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Improved Fluid Characterization for Miscible Gas Floods

by

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Dedication

To the memory of my late father, Matthew Egwuenu, birth mother, Betty Egwuenu,
adoptive parents, Mr. and Mrs. Chidi, I. Egwuenu, and my sister Mrs. Amalaonye
Ebinum for their sacrifices and support through my education.

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Abstract

Improved Fluid Characterization for Miscible Gas Floods

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Injection of gases into a reservoir for enhanced oil recovery results in complex fluid phase behavior that cannot be modeled by black oil simulators. This interaction of flow and phase behavior is best captured by fully compositional simulators. A drawback of fully compositional simulators is that they require accurate reservoir fluid characterizations by equations of state (EOS) to capture the phase interactions in miscible gas floods. Another disadvantage is that EOS are computationally intensive. An EOS is typically tuned to standard PVT data, which may include multicontact experiments and swelling tests. The standard method of tuning, however, does not incorporate important displacement parameters such as the minimum miscibility pressure or enrichment (MMP or MME) or the likely compositions that result in a reservoir from condensing-vaporizing displacements.

The currently available correlations for the estimation of MMP for CO₂ floods in literature are not robust enough for the wide range of reservoir oil types and conditions. The MMP correlation available in literature for impure CO₂ floods is so limited in its application that it is only suitable for a certain West Texas reservoir oil type.

This thesis presents new MMP correlations for the displacement of multicomponent oil by CO₂ and impure CO₂. The approach is to use recently developed analytical theory for MMP calculations from EOS to generate MMP correlations for displacements by pure and impure CO₂. The advantage of this approach is that MMPs for a wide range of temperatures and reservoir fluids can be calculated quickly and accurately without introducing uncertainties associated with slim-tube MMPs and other numerical methods. The improved MMP correlation is based solely on the reservoir temperature, molecular weight of C₇₊, and percentage of intermediates (C₂–C₆) in the oil. The MMPs from the improved correlation are compared to currently used correlations and 41 experimentally measured MMPs. Correlations are also developed for impure CO₂ floods, where the injection stream may contain up to 40% methane. The new correlations are significantly more accurate and applicable than currently used correlations.

An improved tuning procedure for miscible gas floods that can more accurately represent the interaction of flow and phase behavior is also presented. Two displacements are used to demonstrate the approach; an eleven-component CO₂ flood and a twelve-component enriched gas flood. The MOC analytical theory is used to determine the MME (or MMP) of both lumped and unlumped pseudocomponent EOS models.

The results show that by tuning to the MME or MMP, fewer pseudocomponents were required to obtain the same degree of accuracy as the standard approach with more pseudocomponents. The lumped model gave good oil recovery prediction and composition velocities even when lumped to four pseudocomponents. The MME or

MMP is shown to be the key tuning parameter. Furthermore, for the cases studied, the lumped models tuned with the proposed characterization method gave more reliable results compared to traditional tuning methods over a wide range of dispersion found in reservoirs. The reduced number of components will reduce the computational time required for compositional simulators.

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Chapter 1: Introduction

The injection of gases into mature reservoir fields for the purpose of increasing the amount of oil recovered is a well-established tertiary recovery method. The choice of injection gas depends primarily on the reservoir temperature, pressure, oil composition, and economic considerations. Gases commonly injected in enhanced oil recovery projects (EOR) include; flue gases, mixture of hydrocarbon gases (or enriched gases), nitrogen, methane, and carbon dioxide. Gas injection increases the mobility of the remaining or residual oil after primary depletion or secondary water floods by reducing the oil viscosity and density. Repeated mass transfer of components between the gas stream and the reservoir oil also cause the oil to become more miscible with the vapor stream in the reservoir. An increase in the oil miscibility and mobility results in an increase in the displacement efficiency and ultimately the recovery efficiency.

The number of EOR gas injection projects in the U.S. has remained relatively unchanged for the past ten years (Guntis 2004). However, the number of miscible CO₂ floods has continued to grow steadily from 54 in 1994 to 70 in 2004. In addition, the amount of oil recovered by this process has increased steadily from 161,000 barrels/day to 205,000 barrels/day over the last ten years. The rise in the number of CO₂ floods is likely because CO₂ achieves miscibility with the oil at relatively lower pressures than natural gas or flue gas. In addition, CO₂ is available naturally in large deposits (Stalkup 1981) and as a byproduct of many industrial processes. All reservoir fields will eventually reach maturity and as the number of new reserves discovered decline, miscible gas injection will contribute a greater percentage to production around the world.

One goal in the design of miscible floods is to operate the reservoir at conditions favorable for miscibility to develop between the injection gas and reservoir fluid. The

percentage of oil recovered increases when the injected gas and reservoir fluids are near miscibility. When fluids are miscible in all proportions, the flood is described as first contact miscible (FCM). Miscibility may also develop by repeated contact with the reservoir fluid in a multicontact miscible (MCM) process. It is rare to find reservoir conditions that favor first contact miscibility because it usually occurs at very high pressures not attainable in most naturally existing reservoirs. The determination of the minimum miscibility pressure or enrichment (MMP or MME) for MCM flow is very important for design considerations.

The injection of a miscible gas into the reservoir often results in complex phase behavior that can be captured only by compositional simulators. Compositional simulators require accurate EOS fluid characterization to make useful predictions. Several researchers (Whitson 1980, Newley & Merrill 1991, Rafael *et al.* 2002, Liu 1999, Khan & Pope 1992) have developed different methods of characterization. The process of describing reservoir oil with an EOS is an expensive and tedious process. There are a number of important questions that need to be addressed in order to design a successful miscible gas flood as well as provide the necessary EOS characterization required for a good compositional simulation. These questions are:

1. What kind of phase behavior will result from the interaction of the oil and injected gas at the prevailing reservoir condition?
2. What kind of mechanism drives the miscible process?
3. How will the MMP or MME for the reservoir be estimated?
4. What approach will be adopted in characterizing the reservoir oil?
5. What PVT experiments are necessary to develop a good EOS fluid characterization?
6. How will the pseudocomponents be selected?

7. What tuning approach and mixing rule will be applied in the pseudoization process to determine the EOS fluid properties?
8. What is the level of dispersion in the reservoir, how will this affect miscibility and consequently oil recovery?

Extensive studies into these questions have been carried out over the years as are described next.

1.1 DEVELOPMENT OF MISCIBILITY AND DRIVE MECHANISM

When injected gas and oil mix in the reservoir, equilibrium gas and oil may result depending on the phase behavior. When the conditions favor first contact miscibility, only a single phase results. However, when the process is multicontact miscible, as many as three phases may co-exist in equilibrium during the contacting process. Propane or liquid petroleum gas (LPG) mixtures are solvents typically used for first contact miscible floods. Multicontact miscible floods usually involve the injection of CO₂, N₂, CH₄ or a mixture of hydrocarbon gases. When CO₂ contacts reservoir oil at a high temperature, two phases typically develop, a vapor phase and a liquid phase. This forms the basis for most fluid characterization PVT experimental data. However, when the fluids contact at temperatures below 120°F, the phase behavior is more complex because three hydrocarbon phases can form.

Experimental measurements of the phase behavior of CO₂/oil mixtures at low temperatures (Orr & Jessen 1984, Monger *et al.* 1981, Turek *et al.* 1984, Shelton and Yarborough 1977) reveal the existence of a liquid/vapor (LV) region, a liquid/liquid/vapor (LLV) region and a liquid/liquid (LL) region. These phases have been shown to occur within different pressure ranges (Stalkup 1983). Several researchers (Ngheim & Li 1986, Khan & Pope 1992, Turek *et al.* 1984, Negahban & Kremesec 1989) have developed EOS characterizations that predict the three-phase region for CO₂/oil

mixtures. Pontious and Tham (1978) speculated that the mobility of CO₂ in the transition zone, may be affected by the co-existence of an LL and LV phase at the flood front region and therefore improve the sweep efficiency. It has also been suggested that the high recovery of CO₂ floods above a certain pressure (MMP) is a result of the formation of a dense CO₂ rich liquid phase that is efficient in extracting the C₅₊ fraction of the oil (Ngheim & Li 1986).

Multicontact miscibility (MCM) in real displacements occurs by either pure vaporizing or combined condensing-vaporizing drive (CV) mechanisms. Pseudo-ternary diagrams have traditionally being used to explain the mechanism for development of miscibility. In ternary systems, a displacement is MCM only if either the injected gas composition (condensing drive) or the oil composition (vaporizing drive) lies outside the region of tie-line extensions on a ternary phase diagram. The mechanism for miscibility can be either condensing or vaporizing but never both. Studies have since shown that the ternary diagrams are inadequate to describe the displacement process for most MCM floods. Zick (1986) and Stalkup (1987) showed that many multicomponent displacements contain aspects of both drive mechanisms (CV drive). Johns *et al.* (1993) proved that at least four components are required for combined CV displacements. MMPs and MMEs estimated using ternary methods can be significantly different from that observed for CV drives. Therefore, new methods were developed for estimation of MMPs and MMEs.

1.2 METHODS FOR ESTIMATING MMP AND MME

There are three primary methods for estimating the MMP or MME for fluid displacements: experimental methods, numerical methods, and analytical techniques. Experimental methods include slim-tube tests (Jarrell *et al.* 2002), rising bubble apparatus (RBA) etc, while numerical methods include the use of mixing cell models (Zick 1986, Jessen and Orr 2002) and 1-D compositional simulations (Rathmell *et al.*

1971). Analytical techniques (Johns and Orr 1996, Wang and Orr 1998, Yuan *et al.* 2002, Jessen *et al.* 1998) are more recent developments that calculate the MP and MME exactly for dispersion-free displacements. Each of these methods has advantages and disadvantages.

1.2.1 Experimental Methods

Slim-tube experiments remain the most widely used method for estimation of MMP. The apparatus (Klins 1984) is made up of a coil usually 20-200 ft long packed with sand or glass beads. The tubing for the coil has a small diameter to ensure the displacement is approximately one-dimensional (1-D). The tube should be long enough for transitional mixing of MCM flow to take place. The permeability of the slim-tube apparatus is very high so that the whole process remains approximately at constant pressure. The dispersion level is small relative to field scale dispersion. Miscible displacements are carried out in the apparatus at different pressures or injection gas enrichments for a given reservoir temperature. The primary results from slim-tube experiments are plots of cumulative oil recovery at a particular time as a function of pressure.

Figure 1 (Yuan 2003) demonstrates a typical plot of oil recovery with pressure for a slim-tube experiment as well as that for dispersion-free displacement. The dispersion-free displacements show a sharp bend at 100% oil recovery. The pressure at which this occurs is the thermodynamic MMP. The slim-tube however includes dispersion and the MMP is determined using several different criteria. Some of the well-known criteria are:

- Oil recovery of 90% at 1.0 pore volume (PV) of gas injected.
- Oil recovery of 90% at 1.2 PV gas injection.
- Oil recovery of 95% at gas breakthrough or more than 80% at gas breakthrough.
- Oil recovery of 94% when the gas-oil ratio (GOR) reaches 4000 scf/bbl.

- Distinct point of maximum curvature when cumulative recovery of oil at 1.2 PV gas injected is plotted against pressure.
- Distinct point of maximum curvature when recovery of oil at gas breakthrough is plotted versus pressure.

The non-unique nature of the criteria leads to uncertainty in the estimation of MMP. For example, Figure 1 illustrates the determination of the point of maximum curvature by the construction of two tangents to the recovery curve. The point of intersection of the two tangent lines gives the estimated MMP. These tangent lines could be drawn in many ways.

Zhou and Orr (1998) have shown that the rising bubble apparatus gives comparable results to the slim-tube experiments with less time. Zhou and Orr reported that RBA is suitable for predicting MMPs for vaporizing drives but not for CV drives. MMP estimates obtained by this method are also subject to experimental errors.

1.2.2 Numerical Methods

These methods to estimate MMP include fine grid 1-D compositional simulations and mixing cell models. In the 1-D compositional simulation method, simulations of the displacement process are made for relatively constant pressure using different grid-block sizes. The oil recovery at extrapolation to zero-dispersion (infinite number of grid-blocks) is estimated for each pressure and a plot of recovery versus pressure is made (such as Figure 1). The MMP is estimated as the pressure at the point of maximum curvature of the curve. Stalkup *et al.* (1990) have reported that there is not always a clear trend for some of the oils studied. This is caused by numerical dispersion. Numerical dispersion arises from the truncation error that results from the approximation of the partial differential equations governing the displacement.

Figure 1: Estimation of MMP by slim-tube experiments. The smooth curve is slim-tube recovery and the other solid curve is dispersion-free recovery. The thermodynamic MMP is the pressure at the sharp bend of the curve as determined by construction of two intersecting tangent lines (the dashed lines). The pressure at the intersection point is often taken as the slim-tube MMP.

Mixing-cell models are of two types: forward contacting and backward contacting. The models operate in the same way as multicontact experiments. Repeated flash calculations are done for a mixture of equilibrium oil and injection gas (backward contacting) or a mixture of equilibrium gas and reservoir oil (forward contacting). The MMP is estimated to be the pressure at which the fluid mixture remains single phase (i.e. the gas or oil tie line becomes the limiting tie line at the critical point). These calculations assume that the drive mechanism is either purely vaporizing or condensing. Such a major shortcoming makes it unsuitable for CV drive displacements.

