50 recovery factors for gas-rich case in Marcellus shale**
For Marcellus shale gas, the predicted recoveries ranges from 7% to 56%. As compared to Utica, these figures are on the lower side. To illustrate this in a better way, a plot is made to compare the P90 recoveries for both formations for drainage are of 60 acres. This is shown in Figure 7.19 below.
From the figure, one can see that recoveries from Utica shale are, on an average, 18% higher as compared to those from Marcellus. Although there are a number of factors affecting the production performance, with operating conditions being equal, the higher recoveries are obtained due to higher initial reservoir pressure. As a final note, we want to state that the results and analysis presented above are obtained using typical parameter values as obtained from field data, and we might expect different results for individual fields for Marcellus and Utica shale formations. In such cases, the Monte-Carlo exercise needs to be performed again to obtain accurate results.
Chapter 8
Conclusions and Future Work

8.1 Conclusions

Some important conclusions can be made for the study conducted till date:

- In this research, a dual-porosity, dual-permeability, multi-mechanistic, compositional model that accounts for multi-component adsorption and diffusion processes in shales was developed. The model is fully-implicit, and can handle upto four hydrocarbon components.

- The model has the capability of performing simulations in Cartesian as well as Ellipsoidal (Prolate Spheroidal) Coordinates. The development of Ellipsoidal coordinates was considered to be essential in reducing the grid orientation effects in near-wellbore horizontal wells, as well as for proper modeling of the stimulated reservoir volume.

- Both, the Cartesian and the Ellipsoidal grid models, were validated. The Cartesian model was validated against a commercial numerical simulator, while the Ellipsoidal model was validated against an analytical solution available in the literature. The match between the simulator and analytical solution was deemed to be satisfactory.

- A liquid phase adsorption model was developed and implemented in numerical simulator. The model is an extension of ideal adsorbed solution theory (IAST) to calculate the adsorbed phase properties using vapor-liquid equilibria theory.
Standalone calculations were performed for a case study, and it was shown that liquid phase adsorption can account for around 8-12% of the original fluid. Parametric analysis was also performed for overall fluid composition, amount of adsorbent, and adsorbent affinity towards each component. Implementation of liquid phase adsorption model into simulator was also demonstrated with the help of an example.

- Diffusion model based on chemical potential gradient was applied to examples in shale reservoirs. The results were compared against those using effective diffusion coefficient values for concentration-gradient based diffusion model. It was observed that for extremely tight reservoirs (matrix permeability < 100 nD), diffusion contributed to more than 50% of the total fluid recovery. Also, it was observed that effective molecular diffusion coefficient values of 5 ft²/day or more might be unrealistic to be used in modeling of flow in shales. A realistic range might be around 1 to 1.5 ft²/day. Mapping of multi-mechanistic domain was also carried out.

- A geochemical precursor was developed that would aid in fluid characterization using the routinely collected geochemical data. The overall fluid composition was correlated to the thermal maturity values for Barnett shale, and a case study was shown for demonstrating the calculation steps required. This precursor is integrated with the numerical simulator, where the user has the option of presenting only the geochemical information, without the need of providing any fluid composition and Langmuir parametric information to the simulator.
Pressure transient type curves are generated using synthetic data from ellipsoidal model. The aim of this exercise was to check whether the newly developed ellipsoidal model could be used in type curve generation process with satisfactory accuracy. The type curves therefore needed to be validated, and this was performed through the type-curve matching exercise. In addition to the pressure-change type curves, derivatives type curves were also presented. Similar level of accuracy is obtained in both types.

Finally, sensitivity analysis is carried out with respect to drainage area and SRV volume for typical Utica shale reservoir properties. It was found out that, for the reservoir properties considered, the largest economically-allowable drainage area was around 63 acres. Increasing the effectiveness of SRV increased the cumulative production, however, this should be considered in conjunction with economic calculations. Monte-carlo simulation study was carried out for dry-gas and oil-rich regions of Utica shale, and a comparison was performed for dry-gas regions of Utica and Marcellus shales. Again, for the properties considered, the probabilistic recoveries for Utica were found to be larger than that for Marcellus.

8.2 Future Work

Following additions were identified as immediate ways to extend the study presented in this thesis:
• As stated in Chapter 6, the effect of Knudsen diffusion on the calculation of overall diffusion coefficient should be performed. Examples need to be shown illustrating their relative importance.

• The pore compressibility effects were neglected in this study, and future work would entail incorporating these effects into the PVT behavior of fluids in shales.

• A case study will be shown for CO₂ huff and puff process, with the importance of multi-mechanistic flow can be investigated with the help of the new formulation of diffusion.