1.2.3 Analytical Techniques

Analytical techniques for MMP or MME calculation have recently been developed using the method of characteristics (MOC). The calculations are very fast so that MMPs (or MMEs) can be determined for many different reservoir conditions, oil compositions, and gas enrichments. Analytical solutions by MOC were first determined for two-phase, three-component flow by Helfferich (1981). This approach has been extended to other displacements such as surfactant flooding (Hirasaki 1981, Pope 1980).

Monroe *et al.* (1990) extended the analytical method to quaternary systems where they showed that a third key tie line exists, known as the crossover tie line. Johns *et al.* (1993) analytically proved that the crossover tie line controls the development of miscibility for a CV drive for a quaternary system. Furthermore, Johns and Orr (1996) extended the theory to multicomponent displacements where they showed that the displacement path for dispersion-free flow is controlled by n_c-1 key tie lines and n_c-3 crossover tie lines. They showed that MCM is obtained when any of these key tie lines intersects the critical locus as pressure or enrichment is increased.

Wang and Orr (1998) implemented a technique for the calculation of MMP for oil displacements by a multicomponent injection gas based on the geometric construction approach of Johns and Orr (1996). The algorithm developed was modified by Jessen *et al.* (1998) to increase its speed and robustness. However, the number of unknowns to be determined by the modified scheme was still very large, which can cause convergence to false solutions. They reported convergence problems near the critical locus. Yuan *et al.* (2002) have developed a new more robust scheme with fewer unknowns and a well-defined initial guess to improve convergence to the true solution. Johns *et al.* (2002) have also proposed an accurate method for the quantification of the displacement mechanism and demonstrated this for a four-component system.

The small computational time associated with analytical calculations of MMP offers significant promise for the development of new MMP correlations, compositional streamline simulations, and compositional simulations. The main disadvantage of this technique is that it requires an accurate EOS fluid characterization.

1.3 MMP CORRELATIONS

A variety of correlations for the estimation of MMP have been developed from regressions of slim-tube data. Although less accurate, correlations are quick and easy to use and generally require only a few input parameters. Hence, they are very useful for fast screening of reservoirs for potential CO₂ flooding. They are also useful when detailed fluid characterizations are not available. One significant disadvantage of current MMP correlations is that the regressions use MMPs from slim-tube data, which are in themselves uncertain. Some MMP correlations require only the input of reservoir temperature and the API of the reservoir fluid. Other more accurate correlations require reservoir temperature and the total C₂–C₆ content of the reservoir fluid (Johnson and Pollin 1981, Cronquist 1977, Glaso 1985, Yellig, *et al.* 1980, Alston *et al.* 1985, Holm and Josendal 1980). A few require detailed EOS characterizations (Orr and Silva 1987, Kovarik 1985, Ahmed 1997). In nearly all of the correlations, the methane content of the oil is assumed to have negligible effect the MMP. Orr *et al.* (1993) showed why this is true using analytical theory.

The MMP for reservoir oil depends on its composition and that of the injection gas. Lighter oils have lower MMPs than heavier oils. The MMP for nitrogen or methane gas injection is usually higher than that for pure CO₂ injection. However, for high temperature reservoirs, similar MMPs are obtained for these three gases (Jarrell *et al.* 2002).

MMP correlations for impure CO₂ injection (Alston *et al.* 1985, Sebastian *et al.* 1985) have been developed to account for the type and amount of impurity. These correlations, however, are inaccurate for general use as they rely largely on one fluid type. The most widely used correlation by Sebastian *et al.* (1985) is solely based on the pseudocritical temperature of the injected fluid and was primarily developed based on slim-tube data from only one field, the Levelland field. The effect of reservoir temperature and reservoir fluid composition on the MMP is therefore not considered.

Dindoruk *et al.* (1997) used analytical theory to calculate MMPs for injection of nitrogen and methane mixtures. Their paper shows that the MMP depends strongly on the methane content of the injection gas, and at high nitrogen content on the methane content of the reservoir fluid. For small nitrogen contents in the injection gas, however, the MMP is only weakly dependent on the methane concentration in the oil. Hence, correlations for CO₂ injection contaminated with small amounts of nitrogen do not need to incorporate the methane content of the oil.

This thesis uses the analytical theory developed for multicomponent multiphase flow to calculate MMPs for a variety of fluid characterizations, reservoir temperatures, and injection compositions. The primary advantage in this approach is that the analytical calculation is fast and accurate and thus a wider range of input parameters can be considered. The correlations for pure and impure CO₂ injection are developed from regressions of the calculated MMPs. Available MMPs estimated from slim-tube experiments are compared to those predicted from the new correlations.

1.4 DISPERSION

Dispersion is a physical property of a reservoir or porous media that causes' mixing between two fluids in a displacement process because the level of dispersion found in slim-tubes is very small compared to field scale. There is no known way to scale

up dispersivity for cores to field scale. Dispersion adversely affects the local displacement efficiency (Johns, *et al.* 2002, Solano *et al.* 2001) and consequently the ultimate oil recovery. Johns *et al.* (1992) have examined the effect of dispersion on nearly miscible displacements for CV drives. In compositional simulations, adjusting the grid-block sizes approximately captures the effect of dispersion in that numerical dispersion closely mimics the effect of physical dispersion on compositional and saturation profiles.

1.5 EQUATION OF STATE FLUID CHARACTERIZATION

The increase in the number of CO₂-miscible gas projects makes it imperative that good compositional simulators are available to predict oil recovery. Compositional simulators require accurate EOS fluid characterizations. The process of characterizing fluids is complex and not unique. It requires an extended reservoir fluid analysis to obtain single carbon number compositions for developing detailed EOS fluid characterizations.

1.5.1 Reservoir Fluid Analysis

Several experimental methods are available for carrying out extended fluid analysis. The methods that give the greatest amount of information about the fluid are the true boiling point distillation method and gas chromatography. They can give fluid compositions for individual carbon numbers up to C₃₅ (Hoffman, *et al.* 1953). Pedersen *et al.* (1989) carried out an extended reservoir fluid analysis to obtain single carbon number components up to C₂₀ by the modification of the true boiling point distillation method. He also compared this method to the gas chromatography technique and found satisfactory agreement.

1.5.2 Pseudocomponent Selection

After the fluid analysis is complete, the next step is pseudocomponent selection.

The lumping of components together into pseudocomponents is accomplished by the use of some predetermined criteria. Equations of state (EOS) can be calibrated for a large number of components or just a few components to accurately represent the fluid phase behavior. An EOS characterization, which consists of a large number of components, gives an accurate phase behavior prediction. However, excessive computation time and storage will be required to keep track of the simulation.

A detailed multicomponent model (say 24 components) may be necessary to study displacement processes in more detail in a limited section of the reservoir at the pattern scale while a model with a few components could be more applicable for field scale. The usual approach is to first lump the original fluid analysis to as few as 12-15 components, tune the EOS model to match the available PVT data, and then reduce the number of components further by lumping the already characterized model.

The components of the extended fluid analysis can be lumped by several different methods. The simplest methods assign pseudocomponents based on component mole (Cotterman *et al.* 1985) or mass fractions (Pedersen *et al.* 1985). Whitson (1980) proposed a method based on dividing the molecular weight range of the components into intervals. Components in each interval are then lumped together. Mehra *et al.* (1982) proposed a statistical method for lumping components into pseudocomponents. Li *et al.* (1985) proposed a tuning approach that divides components into intervals based on the logarithm of their K-values. Newley & Merrill (1991) proposed a method that is based on minimizing an objective function such that the K-values of the original component are similar to the K-value of the pseudocomponent to which they are assigned.

In the pseudoization of an existing multicomponent model, the heart of the process lies in the selection of an appropriate mixing rule. Some of the already mentioned lumping schemes may not be appropriate to create reduced pseudocomponent models.

Using a poor mixing rule to calculate the properties of reduced pseudocomponent models may result in a significant change in the phase behavior predictions. It is desirable that the reduced model be created with as little adjustment to the properties as possible. The Newley and Merrill (1991) method is an excellent method that calculates EOS properties that require only a little adjustment to match the phase behavior of the reservoir fluids. The method is adopted in this research.

1.5.3 Tuning Process

The goal of the tuning process is to adjust the EOS properties of the pseudocomponents to fit the PVT experimental data generated with the oil or multicomponent EOS model. Typical PVT data used for tuning include:

- Differential liberation test
- Constant composition expansion test
- Swelling test
- Constant volume depletion
- Multiple-contact test
- Separator test

Multicontact tests assume that the drive mechanism is either vaporizing or condensing. Thus, it generally does not provide useful data applicable to CV drives. An EOS tuned to match this data will give poor predictions of the CV displacements. However, when the drive mechanism is mostly vaporizing, the forward-contacting, multicontact test can give useful compositional data along the expected displacement path.

The type and number of PVT experiments required for tuning is dependent on the use of the resulting models. For gas compositional processes, Newley & Merrill (1991) demonstrated that tuning to the differential depletion and swelling test data gave the best results.

Shahin & Kremesec *et al.* (1992) developed a tuning technique for CO₂/oil system, which involved fitting to the MMP. However, they tuned their model to slim-tube MMPs, which often have interpretation uncertainties. They also assumed a vaporizing gas drive mechanism for CO₂ displacement. Displacements by CO₂ have been shown to be CV. In addition the method was designed for EOS characterization of extended fluid analysis. Thus, it may be unsuited for further pseudoization of existing multicomponent EOS models.

Several procedures have been suggested for tuning EOS characterizations (Khan and Pope 1992, Rafael *et al.* 2002, Liu, 1999, Fong et al 1992, Hong 1982). Tuning to match a set of PVT data is more of an art than an exact science. Jhaveri and Youngren (1984) recommend classifying PVT experimental data into volumetric and phase behavior data. Pre-selected EOS parameters are adjusted to match the phase behavior data first and then volumetric data are matched by adjusting the volumetric shift parameters. Whatever approach is adopted, the properties of pure components are usually not adjusted. Adjustments are made to only the most uncertain properties. When components are lumped, the properties of the heaviest pseudocomponents have the greatest level of uncertainty and are therefore, the first choice components parameter adjustment. The critical properties of the heaviest component as well as their binary interaction parameters are adjustable. EOS tuning is usually accomplished by regressing on the available data using a multivariate, non-linear regression tool. EOS tuned to match a specific set of data may not give reliable predictions for other data not included in the regression.

1.6 OBJECTIVES AND ORGANIZATON

This research focuses on two major areas. The first part deals with the development of correlations for pure CO₂ and impure CO₂ miscible displacements. The

second half of the report focuses on an improved tuning approach for EOS characterization suitable for compositional studies. The objectives of this research are to:

- 1 Demonstrate the inadequacy of currently existing correlations for CO₂ floods.
- 2 Show the advantages of the analytical determination of MMP by MOC.
- 3 Develop a more robust MMP correlation for impure CO₂ floods applicable over a wide range of temperature and reservoir fluid types.
- 4 Demonstrate that the general tuning approach currently in use for gas compositional processes is not adequate for lumping multicomponent models to reduced pseudocomponent models.
- 5 Demonstrate that the reduction of multicomponent EOS models to four or five pseudocomponents can be achieved by inclusion of a displacement parameter such as the MMP (or MME) in the regression data.
- 6 Show that the lumped pseudocomponent model predicts the PVT data and matches the 1-D simulation results of the multicomponent model.
- 7 Demonstrate the effects of dispersion on the 1-D simulation results of both the lumped and unlumped models.

Chapter 2 deals with the development of new correlations for pure and impure CO₂ floods. The method of characteristics is used to analytically determine the dispersion-free MMP for different oil types. The impurity in the CO₂ gas stream is limited to only CH₄ and N₂. The analytically generated MMPs along with slim-tube MMPs are used to generate the new correlations.

Chapter 3 focuses on the improved tuning technique for miscible gas floods. The proposed tuning procedure is demonstrated for a 12-component and 11-component oil characterization using the Peng-Robinson EOS (1976). The 12-component model is lumped to four pseudocomponents by matching the MME for displacement using a

multicomponent injection gas. The 11-component model is reduced to a five pseudocomponents by tuning to the MMP for pure CO₂ injection. 1-D simulation results are presented to validate the improved tuning procedure

Chapter 3 also examines the effect of dispersion on both the lumped and unlumped models. Saturation profile at levels of dispersion of the order seen in slim-tubes and that observed at the field scale are compared for both the lumped and unlumped models. Chapter 4 presents conclusions and recommendations for future research.

Equation Chapter 2 Section 2

Chapter 2: New MMP Correlations

All currently available correlations for both pure and impure CO₂ floods are based on the limited available slim-tube MMPs. These correlations do not accurately account for the temperature dependence of MMP and are not applicable to a wide range of reservoir fluid types. In this chapter, new correlations based on the analytically calculated dispersion-free MMPs and the available slim-tube data are presented. Analytical MMPs are calculated based on the analytical theory developed by Johns and Orr (1996) for multicomponent gas floods.

Johns and Orr showed that the displacement path for dispersion-free flow is controlled by n_c-1 key tie lines, which includes n_c-3 crossover tie lines. They showed that the extension of successive key tie lines must intersect in composition hyperspace. Miscibility (MCM) is obtained when any of the key tie lines intersect the critical locus (or has a length of zero) as pressure (MMP) or enrichment (MME) is increased. The analytical approach is implemented in PVTsim, a commercially available software and MMPE, an in-house code developed at the University of Texas for MMP/MME calculations. Both codes are used in this research.

2.1 PVTsim AND MMPE CODES

The two codes differ in their solution approach to the analytical method. PVTsim employs the Jessen *et al.* (1998) approach whereas the Yuan *et al.* (2002) approach, which has substantially reduced number of parameters, is implemented in MMPE. The MMPE code makes both MME and MMP calculations while PVTsim is only capable of MMP calculations. PVTsim uses less computational time than the MMPE code for MMP calculations. The codes give similar MMP results for most of the cases studied (see

appendix A), although, for some EOS models the PVTSim code had computational difficulties. For such cases, the MMPs were determined from the MMPE code.

Figure 2.1 illustrates the calculation of dispersion-free analytical MMP for an example eight-component oil (oil A) displacement by CO₂ using the MMPE code. Oil A is black oil with a bubble-point pressure of 3375.5 psia at 189°F. As shown in Figure 2.1, all key tie-line lengths decrease with pressure. The second crossover tie line (labeled C2), however, intersects the critical locus first (becomes zero length) at a pressure of 3322 ± 1 psia, which is the MMP. Because one of the crossover tie lines controls miscibility, the displacement of oil A by CO₂ is a combined condensing/vaporizing displacement (Johns *et al.* 2002).

Figure 2.2 and 2.3 compare the analytical MMP and MME predictions of the two codes for oil A and an example 12-component oil respectively. As mentioned above, PVTSim does not carry out MME calculations. To determine MMEs using this code, the MMP for different injection gas enrichments are computed instead. The MMP determined is the pressure for which the injection gas composition is at the MME. In Figure 2.2, both codes show consistent results with an average difference in MMP values of only 4 psi. However, in Figure 2.3, the codes show much larger differences in MMP predictions for some gas enrichments considered. The largest difference was 268 psi. This difference is due to convergence errors in the calculation of MME for multicomponent gas displacement by the codes.

Figure 2.1: Tie-line lengths for key tie lines in the displacement of oil A by pure CO₂ at 189°F. The MMP is 3322 psia where one of the key tie lines first reaches zero length.

Figure 2.2: Comparison of MMPs calculated for the displacement of Oil A by gas mixtures containing CO₂ and C₁ at 189°F using PVTsim and MMPE code.

Figure 2.3: Comparison of MMPs calculated for the displacement of 12-component oil by gas mixtures at 182°F using PVTsim and MMPE code.

2.2 NEW MMP CORRELATION FOR PURE CO₂ INJECTION

Elsharkaway *et al.* (1992) reported three trends of MMP for different oils as a function of temperature. Depending on the oil used they observed concave downward, concave upward or linear trends with temperature. Figure 2.4 illustrates a slight concave downward trend in the analytically calculated MMPs with temperature. The trends for the correlations, however, are nearly linear and in some cases have the wrong slope. Figure 2.5 illustrates a similar downward trend, but for a different oil, in this case a volatile oil from Jutila *et al.* (2001) (referred to as oil D here).

Most correlations in the literature predict nearly linear behaviour of MMP with respect to temperature. However, as predicted by the analytical theory and experimental phase behaviour, the increase in MMP should decrease at higher temperatures, owing to the theoretical limit at which the system should transform into a gas/gas system at extreme temperatures. Therefore, we would not expect an indefinite increase in MMP with an increase in temperature.

The analytical MMPs for both oils A and D are fitted to a quadratic function of reservoir temperature with very little error as shown in Figs. 2.4 and 2.5. The approach, therefore, is to develop a new correlation for CO₂ floods based on quadratic fits of analytical MMPs with temperature. The data set used consists of 70 analytically calculated MMPs from nine oils (see Table 2.1). As for other correlations, three input parameters were selected for the estimation of MMP: the molecular weight of C₇₊, the total mole fraction of C₂-C₆, and the reservoir temperature. We found a good fit to the analytical MMPs with the equation:

Figure 2.4: MMP estimated from different correlations and calculated from analytical method for black oil A. The MMPs are fit to a quadratic function.

Figure 2.5: MMPs calculated from analytical method for volatile oil D. The MMPs are fit to a quadratic function.

Table 2.1: Oils used to generate the new MMP correlations for CO₂ floods by analytical method.

Reference	Molecular Weight of C ₇₊	Mole % C ₂ –C ₆	Mole % C ₁	Reservoir Temperature (°F)
Wang and Orr (2002)	140.60**	20.16	34.67	150
Oil A (Yuan, <i>et al.</i> 2002)	194.90**	19.58	47.91	189
Johns et al (2002)	241.30	25.21	30.97	157
Oil B (unpublished)	211.30**	24.68	46.30	180
Oil C (unpublished)	179.50**	18.26	75.60	140
Oil D (Juttila, <i>et al.</i> 2001)	148.90**	14.11	81.92	275
Hong (1982)	245.40**	35.57	31.00	130
Khan <i>et al.</i> (1992)	215	40.36	17.52	94*
Oil E (unpublished)	241.59**	10.39	44.55	165

* These temperatures resulted in three phases and were not used.

** The oils corresponding to these data were used in the impure CO₂ correlation.

$$MMP_{pure} = a_1 + a_2 M_{C_{7+}} + a_3 P_{C_{2-6}} + \left(a_4 + a_5 M_{C_{7+}} + a_6 \frac{P_{C_{2-6}}}{M_{C_{7+}}^2} \right) T + (a_7 + a_8 M_{C_{7+}} + a_9 M_{C_{7+}}^2 + a_{10} P_{C_{2-6}}) T^2 \quad (2.1)$$

where MMP_{pure} is the estimated MMP from the correlation for pure CO₂ injection, a_1 - a_{10} are coefficients determined from a regression of the data, $M_{C_{7+}}$ is the molecular weight of C₇₊, $P_{C_{2-6}}$ is the total molar percentage of C₂-C₆, and T is the reservoir temperature. For the nine oils used in the regression, $M_{C_{7+}}$ ranged from 140 to 245, $P_{C_{2-6}}$ ranged from 11.3 to 40.3%, and the reservoir temperature was varied from 120 to 300°F. The absolute average error of the fit to the 70 MMPs is 6.6%. For example, if the estimated MMP is 3000 psia, the true MMP is likely between 2802 psia and 3198 psia.

Figure 2.6 compares the estimated MMPs from the fit to the analytical MMPs to several other correlations and also to the MMPs estimated from slim-tube experiments (see Table 2.2). As shown, the correlation predicts the slim-tube MMPs about as well as the other correlations. The average absolute error for the 41 slim-tube MMPs is 15.7% for the analytical MMP correlation, 12.6% for Glaso's correlation, 15.3% for Cronquist, 16.7% for Holm and Josendal, and 17.5% for Yellig and Metcalf.

Although the average error is about the same as the other correlations, the fit to the analytical MMPs is significant when considering the nature of the test data set in Table 2.2. First, the analytical MMP correlation is applicable over a wider range of input parameters. For example, the correlation is valid for $M_{C_{5+}} < 180$, where others such as the Holm and Josendal correlation are not. Second, the analytical correlation is significant because the coefficients and charts in the other correlations were determined largely on best fits to the slim-tube MMPs in Table 2.2. Hence, one would expect good predictions by the other correlations for this data set. The coefficients in Glaso's correlation for

Figure 2.6: Comparison of the analytical MMP correlation with other currently used correlations. The correlation is based solely on analytically calculated MMPs.

Figure 2.7: Comparison of the new correlation with other currently used correlations. The correlation is based on both the analytically calculated MMPs and slim-tube MMPs.

Table 2.2: Comparison of MMPs estimated from correlations to slim-tube MMPs for oil displacements by CO₂. Blank spaces indicate data that were not available.

Reference	T (°F)	Mol % C ₁	Mol.% C ₂ -C ₆	M _{C5+}	M _{C7+}	Slim- Tube MMP (psia)	MMP from Eq. 2.1 (psia)	Glaser (1985) MMP (psia)	Cronquist (1977) MMP (psia)	Holm- Josendal (1980) MMP (psia)	Yellig <i>et al</i> (1980) MMP (psia)
Rathmell and Stalkup (1971)	103	28	30	200	223	2000	1428	1376	1703	1550	1247
Rathmell and Stalkup (1971)	109	17	28.8	204	222	1550	1583	1450	1708	1625	1339
Rathmell and Stalkup (1971)	186	45	13	248	268	5000	3548	2909	4658	3700	2317
Holm and Josendal (1980)	135	2	15	183	193	1900	2253	2024	1683	1920	1696
Holm and Josendal (1980)	130		11		175	1750	2026	2458			1631
Holm and Josendal (1980)	71		15		193	1250	959	1289			620
Metcalfe (1982)	105	11	25	188	206	1190	1492	1368	1444	1550	1279
Metcalfe (1982)	135	11	25	188	206	1720	2056	1728	1842	1900	1696
Metcalfe (1982)	90	11	25	188	206	1100	1176	1188	1244	1350	1027
Yellig and Metcalfe (1980)	95		20		201	1150	1063	1245			1116
Yellig and Metcalfe (1980)	118		20		201	1375	1527	1516			1469
Yellig and Metcalfe (1980)	150		20		201	1875	2079	1893			1884
Yellig and Metcalfe (1980)	192		20		201	2350	2637	2388			2388
Alston <i>et al</i> (1985)	219		3		195	4390	4023	4452			2716
Alston <i>et al</i> (1985)	230	33	36	181	185	2930	2678	2770	3544		2852
Alston <i>et al</i> (1985)	160	41	7	221	227	3400	3392	3423	3317	2500	2005
Alston <i>et al</i> (1985)	216	51	10	205	210	4085	3864	3652	4490		2679
Alston <i>et al</i> (1985)	100	4.9	2	236	245	2400	2695	3303	1687		1199
Alston <i>et al</i> (1985)	154	31	23	204	210	2450	2477	1971	2676	2280	1933

Table 2.2 cont'd.

Reference	T (°F)	Mol % C ₁	Mol % C ₂ -C ₆	M _{C5+}	M _{C7+}	Slim- Tube MMP (psia)	MMP from Eq. 2.1 (psia)	Glaso (1985) MMP (psia)	Cronquist (1977) MMP (psia)	Holm- Josendal (1980) MMP (psia)	Yellig <i>et al</i> (1980) MMP (psia)
Alston <i>et al</i> (1985)	234	33	28	214	220	3502	3111	3032	4402		2902
Alston <i>et al</i> (1985)	176	53	9	241	245	3880	3657	3542	4514	3150	2197
Sebastian <i>et al.</i> (1985)	88	12	24.2	205	240	1175	1495	1221	1339	1325	990
Abdassah <i>et al.</i> (2000)	250	0.4	12.3	259	278	3160	3432	4790	4732		3106
Dichary <i>et al.</i> (1973)	130	29	40.4	171	197.4	1550	1368	1652	1871	1675	1631
Cardenas <i>et al.</i> (1984)	164	49	8.84	210	218	3500	3281	3199	3397	2500	2053
Zain <i>et al.</i> (2001)	215	9.8	31.9		196	2875	2761	3414	2978		2667
Zhou <i>et al.</i> (1999)	180	4.4	24	185	234	3250	2923	2452	2283	2550	2245
Chaback <i>et al</i> (1986)	130		36.6		198	1550	1499	1653			1631
Spence <i>et al.</i> (1980)	104	24	30.7	202	221	1316	1404	1384	1700	1600	1263
Spence <i>et al.</i> (1980)	109	17	23.4	221	235	1822	1910	1494	1861	1700	1339
Frimodig <i>et al.</i> (1983)	130		13.4		319.7	3970	3084	3067			1631
Chaback (1988)	220	43	30.8	154	273	3190	2425	3543	3152		2728
Chaback (1988)	130	30	37.3	169	190	1708	1424	1645	1847		1631
Hamoodi (1986)	110	54	43.5	160	284	1572	1384	1792	1790		1354
Metcalfe <i>et al.</i> (1979)	160		25		142	1900	1861	2179			2005
Metcalfe <i>et al.</i> (1979)	160		30		142	1900	1840	2179			2005
Metcalfe <i>et al.</i> (1979)	120		21		142	1700	1240	1716			1497
Whiston (1984)	150		20		139	2030	1706	2101			1884
Henry <i>et al.</i> (1983)	120	16	31	214	227	1535	1744	1610	1960	1750	1497
Henry <i>et al.</i> (1983)	104	8.3	31	191	205	1274	1252	1355	1432	1500	1263
Jacobson	188		31.1		200	2500	2543	2337			2341

example was developed using most of the data points (23 out of 41). When the other independent (non-fitted slim-tube MMPs) are considered, the error in the MMPs from Glaso's correlation increases to over 15%. Glaso used a total of 28 experimental data points, four of which did not have reported C₂-C₆ mole fractions.