In this study, only ellipsoidal model was developed to approximate the rubble zone as well as the original reservoir region. An extension of this study would be to generate a hybrid model, where the rubble zone will still be represented by ellipsoidal model, but the region beyond that can be modeled using Cartesian coordinates. It is postulated that this model will lead to further accurate analysis of the flow regime.
REFERENCES


Appendix A

Permeability Transformation

Since permeability is a tensor, it needs to be transformed into prolate spheroidal coordinates before it can be used in that coordinate system. Following is the transformation used between permeability values in Cartesian coordinates and that in prolate spheroidal coordinates.

We obtain the following correlation for transformation from Moon and Spencer (1961).

\[ k_x = \sum_{i=1}^{3} \frac{1}{(g_{ii})^{\frac{1}{3}}} \cdot \frac{\partial x}{\partial u^i} \cdot (k)_i \] (A.1)

\[ k_y = \sum_{i=1}^{3} \frac{1}{(g_{ii})^{\frac{1}{3}}} \cdot \frac{\partial y}{\partial u^i} \cdot (k)_i \] (A.2)

\[ k_z = \sum_{i=1}^{3} \frac{1}{(g_{ii})^{\frac{1}{3}}} \cdot \frac{\partial z}{\partial u^i} \cdot (k)_i \] (A.3)

where the relation between Cartesian and prolate spheroidal coordinates were given in Equation 4.6, and reproduced below:

\[ x = d \cdot \sinh \xi \cdot \sin \eta \cdot \cos \psi, \]

\[ y = d \cdot \sinh \xi \cdot \sin \eta \cdot \sin \psi, \]

\[ z = d \cdot \cosh \xi \cdot \cos \eta \]

The parameter \( i \) varies from 1 to 3, since the prolate spheroidal coordinates contain three orthogonal axes (similar to \( x, y, \) and \( z \) in Cartesian coordinates). \( g_{ii} \) are metric coefficients, while \( u \) corresponds to different prolate spheroidal coordinates.

Substituting the relations between Cartesian and prolate spheroidal coordinates in Equation A.1, we get:
Making the subsequent mathematical modifications, we get:

\[
k_x = \frac{k_\xi}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot d\cosh \xi \sin \eta \cos \psi \\
+ \frac{k_\eta}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot d\sinh \xi \cos \eta \cos \psi \\
- \frac{k_\nu}{d\sinh \xi \sin \eta} \cdot d\sinh \xi \sin \eta \sin \psi
\]  \hspace{1cm} (A.4)

Similarly, we have:

\[
k_y = \frac{k_\xi}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot d\cosh \xi \sin \eta \sin \psi \\
+ \frac{k_\eta}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot d\sinh \xi \cos \eta \sin \psi \\
+ \frac{k_\nu}{d\sinh \xi \sin \eta} \cdot d\sinh \xi \sin \eta \cos \psi
\]  \hspace{1cm} (A.5)

Again, making the mathematical modifications, we get:

\[
k_y = \frac{\cosh \xi \cdot \sin \eta \cdot \cos \psi \cdot k_\xi}{\sqrt{\sinh^2 \xi + \sin^2 \eta}} + \frac{\sinh \xi \cdot \cos \eta \cdot \cos \psi \cdot k_\eta}{\sqrt{\sinh^2 \xi + \sin^2 \eta}} - \sin \psi \cdot k_\nu
\]  \hspace{1cm} (A.6)

And finally, for permeability vector in z-direction, we have:

\[
k_z = \frac{k_\xi}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot d\sinh \xi \cos \eta \\
- \frac{k_\eta}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot d\cosh \xi \sin \eta \\
+ \frac{k_\nu}{d\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot (0)
\]  \hspace{1cm} (A.7)

This leads to the following relation:
Therefore, we have three unique correlations between permeability vectors in Cartesian and prolate spheroidal coordinates. Therefore, we can then calculate the prolate spheroidal permeability vectors as a function of permeability vectors in Cartesian coordinates.

\[ k_z = \frac{\sinh \xi \cdot \cos \eta}{\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot k_z - \frac{\cosh \xi \cdot \sin \eta}{\sqrt{\sinh^2 \xi + \sin^2 \eta}} \cdot k_q \] (A.9)
VITA

Vaibhav Rajput

Vaibhav Rajput was born and brought up in Jalgaon District of Maharashtra, India. He finished his Bachelor’s degree in Chemical Engineering from Institute of Chemical Technology, Mumbai, after which he came to Penn State to pursue graduate studies. He completed M.S. in petroleum and natural gas engineering, and continued his PhD at the same institution. During his graduate studies, he completed two summer internships, at Shell (2014) and Baker Hughes (2013).