The analytical correlation is based only on nine EOS characterizations and is therefore limited to oils of similar type. The 15.7% average error in the prediction of the analytical correlation for the slim-tube data of Table 2.2, is due principally to three data points that fall outside the range of the nine EOS characterization ($M_{C7+} > 245$) used to develop the correlation (see Figure 2.6). Excluding these three data points, the average error of prediction of the generated analytically correlation drops to 10.3% for the same independent data set. Therefore, in order to improve the predictability of our correlation (especially in the aforementioned data range), the 70 analytical MMPs (see Table 2.3) and 41 experimental slim-tube MMPs (see Table 2.2) were regressed to obtain a new set of coefficients. All the MMPs were weighted equally in the regression. The best fit coefficients for Eq. 1 were found to be

$$\begin{aligned} a_1 &= -1.4634 \text{ E}+03 \\ a_2 &= 0.6612 \text{ E}+01 \\ a_3 &= -4.4979 \text{ E}+01 \\ a_4 &= 0.2139 \text{ E}+01 \\ a_5 &= 1.1667 \text{ E}-01 \\ a_6 &= 8.1661 \text{ E}+03 \\ a_7 &= -1.2258 \text{ E}-01 \\ a_8 &= 1.2883 \text{ E}-03 \\ a_9 &= -4.0152 \text{ E}-06 \\ a_{10} &= -9.2577 \text{ E}-04 \end{aligned}$$

Table 2.3: Comparison of MMPs estimated from correlations for oil displacements by CO₂ to analytically calculated MMPs.

Reference	Temperature (°F)	Molecular Weight of C ₇₊	Mole % C ₂ –C ₆	Analytical MMP (psia)	MMP from Eq. 2.1 (psia)
Wang and Orr (2002)	120	140.56	20.16	1320	1236
Wang and Orr (2002)	150	140.56	20.16	1879	1721
Wang and Orr (2002)	180	140.56	20.16	2162	2134
Wang and Orr (2002)	200	140.56	20.16	2308	2371
Wang and Orr (2002)	220	140.56	20.16	2421	2575
Wang and Orr (2002)	240	140.56	20.16	2502	2748
Wang and Orr (2002)	260	140.56	20.16	2552	2890
Wang and Orr (2002)	280	140.56	20.16	2575	3000
Oil A (Yuan, <i>et al.</i> 2002)	140	194.88	19.581	2856	2214
Oil A (Yuan, <i>et al.</i> 2002)	160	194.88	19.581	3034	2542
Oil A (Yuan, <i>et al.</i> 2002)	180	194.88	19.581	3234	2837
Oil A (Yuan, <i>et al.</i> 2002)	189	194.88	19.581	3322	2959
Oil A (Yuan, <i>et al.</i> 2002)	200	194.88	19.581	3430	3098
Oil A (Yuan, <i>et al.</i> 2002)	220	194.88	19.581	3612	3325
Oil A (Yuan, <i>et al.</i> 2002)	240	194.88	19.581	3780	3519
Oil A (Yuan, <i>et al.</i> 2002)	260	194.88	19.581	3928	3679
Oil A (Yuan, <i>et al.</i> 2002)	280	194.88	19.581	4058	3805
Oil A (Yuan, <i>et al.</i> 2002)	300	194.88	19.581	4170	3897
Johns <i>et al.</i> (2002)	100	241.26	25.21	1771	1717
Johns <i>et al.</i> (2002)	120	241.26	25.21	1924	2090
Johns <i>et al.</i> (2002)	150	241.26	25.21	2170	2547
Johns <i>et al.</i> (2002)	220	241.26	25.21	2730	3131
Johns <i>et al.</i> (2002)	240	241.26	25.21	2876	3174
Johns <i>et al.</i> (2002)	250	241.26	25.21	2946	3175
Johns <i>et al.</i> (2002)	260	241.26	25.21	3014	3162
Johns <i>et al.</i> (2002)	280	241.26	25.21	3145	3095
Johns <i>et al.</i> (2002)	300	241.26	25.21	3269	2972
Oil D (Juttila <i>et al.</i> 2001)	120	148.92	14.11	1276	1402
Oil D (Juttila <i>et al.</i> 2001)	140	148.92	14.11	1637	1725
Oil D (Juttila <i>et al.</i> 2001)	160	148.92	14.11	1941	2021
Oil D (Juttila <i>et al.</i> 2001)	180	148.92	14.11	2222	2292
Oil D (Juttila <i>et al.</i> 2001)	200	148.92	14.11	2482	2536
Oil D (Juttila <i>et al.</i> 2001)	220	148.92	14.11	2722	2753
Oil D (Juttila <i>et al.</i> 2001)	240	148.92	14.11	2943	2945
Oil D (Juttila <i>et al.</i> 2001)	250	148.92	14.11	3048	3031
Oil D (Juttila <i>et al.</i> 2001)	260	148.92	14.11	3150	3110
Oil D (Juttila <i>et al.</i> 2001)	275	148.92	14.11	3298	3217

Table 2.3 cont'd.

Reference	Temperature (°F)	Molecular Weight of C ₇₊	Mole % C ₂ -C ₆	Analytical MMP (psia)	MMP from Eq. 2.1 (psia)
Oil D (Juttila <i>et al.</i> 2001)	280	148.92	14.11	3346	3249
Oil D (Juttila <i>et al.</i> 2001)	300	148.92	14.11	3533	3362
Hong (1982)	120	245.40	35.57	1597	1685
Hong (1982)	130	245.40	35.57	1712	1838
Hong (1982)	140	245.40	35.57	1821	1974
Hong (1982)	150	245.40	35.57	1923	2095
Hong (1982)	160	245.40	35.57	2017	2199
Hong (1982)	180	245.40	35.57	2177	2358
Hong (1982)	200	245.40	35.57	2302	2453
Hong (1982)	220	245.40	35.57	2394	2482
Khan <i>et al.</i> (1992)	180	229.00	34.71	1751	2401
Khan <i>et al.</i> (1992)	200	229.00	34.71	1895	2552
Khan <i>et al.</i> (1992)	250	229.00	34.71	2293	2683
Oil B (unpublished)	140	211.27	24.68	2633	2201
Oil B (unpublished)	160	211.27	24.68	2760	2511
Oil B (unpublished)	180	211.27	24.68	2923	2780
Oil B (unpublished)	200	211.27	24.68	3088	3007
Oil B (unpublished)	220	211.27	24.68	3242	3192
Oil B (unpublished)	240	211.27	24.68	3379	3334
Oil B (unpublished)	250	211.27	24.68	3440	3390
Oil B (unpublished)	260	211.27	24.68	3496	3435
Oil B (unpublished)	280	211.27	24.68	3592	3494
Oil B (unpublished)	300	211.27	24.68	3667	3511
Oil C (unpublished)	120	179.49	18.26	1335	1709
Oil C (unpublished)	140	179.49	18.26	1673	2067
Oil C (unpublished)	300	179.49	18.26	3495	3849
Oil E (unpublished)	140	241.59	10.387	2493	3058
Oil E (unpublished)	165	241.59	10.387	2833	3430
Oil E (unpublished)	180	241.59	10.387	3024	3620
Oil E (unpublished)	200	241.59	10.387	3260	3836
Oil E (unpublished)	220	241.59	10.387	3469	4006
Oil E (unpublished)	250	241.59	10.387	3733	4180
Oil E (unpublished)	300	241.59	10.387	4040	4247

The inclusion of the experimental data increased the absolute average error from 6.6% to 10.3% for all the data fitted. The absolute average error of estimation of the slim-tube MMPs, however, decreased from 15.7% to 11.9%. This level of error is on the order of measurement errors in slim-tube MMPs.

The new correlation with the above coefficients is based on all 111 MMPs. For that data, M_{C7+} ranged from 139 to 319, P_{C2-6} ranged from 2.0 to 40.3%, and the reservoir temperature was varied from 71 to 300°F. The new correlation incorporating the slim-tube MMPs is still weighted in favour of the more accurate analytical data. The calculated MMPs using the new correlation are shown in Tables 2.2 and 2.3. A comparison of the new correlation and other available correlations from literature to the slim-tube MMPs is shown in Figure 2.7. As shown the new correlation is superior to all others.

2.3 ANALYTICAL MMP CORRELATION FOR IMPURE CO₂ FLOODS.

The injection stream in CO₂ floods often contains impurities such as methane, nitrogen, hydrogen sulfide, or ethane that are mostly the result of recycling and separation inefficiencies. Because achieving greater CO₂ purity is quite costly, the maximum allowable dilution (MAD) is an important economic parameter. Methane is the most prevalent impurity found associated with naturally occurring CO₂ deposits. In this section, we derive a new MMP correlation that accounts for the oil and gas composition, as well as the reservoir temperature. Analytical techniques bring a significant advantage to MMP calculations. They give very quick calculations, so that we can examine the effect of several factors like temperature and gas composition on MMP. Yuan *et al.* (2002) have demonstrated that MMP has a quadratic dependence on temperature.

The correlation for injection of CO₂ contaminated with methane is developed from seven of the oil characterizations. Table 2.1 shows the properties of the seven oils

used in the regression. $M_{C_{7+}}$ ranged from 140 to 245, C_{2-6} ranged from 10.4 to 24.7%, and the reservoir temperature was varied from 110 to 300°F. MMPs were calculated for displacements of the oils by various gas mixtures of CO₂ and C₁. For example, Figure 2.8 shows the MMP ratio (MMP for impure CO₂ injection divided by the MMP for pure CO₂ injection) for oil A as a function of CO₂ content in the injection gas at different reservoir temperatures. As expected, the MMP ratio increases as the methane content in the injection gas increases at constant temperature and decreases as the reservoir temperature is increased at constant gas composition.

Figure 2.9 shows a similar plot of the MMP ratio for oil D. The MMP ratio for the volatile oil (oil D) is substantially greater than the black oil (oil A), especially for gas mixtures that contain significant amounts of methane. Sebastian's correlation (1985) is the widely reported correlation for impure CO₂ floods. His correlation gives the MMP ratio as a function of the average critical temperature of the injection gas alone. This means that the composition and temperature of the reservoir were considered irrelevant. Figs. 2.8 and 2.9 demonstrate that this is incorrect. Figure 2.8 shows values from Sebastian's correlation for the MMP ratios at the different temperatures. The correlation predicts inaccurate MMP ratios for this oil sample. It has only one curve to represent the four curves given for oil A. The correlation has been shown to work effectively (Sebastian, *et al.* 1985) for only oil samples from the West Texas field from which it was developed.

Figure 2.8: MMP ratios calculated from the analytical method and Sebastian's correlation for displacement of oil A (black oil) by mixtures of CO_2 and C_1 at different reservoir temperatures.

Figure 2.9: MMP ratios calculated from the analytical method for displacement of oil D (light oil) by mixtures of CO_2 and C_1 at different reservoir temperatures.

For both oils A and D, the trends in the MMP ratio are concave upward. However, the trends in the region of interest (small methane contamination) are nearly linear between pure CO₂ injection and injection of a gas mixture with about 60% CO₂ and 40% C₁. Only the linear portions were used in the development of the new correlation. Based on seven oil characterizations, 119 analytical MMPs (see Table 2.2) were calculated and regressed to give the new correlation for impure CO₂ as,

$$\frac{MMP_{imp}}{MMP_{pure}} = 1 + m(P_{CO_2} - 100) \quad (2.2)$$

$$m = f(M_{C_{7+}}, P_{C_{2-6}}, T)$$

with

$$m = a_1 + a_2 M_{C_{7+}} + a_3 P_{C_{2-6}} + \left(a_4 + a_5 M_{C_{7+}} + a_6 \frac{P_{C_{2-6}}}{M_{C_{7+}}^2} \right) T + (a_7 + a_8 M_{C_{7+}} + a_9 M_{C_{7+}}^2 + a_{10} P_{C_{2-6}}) T^2 \quad (2.3)$$

and

$$a_1 = 6.5996E-02$$

$$a_2 = -1.5246E-04$$

$$a_3 = 1.3807E-03$$

$$a_4 = 6.2384E-04$$

$$a_5 = -6.7725E-07$$

$$a_6 = -2.7344E-02$$

$$a_7 = -2.6953E-06$$

$$a_8 = 1.7279E-08$$

$$a_9 = -3.1436E - 11$$

$$a_{10} = -1.9566E - 08$$

Sebastian's correlation is given by:

$$\frac{MMP_{imp}}{MMP_{pure}} = 1.0 - A(0.0213 - 2.51 \times 10^{-4} A + 2.35 A^2) \quad (2.4)$$

where

$$A = \frac{\left(\sum_{i=1}^{n_c} y_i T_{ci} - 87.89 \right)}{1.8} \quad (2.5)$$

The correlation given by Eq. 2.2 is strictly valid only for methane contents in the gas up to 40 %.

Figure 2.10 and Table 2.4 compare the MMP ratio estimated from the new correlation and those calculated from the analytical method. As is shown, a good match is obtained with an average error of only 3% in the MMP ratio.

There is limited slim-tube data in the literature to validate the new correlation. The only usable slim-tube MMP data we could find are from the Levelland field (Sebastian, *et al.* 1985). Because the Levelland oil was also used by Sebastian *et al* (1985) in their correlation, it does not represent an independent set of data to compare both correlations. As also shown by Kovarik (1985), their correlation is likely inaccurate for other oils. The new correlation developed here predicted the Levelland MMPs with good accuracy with a maximum average error of 9% in the MMP ratio for an injection stream

that contains about 10 to 20% methane (see Table 2.5). The accuracy of the new correlation could be improved if additional EOS characterizations become available.

Figure 2.10: Comparison of estimated MMP ratios from the new correlation and those calculated from the analytical method.

Table 2.4: Comparison of MMP ratio estimated from new correlation to analytically calculated MMP ratios for oil displacements by impure CO₂.

Reference	Mole % C ₂ -C ₆	Molecular Weight of C ₇₊	Temperature (°F)	% CO ₂ in injection gas	$\frac{\text{MMP}_{\text{imp}}}{\text{MMP}_{\text{pure}}}$ (Analytical)	$\frac{\text{MMP}_{\text{imp}}}{\text{MMP}_{\text{pure}}}$ (from Eq. 2.2)
Wang and Orr (2002)	20.16	140.6	120	100	1.00	1.00
Wang and Orr (2002)	20.16	140.6	120	90	1.18	1.18
Wang and Orr (2002)	20.16	140.6	120	80	1.36	1.36
Wang and Orr (2002)	20.16	140.6	120	70	1.55	1.54
Wang and Orr (2002)	20.16	140.6	120	60	1.74	1.72
Wang and Orr (2002)	20.16	140.6	140	100	1.00	1.00
Wang and Orr (2002)	20.16	140.6	140	90	1.13	1.15
Wang and Orr (2002)	20.16	140.6	140	80	1.28	1.29
Wang and Orr (2002)	20.16	140.6	140	70	1.42	1.44
Wang and Orr (2002)	20.16	140.6	140	60	1.57	1.58
Wang and Orr (2002)	20.16	140.6	160	100	1.00	1.00
Wang and Orr (2002)	20.16	140.6	160	90	1.12	1.12
Wang and Orr (2002)	20.16	140.6	160	80	1.24	1.25
Wang and Orr (2002)	20.16	140.6	160	70	1.36	1.37
Wang and Orr (2002)	20.16	140.6	160	60	1.49	1.49
Wang and Orr (2002)	20.16	140.6	180	100	1.00	1.00
Wang and Orr (2002)	20.16	140.6	180	90	1.10	1.11
Wang and Orr (2002)	20.16	140.6	180	80	1.20	1.22
Wang and Orr (2002)	20.16	140.6	180	70	1.30	1.33
Wang and Orr (2002)	20.16	140.6	180	60	1.40	1.44
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	160	100	1.00	1.00
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	160	90	1.04	1.15
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	160	80	1.10	1.31
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	160	70	1.19	1.46
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	160	60	1.28	1.62
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	189	100	1.00	1.00
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	189	90	1.04	1.11
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	189	80	1.10	1.21
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	189	70	1.17	1.32
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	189	60	1.25	1.43
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	220	100	1.00	1.00
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	220	90	1.04	1.07
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	220	80	1.10	1.15
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	220	70	1.16	1.22
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	220	60	1.22	1.29
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	260	100	1.00	1.00
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	260	90	1.04	1.06
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	260	80	1.08	1.11
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	260	70	1.13	1.17
Oil A (Yuan, <i>et al.</i> 2002)	19.58	194.9	260	60	1.19	1.23
Oil A (Yuan, <i>et al.</i> 2002)	14.11	148.9	140	100	1.00	1.00
Oil A (Yuan, <i>et al.</i> 2002)	14.11	148.9	140	90	1.18	1.20
Oil A (Yuan, <i>et al.</i> 2002)	14.11	148.9	140	80	1.37	1.40

Table 2.4 cont'd

Reference	Mole % C ₂ –C ₆	Molecular Weight of C ₇₊	Temperature (°F)	% CO ₂ in injection gas	$\frac{\text{MMP}_{\text{imp}}}{\text{MMP}_{\text{pure}}}$ (Analytical)	$\frac{\text{MMP}_{\text{imp}}}{\text{MMP}_{\text{pure}}}$ (from Eq. 2.2)
Oil A (Yuan, <i>et al.</i> 2002)	14.11	148.9	140	70	1.59	1.60
Oil A (Yuan, <i>et al.</i> 2002)	14.11	148.9	140	60	1.84	1.80
Oil A (Yuan, <i>et al.</i> 2002)	14.11	148.9	160	100	1.00	1.00
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	160	90	1.15	1.16
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	160	80	1.31	1.33
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	160	70	1.49	1.49
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	160	60	1.71	1.65
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	180	100	1.00	1.00
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	180	90	1.13	1.14
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	180	80	1.27	1.27
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	180	70	1.43	1.41
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	180	60	1.61	1.55
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	200	100	1.00	1.00
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	200	90	1.11	1.12
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	200	80	1.24	1.24
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	200	70	1.38	1.36
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	200	60	1.55	1.48
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	220	100	1.00	1.00
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	220	90	1.10	1.11
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	220	80	1.21	1.22
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	220	70	1.34	1.33
Oil D (Juttila, <i>et al.</i> 2001)	14.11	148.9	220	60	1.50	1.44
Hong (1982)	35.57	245.4	110	100	1.00	1.00
Hong (1982)	35.57	245.4	110	90	1.17	1.18
Hong (1982)	35.57	245.4	110	80	1.36	1.37
Hong (1982)	35.57	245.4	110	70	1.54	1.55
Hong (1982)	35.57	245.4	110	60	1.72	1.73
Hong (1982)	35.57	245.4	130	100	1.00	1.00
Hong (1982)	35.57	245.4	130	90	1.14	1.15
Hong (1982)	35.57	245.4	130	80	1.29	1.29
Hong (1982)	35.57	245.4	130	70	1.43	1.44
Hong (1982)	35.57	245.4	130	60	1.58	1.58
Hong (1982)	35.57	245.4	160	100	1.00	1.00
Hong (1982)	35.57	245.4	160	90	1.11	1.10
Hong (1982)	35.57	245.4	160	80	1.21	1.21
Hong (1982)	35.57	245.4	160	70	1.32	1.31
Hong (1982)	35.57	245.4	160	60	1.43	1.42
Hong (1982)	35.57	245.4	200	100	1.00	1.00
Hong (1982)	35.57	245.4	200	90	1.07	1.08
Hong (1982)	35.57	245.4	200	80	1.15	1.16
Hong (1982)	35.57	245.4	200	70	1.22	1.23
Hong (1982)	35.57	245.4	200	60	1.30	1.31
Hong (1982)	35.57	245.4	220	100	1.00	1.00
Hong (1982)	35.57	245.4	220	90	1.06	1.08
Hong (1982)	35.57	245.4	220	80	1.13	1.15
Hong (1982)	35.57	245.4	220	70	1.19	1.23
Hong (1982)	35.57	245.4	110	100	1.00	1.00

Table 2.4 cont'd

Reference	Mole % C ₂ – C ₆	Molecular Weight of C ₇₊	Temperature (°F)	% CO ₂ in injection gas	$\frac{MMP_{imp}}{MMP_{pure}}$ (Analytical)	$\frac{MMP_{imp}}{MMP_{pure}}$ (from Eq. 2.2)
Hong (1982)	35.57	245.4	110	90	1.17	1.18
Hong (1982)	35.57	245.4	110	80	1.36	1.37
Hong (1982)	35.57	245.4	110	70	1.54	1.55
Hong (1982)	35.57	245.4	110	60	1.72	1.73
Hong (1982)	35.57	245.4	130	100	1.00	1.00
Hong (1982)	35.57	245.4	130	90	1.14	1.15
Hong (1982)	35.57	245.4	130	80	1.29	1.29
Hong (1982)	35.57	245.4	130	70	1.43	1.44
Hong (1982)	35.57	245.4	130	60	1.58	1.58
Hong (1982)	35.57	245.4	160	100	1.00	1.00
Hong (1982)	35.57	245.4	160	90	1.11	1.10
Hong (1982)	35.57	245.4	160	80	1.21	1.21
Hong (1982)	35.57	245.4	160	70	1.32	1.31
Hong (1982)	35.57	245.4	160	60	1.43	1.42
Hong (1982)	35.57	245.4	200	100	1.00	1.00
Hong (1982)	35.57	245.4	200	90	1.07	1.08
Hong (1982)	35.57	245.4	200	80	1.15	1.16
Hong (1982)	35.57	245.4	200	70	1.22	1.23
Hong (1982)	35.57	245.4	200	60	1.30	1.31

Table 2.5: Comparison of MMP ratio estimated from correlations to slim-tube MMP ratios for oil displacements by impure CO₂

Reference	Mole % C ₁	Mole % C ₂ –C ₆	Molecular Weight of C ₇₊	Temp (°F)	% CO ₂ in injection gas	$\frac{MMP_{imp}}{MMP_{pure}}$ (slim-tube)	$\frac{MMP_{imp}}{MMP_{pure}}$ (from Eq. 2.2)	$\frac{MMP_{imp}}{MMP_{pure}}$ Sebastian's Correlation (1985)
Sebastian <i>et al</i> (1985)	16.48	23.62	240	106	90	1.33	1.31	1.28
Sebastian <i>et al</i> (1985)	16.48	23.62	240	106	81	1.54	1.60	1.60
Sebastian <i>et al</i> (1985)	10.5	24.4	206	105	90	1.33	1.25	1.28
Sebastian <i>et al</i> (1985)	10.5	24.4	206	105	80	1.83	1.50	1.60
Sebastian <i>et al</i> (1985)	10.5	24.4	206	137	90	1.29	1.17	1.28
Sebastian <i>et al</i> (1985)	10.5	24.4	206	137	80	1.59	1.35	1.60

Chapter 3 Improved Fluid Characterizations Using Equations of State

An improved tuning procedure for EOS fluid characterizations that is more reliable for miscible gas compositional simulation is presented. MMP and MME are shown to be the two key displacement parameters that improve the tuning process. The Peng-Robinson (1976) EOS was used for all the characterized models. The EOS model is tuned to match some PVT data and then, the MMP (or MME). The tuning procedure is validated by the successful lumping of a 12-component oil EOS to four pseudocomponents and an 11-component EOS model to five pseudocomponents. 1-D compositional simulations are made to compare the pseudocomponent models to the original multicomponent model. The effect of different levels of dispersion on the oil recovery is also demonstrated.

The process of characterization proceeds in four steps:

1. Generate analytical PVT data using a detailed EOS model as the truth.
2. Select pseudocomponent
3. Tune lumped EOS model using a non-linear regression tool.
4. Validate the model with compositional simulation results.

3.1 PVT DATA

PVT experiments are carried out to provide phase equilibria and volumetric data for tuning EOS characterizations. In this research, PVT data are generated analytically from the original multicomponent EOS characterizations using PVTsim. The detailed EOS characterizations are taken as truth models to compare with lumped models derived from further pseudoization of the multicomponent models. Data from differential liberation tests (DD), separator tests, constant mass expansion (CME), and swelling tests (SWT) were generated. Multicontact experimental data are not used in this research

because the drive mechanism for all the cases considered is CV. A brief description of each experiment is given below.

Differential Liberation Test

This experiment provides important information about the solution gas-oil ratio (R_s), oil formation volume factor (B_o), density of the reservoir fluid at different pressures, gas specific gravity, gas formation volume factor (B_g), and compressibility factor Z . Reservoir fluid is charged to a PVT cell at the reservoir temperature and pressure above the oil bubble point pressure. Pressure is reduced in increments. After each reduction, the system is allowed to equilibrate and the vapor phase is removed by bleeding. The volume of the cell before and after the pressure reduction is measured to determine liquid saturation for B_o calculation. The bled gas stream is used to compute R_s . The process of pressure reduction is continued for the range of pressure depletion expected in the reservoir. In the final stage, the vapor is bled to atmospheric pressure and the density of the remaining liquid is measured.

Constant Mass Expansion Test

Constant mass expansion tests simulate the depletion of a black oil reservoir from pressures above the bubble point to those below the bubble point pressure. In this experiment, the mass of the total system is fixed (i.e. no fluid is withdrawn from the PVT cell). Reservoir oil is placed in a PVT cell at a pressure far above the bubble point pressure of the oil. The pressure of the cell is reduced in increments. At each reduction, single-phase compressibility, liquid volume normalized with the bubble point liquid volume, etc... are measured. This process is carried out over a pressure range above and below the bubble point pressure.

Swelling Test

The objective of this test is to provide PVT and phase equilibrium information for oil/injected gas mixtures that might reflect compositional changes that occur as the displacement takes place in the reservoir. The constant mass expansion test can be performed as part of this test. In this test, a reservoir fluid is charged to a PVT cell and a fixed amount of the injection gas is added to it. The pressure of the system is raised to single-phase conditions and then gradually reduced until the saturation vapor pressure (SVP) is reached. The SVP value and total volume are measured. This process is repeated with incremental additions of the injection gas. The composition of the injection gas/oil critical mixture is also useful information obtained from this test.

Separator Test

Separator tests are designed to give information about the behavior of the reservoir fluids at surface conditions. Information obtained from this test includes; the total gas-oil ratio (GOR), stage GOR, formation volume factor of the oil, density and molecular weight of the stock tank oil. This test can be done in multiple stages and the relevant PVT data measured. The final stage is the stock tank stage at standard temperature and pressure.

3.2 PSEUDOCOMPONENT SELECTION

The successful assignment of components or groups of components to pseudocomponents may depend on the lumping criterion selected. The lumping schemes work well for EOS characterization of extended fluid analysis. Some of the methods may be inaccurate for the pseudoization of an existing multicomponent EOS characterization. The Newley and Merrill (1991) scheme gives very good results for the pseudoization of detailed multicomponent EOS characterizations. This is the scheme used in this research. A brief outline of the method is given below.

The Newley and Merrill Methodology

This lumping scheme is based on the K-values of the components. The scheme aims to minimize the difference between the K-values of components or group of components and the K-value of the pseudocomponent to which it is assigned. This ensures that the predicted phase behavior agrees with that of the detailed EOS model. A well-behaved objective function is defined and minimized to give the best lumping of components.

The pseudocomponents K-values are defined as

$$K_m = \frac{\sum_{i \in m} y_i}{\sum_{i \in m} x_i} \quad (3.1)$$

where K_m is the effective pseudocomponent K-value of a pseudocomponent m . x_i and y_i are the equilibrium phase compositions determined at an appropriate feed composition. The objective function is defined as

$$\sigma = \sum_m \sum_{i \in m} \frac{(K_m - K_i)}{K_i^2} \quad (3.2)$$

K_i is the K-value of the individual component or group of components making up a particular pseudocomponent. Thus, the procedure is reduced to minimizing the objective function by grouping components of similar K-values into the same pseudocomponent.

The first step is to flash an appropriate feed composition of the multicomponent EOS. This is usually at the saturation vapor pressure of the oil or at a composition close to the critical point. The components are then ordered according to their K-values. The initial grouping of components can be made on an equal mole fraction basis by lumping

successive components into the same pseudocomponent. This initial grouping is modified by moving components between adjacent pseudocomponents and σ is calculated for each realization. The realization with the least σ is the best component grouping. The displacement process depends on the K-values of the components. Thus, the average critical properties of the lumped pseudocomponent model can be determined by using a mixing rule based on K-value weighting. The equations are given as:

$$\beta_{cm} = \sum_{i \in m} \beta_{ci} Z_i K_i^{-1/2} / \sum_{i \in m} Z_i K_i^{-1/2} \quad (3.3)$$

where $\beta_{cm} = T_{cm}, V_{cm}, P_{cm}$ or ω_{cm} , and Z_i is overall component composition. These are the average critical properties of the pseudocomponents. The pseudocomponents molecular weights are based on the detailed fluid composition and component molecular weights and are given by:

$$M_m = \sum_{i \in m} M_i Z_i / \sum_{i \in m} Z_i \quad (3.4)$$

Binary interaction parameters are determined from

$$\delta_{mn} = \frac{\sum_{i \in m} \sum_{j \in n} Z_i Z_j \delta_{ij} K_i^{-1/2} K_j^{-1/2}}{\sum_{i \in m} \sum_{j \in n} Z_i Z_j K_i^{-1/2} K_j^{-1/2}} \quad (3.5)$$

where m and n represent two distinct pseudocomponents.

To summarize, the steps are:

1. Flash the detailed multicomponent EOS oil characterization at an appropriate feed composition close to the critical point to obtain representative K-values for the

components. This is could also be done at the bubble point of the oil at the reservoir temperature.

2. Order the components according to their K-values.
3. Lump successive components on equal mole fraction basis. This is only an initial components grouping.
4. Move the component between adjacent pseudocomponents to minimize the objective function.
5. Calculate the average critical properties of the pseudocomponents using the mixing rule in Eq. 3.3

For the purpose of this research, the above steps were implemented in a fortran code (see appendix D). The lumping scheme is implemented for two multicomponent EOS characterizations: a 12-component EOS model lumped to four pseudocomponents and an 11-component EOS model lumped to five pseudocomponents. Tables 3.1-3.6 show the critical properties of the 12-component and the lumped four-pseudocomponent EOS models, while Tables 3.7-3.12 show the properties of the 11-component and the five-pseudocomponent EOS model. These models are the starting points for further tuning.

3.3 IMPROVED TUNING PROCEDURE FOR EOS

Tuning is an art in that there is no unique way to match relevant data. We follow the philosophy that only pseudocomponent properties with a large degree of uncertainty are adjusted in the tuning process. The properties of the heavier pseudocomponents have large uncertainties because they contain many components lumped as a single pseudocomponent. The only measured property of the heaviest pseudocomponent from extended fluid analysis is the molecular weight. This has a measurement error of about 10% (Christensen 1999). All other properties are determined from correlations. These

Table 3.1: Component properties for twelve-component EOS model.

Component	Mole %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	4.484	44.01	87.56	1071.34	1.50	0.225	0.45724	0.0778
CH ₄ -N ₂	36.918	16.00	-117.07	671.17	1.59	0.013	0.45724	0.0778
C ₂	3.205	30.07	89.72	708.35	2.37	0.097	0.45724	0.0778
C ₃	2.333	44.10	205.82	617.38	3.25	0.152	0.45724	0.0778
C ₄	1.532	58.12	294.58	543.31	4.09	0.187	0.45724	0.0778
C ₅	0.877	72.15	366.46	475.28	4.87	0.252	0.45724	0.0778
C ₆	1.265	86.18	439.41	419.54	5.98	0.314	0.45724	0.0778
C ₇₊	9.168	108	584.35	417.69	7.03	0.374	0.45724	0.0778
C ₁₀₊	11.185	152	670.78	407.14	8.11	0.549	0.45724	0.0778
C ₁₄₊	11.220	213	808.24	314.34	12.21	0.755	0.45724	0.0778
C ₂₀₊	9.094	312	954.60	205.28	21.74	0.875	0.45724	0.0778
C ₃₀₊	8.719	451	1136.59	171.07	30.64	1.026	0.45724	0.0778

Table 3.2: Non-zero binary interaction parameters for twelve-component EOS model.

	CO ₂	CH ₄ -N ₂	C ₂	C ₃	C ₄
CO ₂	0.0000				
CH ₄ -N ₂	0.1000				
C ₂	0.1300				
C ₃	0.1350				
C ₄	0.1300				
C ₅	0.1250				
C ₆	0.1200	0.0200	0.0300	0.0300	0.0300
C ₇₊	0.1200	0.0300	0.0300	0.0300	0.0300
C ₁₀₊	0.1200	0.0400	0.0300	0.0300	0.0300
C ₁₄₊	0.1200	0.0600	0.0300	0.0300	0.0300
C ₂₀₊	0.2250	-0.0239	0.0400	-0.0175	0.0400
C ₃₀₊	0.2250	0.2000	0.0400	0.1417	0.0400

Table 3.3: Pseudocomponents selection for twelve-component EOS model.

Components	CH ₄ -N ₂	CO ₂	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇₊	C ₁₀₊	C ₁₄₊	C ₂₀₊	C ₃₀₊
CH ₄ -N ₂	X											
C ₂₊		X	X	X	X							
C ₅₊						X	X	X	X	X	X	
C ₃₀₊												X

Table 3.4: Injection gas composition and the flash data for twelve-component feed composition at 200°F.

Component	Oil Mole Fraction	Injection Gas Mole Fraction	Feed Composition for Pseudocomponent Selection	Y _i	X _i	K _i
CO ₂	0.0448	0.2081	0.1831	0.1921	0.1308	1.4687
CH ₄ -N ₂	0.3692	0.3277	0.3340	0.3545	0.2155	1.6450
C ₂	0.0321	0.2008	0.1750	0.1786	0.1537	1.1620
C ₃	0.0233	0.2223	0.1918	0.1964	0.1657	1.1853
C ₄	0.0153	0.0411	0.0372	0.0367	0.0396	0.9268
C ₅	0.0088		0.0013	0.0013	0.0018	0.7222
C ₆	0.0127		0.0019	0.0017	0.0030	0.5667
C ₇₊	0.0917		0.0140	0.0113	0.0296	0.3818
C ₁₀₊	0.1119		0.0171	0.0119	0.0475	0.2505
C ₁₄₊	0.1122		0.0172	0.0086	0.0670	0.1284
C ₂₀₊	0.0909		0.0139	0.0061	0.0594	0.1027
C ₃₀₊	0.0872		0.0133	0.0008	0.0864	0.0093

Table 3.5: Component properties for untuned four-component EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CH ₄ -N ₂	36.918	16.00	-117.07	671.17	1.59	0.013	0.45724	0.0778
C ₂₊	11.554	40.72	142.80	769.79	2.54	0.159	0.45724	0.0778
C ₅₊	42.809	208.34	775.05	322.86	13.06	0.674	0.45724	0.0778
C ₃₀₊	8.719	451	1136.59	171.07	30.64	1.026	0.45724	0.0778

Table 3.6: Binary interaction parameters for untuned four-component EOS model.

	CH ₄ -N ₂	C ₂₊	C ₅₊	C ₃₀₊
CH ₄ -N ₂	0.0000			
C ₂₊	0.0286	0.0000		
C ₅₊	0.0258	0.0607	0.0000	
C ₃₀₊	0.2000	0.1269	0.0000	0.0000

Table 3.7: Component properties for eleven-component EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	0.1	44.01	87.62	1071.34	1.51	0.225	0.45724	0.0778
C ₁	34.67	16.043	-116.58	667.80	1.59	0.010	0.45724	0.0778
C ₂	3.13	30.07	89.72	708.40	2.37	0.099	0.45724	0.0778
C ₃	3.96	44.097	205.82	617.40	3.25	0.152	0.45724	0.0778
C ₄	5.95	58.124	294.60	543.30	4.08	0.187	0.45724	0.0778
C ₅	4.06	72.151	366.52	475.30	4.87	0.252	0.45724	0.0778
C ₆	3.06	86.178	453.92	431	5.93	0.296	0.45724	0.0778
C ₇	4.95	100.205	512.92	397	6.92	0.351	0.45724	0.0778
C ₈₊	4.97	114.232	564.42	264	7.88	0.394	0.45724	0.0778
C ₁₀₊	30.11	142.285	647.62	320	9.66	0.491	0.45724	0.0778
C ₁₄₊	5.04	198.4	790.02	230	13.30	0.755	0.45724	0.0778

Table 3.8: Non-zero binary interaction parameters for eleven-component EOS model.

	CO ₂	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈₊	C ₁₀₊	C ₁₄₊
CO ₂		0.100	0.130	0.135	0.130	0.130	0.140	0.140	0.140	0.140	0.140
C ₁							0.020	0.030	0.035	0.040	0.060

Table 3.9: Pseudocomponent selection for eleven-component model.

	CO ₂	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈₊	C ₁₀₊	C ₁₄₊
CO ₂	X										
C ₁₊		X	X								
C ₃₊				X	X	X	X				
C ₇₊								X	X	X	
C ₁₄₊											X

Table 3.10: Eleven-component EOS model flash data at 1553 psia and 150°F.

Component	Oil Mole Fraction	Y _i	X _i	K _i
CO ₂	0.1000	0.00166	0.0010	1.6600
C ₁	0.3467	0.92131	0.34613	2.6617
C ₂	0.3130	0.02952	0.03130	0.9431
C ₃	0.3960	0.01888	0.03962	0.4765
C ₄	0.5950	0.01559	0.05954	0.2618
C ₅	0.4060	0.00593	0.04063	0.1460
C ₆	0.3060	0.00209	0.03063	0.0682
C ₇	0.4950	0.00182	0.04955	0.0367
C ₈₊	0.4970	0.00118	0.04975	0.0237
C ₁₀₊	0.3011	0.00202	0.30140	0.0067
C ₁₄₊	0.5040	0.00002	0.05045	0.0004

Table 3.11: Component properties for untuned five-component EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	0.10	44.01	87.89	1069.87	1.51	0.2250	0.45724	0.0778
C ₁₊	37.80	17.84	-89.41	673.15	1.60	0.0217	0.45724	0.0778
C ₃₊	17.03	67.99	348.03	502.67	4.72	0.2310	0.45724	0.0778
C ₇₊	40.03	137.33	633.15	320.43	9.36	0.4750	0.45724	0.0778
C ₁₄₊	5.04	198	790.02	230	13.30	0.7550	0.45724	0.0778

Table 3.12: Binary interaction parameters for untuned five-component EOS model.

	CO ₂	C ₁₊	C ₃₊	C ₇₊	C ₁₄₊
CO ₂	0.0000				
C ₁₊	0.1040	0.0000			
C ₃₊	0.1337	0.0051	0.0000		
C ₇₊	0.1400	0.0339	0.0000	0.0000	
C ₁₄₊	0.1400	0.0521	0.0000	0.0000	0.0000

correlations also have error margins. Therefore, the critical properties of the heavier pseudocomponents are adjustable. The binary interaction parameters between the lightest components and heaviest components have large uncertainties. They are adjustable too. The tuning approach adopted in this study is summarized below:

- Lump the components into pseudocomponents by the Newley and Merrill approach.
- Generate PVT data from differential liberation tests, swelling test, separator test and constant mass expansion using the detailed multicomponent characterization as a truth model.
- Calculate the bubble point pressure of the oil at the reservoir temperature.
- Match the PVT data using the critical temperature, pressure and accentric factor of the two heaviest pseudocomponents.
- Adjust the binary interaction parameters (BIP) between CO₂ and the heaviest component to match the MMP analytically determined from the multicomponent EOS model. Adjust the BIP between the two lightest components in the injection gas and the heaviest component in the lumped models to match both the MME and SVP determined from the multicomponent EOS model. Do a sensitivity analysis to determine the most sensitive BIPs to tune the EOS models. The process of matching the MMP proceeds by repeated adjustment of the suggested BIPs and calculation of the analytical MMP.
- Check to ensure that none of other PVT data predictions have been adversely affected after tuning to the MMP or MME. Otherwise, the process is repeated until a reasonable match is obtained for all the data considered.

The procedure is demonstrated for two EOS characterizations. All regressions were done using the PVTsim regression tool. PVTsim allows the user to weight the PVT data for regression differently as well as assign maximum adjustment that should be made to any of the EOS parameters during the tuning process. Therefore, it is possible to get a good match to PVT data considered to be more important by assigning larger weights to those data. Assigning an upper limit for EOS parameter adjustment ensures that properties are not reduced to unphysical values. Appendix D contains illustrations from the PVTsim regression tool.

3.4 VALIDATION OF EOS MODELS

This is the final step in the fluid characterization procedure. After the models have been tuned to match the PVT and MMP data of the original multicomponent model, it is important to verify that they can adequately simulate the displacement process for miscible gas floods. In this section, 1-D compositional simulations are carried out to compare saturation and compositional profiles. Recovery plots are also generated to compare compositional and cumulative oil recovery from the reservoir. The results for the lumped models are compared to those of the original multicomponent models.

Compositional Simulation Model

The simulator used for all the simulations in this section of the report is the commercially available Computer Modeling Group (CMG) compositional simulator called GEM (2003). All simulations were done at relatively constant pressure to ensure that the phase behavior remains approximately unchanged during the simulation. A reservoir of 1000 ft length and 20 ft thickness was used. The relative permeability model used is a simple Corey-type relative permeability model with arbitrary end point values of 0.64 for the oil and gas phase. The relative permeability exponents are two. The residual oil saturation (S_{or}) is 0.20 with zero critical gas saturation and zero initial water

saturation. The Peng-Robinson EOS is used for all the simulation calculations. The number of grid-blocks for the simulations is varied from 200 to 4000 grid-blocks. This wide range is important for showing the effect of different levels of dispersion on the EOS models. GEM variable time step option was employed for all the simulations. A sample input file used for the simulation is given in appendix F.

3.5 APPLICATION OF THE IMPROVED TUNING TECHNIQUE

The detailed tuning procedure outlined above is tested for two oil samples: a 12-component EOS characterization and an 11-component EOS characterization. These two multicomponent models are taken as the truth models. The 12-component model is lumped to a four pseudocomponent model by tuning to the MME while the 11-component model is lumped to a five pseudocomponent model by tuning to the MMP.

3.5.1 Twelve-Component EOS Pseudoization

A 12-component EOS characterization (Table 3.1) was lumped to a four-pseudocomponent model using the lumping scheme and tuning technique outlined in section 3.3. In lumping the components, $\text{CH}_4\text{-N}_2$ was selected as a separate pseudocomponent so that its composition in the injection gas can be varied. C_{30+} was also selected as a separate pseudocomponent because it has a very low K-value (see Table 3.4). The other two pseudocomponents are defined when the objective function is minimum. Table 3.5 shows the resulting lumped, four-pseudocomponent model.

The pseudocomponent model was then tuned to PVT data and the MME for the oil. At the end of the tuning, two primary models result: one tuned to only the PVT data and the other tuned to both the PVT data and the MME. The PVT data were generated from the 12-component, truth model at 200°F.

Tables 3.13-3.16 show the properties of the tuned pseudocomponent models. Four lumped models were developed from the 12-component model to illustrate the impact of obtaining an accurate match to either the pressure-composition data (P-X) data or MME. The models are:

1. 4-PVT: model tuned to PVT data, which excludes the P-X data.
2. 4-PVTX: model tuned to all the available PVT data.
3. 4-PVT & MME: model tuned to PVT data and MME, which excludes the P-X data.
4. 4-MME & PVTX: model tuned to all the available PVT data and the MME.

Table 3.17 compares how well the four-component models predict the SVP and MMP of the 12-component model at 200°F. Figures 3.1–3.9 show the match of the models to the analytical PVT data from the different PVT tests.

To match the PVT data, the critical temperature and pressure of C_{30+} was adjusted by 2% and 5% respectively. It was difficult to get a good match to the P-X data from the swelling test and the MME simultaneously. The MME was given a greater weight in the tuning process. All other swelling test data (GOR, swollen volume, etc) were well matched. A match to the SVP, and MME was obtained by adjusting the BIP between CH_4-N_2 and C_{30+} by 10% (0.20 to 0.1809), C_{2+} and C_{5+} by 45% (0.0607 to 0.0335), and C_{2+} and C_{30+} from 0.1269 to 0.127.

BIPs are usually adjusted to get a match to the P-X data and the MME (or MMP). When the BIPs were adjusted to match the P-X data without considering the match to MME, the resulting EOS model did not give accurate simulation predictions for the displacement process (see Figure 3.10). Adjusting a particular BIP could have opposite effects on the MME and P-X data predictions.

Table 3.13: Component properties for four-component EOS model tuned to only PVT data at 200°F.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CH ₄ -N ₂	36.918	16.00	-117.07	671.17	1.59	0.013	0.45724	0.0778
C ₂₊	11.554	40.72	142.80	769.79	2.54	0.159	0.45724	0.0778
C ₅₊	42.809	208.34	775.05	322.58	13.06	0.674	0.45724	0.0778
C ₃₀₊	8.719	451	1104.67	162.68	30.64	1.026	0.45724	0.0778

Table 3.14: Binary interaction parameters for four-component model tuned to only PVT data.

	CH ₄ -N ₂	C ₂₊	C ₅₊	C ₃₀₊
CH ₄ -N ₂	0.0000			
C ₂₊	0.0286	0.0000		
C ₅₊	0.0258	0.0607	0.0000	
C ₃₀₊	0.2000	0.1269	0.0000	0.0000

Table 3.15: Component properties for four-component EOS model tuned to both the PVT data and MME at 200°F.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CH ₄ -N ₂	36.918	16	-117.07	671.17	1.59	0.013	0.45724	0.0778
C ₂₊	11.554	40.72	142.80	769.79	2.54	0.159	0.45724	0.0778
C ₅₊	42.809	208.34	775.05	322.86	13.06	0.674	0.45724	0.0778
C ₃₀₊	8.719	451	1136.59	171.07	30.64	1.026	0.45724	0.0778

Table 3.16: Binary interaction parameters for four-component model tuned to both PVT data and MME.

	CH ₄ -N ₂	C ₂₊	C ₅₊	C ₃₀₊
CH ₄ -N ₂	0.0000			
C ₂₊	0.0286	0.0000		
C ₅₊	0.0258	0.0335	0.0000	
C ₃₀₊	0.1809	0.1270	0.0000	0.0000

Table 3.17: Prediction of MMP and SVP by four-component EOS models.

EOS Model	Temperature (°F)	SVP (psia)	MMP (psia)
12-component	200	3200.37	3311.80
4-PVT	200	3201.75	3949.75
4-PVTX	200	3218.71	4248.81
4-PVT & MME (no P-X)	200	3202.00	3311.12
4-MME & PVTX	200	3188.03	3426.01

However, when the P-X data was not matched at all, the 1-D simulation results obtained were unstable with oscillations in the saturation velocities. Table 3.17 compares the MMP predictions for the four lumped models developed by tuning to different combinations of PVT data and the MME. The most inaccurate predictions were by the models tuned to only PVT data. The 4-PVTX model over predicted the MMP by 638 psia. The results obtained suggest that the best approach would be to give more weight to the MMP or MME while ensuring a reasonable match to the P-X data. A fair match to the P-X data ensured stability of the simulations while a match to the MMP or MME ensured accuracy of prediction of the displacement process.

In the separator test, the four-component model predicted a total GOR (at 14.7 psia and 60°F) of 463 scf/stb, which compared well with the 12-component model total GOR of 462 scf/stb.

Figures 3.1 and 3.3-3.8 generally show a good match to the PVT data. Figure 3.2 shows a relatively poor fit to the solution gas/oil ratio (R_s). This is due to the inherent difficulty of matching all PVT data simultaneously. A better match of the R_s data resulted in a poorer prediction of the densities. A match to the density data could be achieved by adjusting the volume shift parameters but this adversely impacts the prediction of R_s . The best fit obtained for both data is a trade off between an excellent match to the densities and a fair match to the R_s .

Validation of the lumped four-component EOS models.

The MMP of the oil at 200°F for displacement by injection gas of fixed composition (67.23% C_{2+} enrichment) is 3311 psia. Therefore, to investigate miscible gas floods above the MMP for this oil, a pressure of 3650 psia at 200°F was selected for the compositional simulations.

1-D, 400 grid-blocks simulation was made to compare the four lumped models developed from tuning to different combinations of the PVT data and MMP. Figure 3.9 compares the simulated gas saturation velocity distribution for the models for 0.5 HCPVI. Figure 3.10 compares the model tuned to only PVT data and that tuned to both the PVT data and MME with the 12-component model for analytically calculated MME predictions at different pressures (or the MMP at different injection gas enrichment). The 4-PVT & MME model closely predicts the 12-component model MME data than the 4-PVT model. There is a perfect match at 67.23% C_{2+} enrichment because this was the MME at which the model was tuned. However, there is an increase in the deviation from the 12-component model MME predictions as the pressure is decreased. As the pressure decreases, the 4-PVT & MME model predicts a lower MME value than the multicomponent model. The 4-PVT model consistently over predicts the MMEs.

The tuned models (4-PVT and 4-MME & PVT) are further compared to the 12-component model by making 1-D simulations at 3650 psia, 200°F and fixed injection gas enrichment (67.23% C_{2+}). The simulations were made for 1000 grid-blocks to minimize the effect of numerical dispersion. Figure 3.11 compares the gas saturation velocity distribution for the EOS models while Figures 3.12-3.15 compare the component velocities. The velocities were generated for 0.3 HCPVI. Figures 3.16-3.18 compare the 1-D simulation oil recoveries to that of the 12-component model.

Figure 3.9 shows that the 4-PVT & MME model gave as good a prediction of the 12-components EOS gas saturation velocities as the 4-MME & PVTX model. This suggests that a rigorous match to the P-X data may not be required to give a good prediction of the miscible displacement. This result is likely because the P-X data may not represent the true CO_2 -oil mixture compositions that occur along the composition path.

Figure 3.1: Tuned four-component model prediction for oil formation volume factor from differential liberation test at 200°F.

Figure 3.2: Tuned four-component model prediction for solution gas-oil ratio from differential liberation test at 200°F.

Figure 3.3: Tuned four-component model prediction for gas formation volume factor from differential liberation test at 200°F.

Figure3.4: Tuned four-component model prediction for oil viscosity from differential liberation test at 200°F.

Figure 3.5: Four-component model predictions for the pressure composition data from swelling test at 200°F.

Figure 3.6: Tuned four-component model prediction for the swollen volume from swelling test at 200°F.

Figure 3.7: Tuned four-component model prediction for the oil/gas mixture density from swelling test at 3200 psia and 200°F.

Figure 3.8: Four-component model prediction for relative volume from constant mass expansion test at 200°F.

The other two models (4-PVT and 4-PVTX) showed a poorer fit to the 12-component EOS model profile. Although the 4-PVTX model was tuned to match all the PVT data, it over predicts the MMP for displacement by the injection gas. The MMP for the 12-component model at 200°F is 3311 psia, 3950 psia for 4-PVT, and 4249 psia for 4-PVTX model. This shows a disadvantage of fitting to only PVT data.

Figure 3.10 shows that the four-component model may not accurately predict the displacement process at higher enrichments. The model would be adequate for 67.23%-80% C_{2+} enrichment. The model will require tuning to a new MME value for enrichment levels higher than 80% C_2 .

The 4-MME & PVT model composition and saturation velocity distributions are a closer fit to that of the 12-component model than the 4-PVT model. At the simulation pressure (3650 psia) and injection gas enrichment, the 4-PVT model predicted a more immiscible flood. The model predicted the MMP to be 3950 psia. This implies that the simulated flood is completely in the two-phase region (i.e. miscibility is never developed). The plots show that the 4-MME & PVT model closely predicts the performance of the 12-component model. However, the 4-MME & PVT model predicts a delayed gas front and as such overestimates the oil recovery given by the 12-component model by a small amount. This probably indicates that lumping to a higher number of pseudocomponents (say five pseudocomponents) would capture better the details of the 12-component predictions.

This research effort was aimed at demonstrating the significance of tuning EOS models to a displacement parameter like the MME or MMP and not to find the minimum number of pseudocomponents required to get a perfect fit.

Figure 3.9: Comparison of simulated gas saturation velocities for four-component models at 0.3 HCPVI, 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.10: Analytical MME predictions by EOS models at 200°F and different pressures.

Figure 3.11: Comparison of 12- and four-component EOS models simulated gas saturation velocities for 0.3 HCPVI at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.12: Comparison of 12- and four-component EOS models simulated C₁N₂ component velocities for 0.3 HCPVI at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.13: Comparison of 12- and four-component EOS models simulated C_{2+} component velocities for 0.3 HCPVI at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.14: Comparison of 12- and four-component EOS models simulated C_{5+} component velocities for 0.3 HCPVI at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.15: Comparison of 12- and four-component EOS models simulated C_{30+} component velocities for 0.3 HCPVI at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.16: Comparison of 12- and four-component EOS models simulated C_{5+} component recovery at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.17: Comparison of 12- and four-component EOS models simulated C_{30+} component recovery at 3650 psia, 200°F and fixed injection gas enrichment.

Figure 3.18: Comparison of 12- and four-component EOS models simulated oil recovery at 3650 psia, 200°F and fixed injection gas enrichment.

However, it is interesting to observe that only a few pseudocomponents can be used to adequately describe the reservoir oil using the proposed tuning technique. Such a reduced pseudocomponent model would significantly improve the speed of compositional simulations.

3.5.2 Eleven-Component EOS Pseudoization

The 11-component model was lumped to five pseudocomponents. The key displacement parameter included in the tuning process is the MMP for displacement by pure CO₂ at 150°F. In selecting the pseudocomponents, CO₂ was selected as a separate pseudocomponent because it is present in both the oil and gas. This reduces the number of components tracked in a compositional simulation for CO₂ floods. C₁₄₊ was also selected as a separate component because of its very low K-value. The other pseudocomponents were selected by the approach of Newley and Merrill. The representative K-values (Table 3.10) used for the lumping and properties calculation were determined at 1553 psia and 150°F.

Tables 3.19-3.20 show the critical properties of the final five-component model tuned to PVT data and MMP for pure CO₂ injection. Figures 3.19-3.26 compare the match of the final lumped model to the 11-component model for the different PVT experiments. The five-component model gave good predictions for most of the PVT data generated from the 11-component model without requiring adjustment to the critical properties of the components. This shows the advantage of the Newley & Merrill approach to lumping pseudocomponents and calculation of EOS properties based on K-value averaged mixing rule. To get a perfect match to the SVP, a 2.2% and 1.3 % adjustment was made to the critical pressure and temperature of C₁₄₊ respectively otherwise the adjustment was unnecessary.

Table 3.18: Prediction of MMP and SVP by five-component EOS models.

EOS Model	Temperature (°F)	SVP (psia)	MMP (psia)
11-component	150	1553.12	1876
5- PVTX	150	1553.52	1868
5-PVT	150	1553.52	2158
5-PVT & MMP	150	1553.52	1876

Table 3.19: Component properties for five-component EOS model tuned to PVT data and MMP at 150°F.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	0.10	44.01	87.89	1069.87	1.51	0.2250	0.45724	0.0778
C ₁₊	37.80	17.84	-89.41	673.15	1.60	0.0217	0.45724	0.0778
C ₃₊	17.03	67.99	348.03	502.67	4.72	0.2310	0.45724	0.0778
C ₇₊	40.03	137	633.15	320.43	9.36	0.4750	0.45724	0.0778
C ₁₄₊	5.04	198	800	235	13.30	0.7550	0.45724	0.0778

Table 3.20: Binary interaction parameters for tuned five-component model.

	CO ₂	C ₁₊	C ₃₊	C ₇₊	C ₁₄₊
CO ₂	0.0000				
C ₁₊	0.1040	0.0000			
C ₃₊	0.1337	0.0051	0.0000		
C ₇₊	0.1210	0.0339	0.0000	0.0000	
C ₁₄₊	0.1160	0.0521	0.0000	0.0000	0.0000

Figure 3.19: Tuned five-component model prediction for oil formation volume factor from differential liberation test at 150°F.

Figure 3.20: Tuned five-component model prediction for solution gas-oil ratio from differential liberation test at 150°F.

Figure 3.21: Tuned five-component model prediction for gas formation volume factor from differential liberation test at 150°F.

Figure 3.22: Tuned five-component model prediction for oil viscosity from differential liberation test at 150°F.

Figure 3.23: Tuned five-component model prediction for the pressure composition data from swelling test at 150°F.

Figure 3.24: Tuned five-component model prediction for the swollen volume from swelling test at 150°F.

Figure 3.25: Tuned five-component model prediction for the oil/CO₂ mixture density from swelling test at 150°F.

Figure 3.26: Tuned five-component model prediction for relative volume from constant mass expansion test at 150°F.

The five-component model generally gave a good match to the PVT data. The density and P-X data predictions were fair. Similar to the 12-component example, the primary goal was to match the MMP of the oil and then the P-X data. The density data can be matched by adjusting the volume shift parameters but this also affects the match to solution gas/oil ratio and oil formation volume factor. Attempts to improve the match to the density data resulted in a poorer fit to the R_s and B_o data. This suggests more pseudocomponents are required to represent the oil in order to increase the degrees of freedom in the parameters available to match the density data. For the purpose of this research, an excellent match to the density was not required because all simulations were 1-D.

The MMP determined analytically for the CO₂-oil displacement was 1876 psia (Table 3.18). PVTsim had difficulties in the calculation of MMPs for the five-component model. All MMP calculations for this model were made with the MMPE code. The binary interaction parameter between CO₂ and C₅₊ was adjusted from 0.14 to 0.121 while that of CO₂-C₁₄₊ was adjusted from 0.14 to 0.116 to get an exact match to the MMP. The P-X data for the 11-component model was matched exactly after the model was successfully tuned to the MMP. This may be just a coincidence. Perhaps, if the lumped model's pseudocomponent properties are computed such that only a small adjustment is required to give a good match to the original multicomponent model, then both data may be well matched. However, if a multicomponent gas is used as the displacement injection gas, it is reasonable not to expect a simultaneous match to the MMP and P-X data because of the opposite effects that may occur from adjusting more than one binary interaction parameter to match either data. For the purpose of illustrating the effect of a poor prediction of the P-X data (see 1-D compositional simulation results), the model was tuned to PVT data, which excluded the P-X data.

Validation of Tuned Five-Component EOS Model.

The 11-component EOS model was lumped and tuned to give two, five-component EOS models. One of the lumped models was tuned to the PVT data and CO₂/oil displacement MMP at 150°F while the other was fitted only to the PVT data (excluding P-X data).

The simulation results of the lumped models were compared to that of 11-component model for a 400 grid-blocks simulation at 2200 psia and 150°F. The displacement is a MCM flood above the MMP. Figure 3.27 compares the saturation velocities of the models for 0.3 HCPVI. In the plot, the 5-PVT represents a model tuned to PVT data, which excludes the P-X data while 5-PVTX is the model tuned to all the PVT data. The model tuned to all the PVT data and the MMP is represented by 5-PVT & MMP.

Figure 3.28 compares the models' MMP predictions at different temperatures. The MMP for the 5-PVT & MMP model coincides with that of the 11-component model at 150°F. As the temperature is increased, the model's MMP predictions deviate from that of the 11-component model. The error grows with increasing temperature.

1-D simulations were made for a 1000 grid-blocks reservoir at a pressure of 2200 psia and 150°F to compare saturation and composition velocities as well as component recoveries for all the models. The injection gas was pure CO₂. Figure 3.29 shows the simulated saturation velocity distribution for 0.3 HCPVI. Figures 3.30-3.34 show the composition velocities while Figures 3.35-3.36 show the cumulative component recoveries. The 5-PVT & MMP model predicts similar saturation and composition velocity distribution as the 11-component model while the 5-PVT model predictions deviate from the 11-component model velocities.

Figure 3.27: Comparison of 11- and five-component EOS simulated gas saturation velocities at 0.3 HCPVI, 2200 psia and 150°F.

Figure 3.28: Comparison of 11- and five-component EOS models analytical MMP predictions for pure CO₂ injection.

Figure 3.29: Comparison of 11- and five-component EOS simulated gas saturation velocities at for 0.3 HCPVI at 2200 psia 150°F. The displacement is by pure CO₂.

Figure 3.30: Comparison of 11- and five-component EOS models simulated CO₂ component velocities for 0.3 HCPVI at 2200 psia, 150°F. The displacement is by pure CO₂.

Figure 3.31: Comparison of 11- and five-component EOS models simulated C_{1+} component velocities for 0.3 HCPVI at 2200 psia and 150°F. The displacement is by pure CO_2 .

Figure 3.32: Comparison of 11- and five-component EOS models simulated C_{3+} component velocities for 0.3 HCPVI at 2200 psia and 150°F. The displacement is by pure CO_2 .

Figure 3.33: Comparison of 11- and five-component EOS models simulated C_{7+} component velocities for 0.3 HCPVI at 2200 psia, and 150°F. The displacement is by pure CO_2 .

Figure 3.34: Comparison of 11- and five-component EOS models simulated C_{14+} component velocities for 0.3 HCPVI at 2200 psia, and 150°F. The displacement is by pure CO_2 .

Figure 3.35: Comparison of 11- and five-component EOS models simulated C_{7+} component cumulative mole percent recovery at 2200 psia and 150°F.

Figure 3.36: Comparison of 11- and five-component EOS models simulated C_{14+} component cumulative mole percent recovery at 2200 psia and 150°F.

The 11-and 5-PVT & MMP model components recoveries overlap while that of the 5-PVT model consistently predicted lower components recovery for all recovery plots. Figure 3.28 demonstrates that the MMP model and the PVTX model compares very well with the 11-component model. The PVTX model predicts a gas saturation front speed only slightly lower than that of the MMP and 11-component models. The 5-PVT model gave the worst saturation predictions. The 5-PVTX model predicted the MMP within a 0.42% error margin. The CO₂-MMP for the 11-component oil is 1876 psia while that for 5-PVTX is 1868 psia. The 5-PVT model over predicts the MMP by 282 psi.

In Figure 3.28, the 5-PVT & MMP model gave a better prediction of the 11-component MMP than the 5-PVT model. The MMP model can adequately represent the 11-component oil within the temperature range of 150-220°F. The model may have to be tuned to a new MMP outside of this temperature range.

The 5-PVT & MMP and 11-component models' component velocities also compare very well with each other. The 5-PVT model velocity distribution deviates from that of the truth model. There is a spike observed in the lumped C₁₊ component velocity distribution, which is completely unobserved in the truth model. This is due to instability in the solution, which may be due to the inadequate match to the P-X data. The recovery plot for C₇₊ and C₁₄₊ components further confirm the 5-PVT & MMP to be the best characterized model. The 5-PVT model predicts a lower component recovery than the other models. This is expected because the model predicts an earlier gas saturation front break through time than either the 11-component or 5-PVT & MMP EOS model.

The importance of including a displacement parameter like the MMP or MME in the process of oil characterization cannot be overemphasized. It is evident from all the discussions and case studies, that a few pseudocomponents can adequately represent the

multicomponent EOS model without any significant loss in accuracy when the improved tuning approach is adopted.

3.6 EFFECT OF DISPERSION ON RECOVERY USING THE EOS MODELS

Numerical dispersion is often used to account for the physical dispersivity. Dispersion causes an otherwise MCM flow to become two-phase flow and thus, miscibility is not attained. Numerical dispersion produces the same dissipating effect on the velocities as physical dispersion. It is usually adjusted by changing the grid-block size. According to Lantz (1971), the numerical Peclet number (P_e) can be estimated as:

$$P_e = \frac{2 * L}{\Delta x}$$

$$\alpha = \frac{\Delta x}{2}$$

where α is the numerical dispersivity, Δx is the size of a grid-block, and L is reservoir length. The effect of dispersion on the calibrated EOS models was studied by carrying out numerical simulations for 200-4000 grid-blocks. The length of the reservoir was 1000 ft. For the 12-and four-component EOS models, simulations were made at 3650 psia, 200°F for 200, 400 and 1000 grid-blocks. The 11- and five-component models were studied at 2200 psia and 150°F for 400, 1000 and 4000 grid-blocks. Table 3.21 gives a summary of the number of grid-blocks and the corresponding Peclet number.

Table 3.21: Summary of grid-blocks used, Peclet numbers and dispersivities.

Number of Grid-blocks	Numerical Dispersivity	Peclet Number
200	2.500	400
400	1.250	800
1000	0.500	2000
4000	0.125	8000

Figures 3.37-3.40 show the simulated saturation velocities for the different models for different levels of dispersion. The gas saturation velocities for the 12-component (Figure 3.37) and four-component (Figure 3.38) EOS models approach the dispersion-free solution closely. At 3650 psia, the process is at a pressure above the MMP (3311 psia) for the injection gas mixture/oil displacement. The dispersion-free solution is a piston like displacement with a gas saturation front dimensionless velocity of unity. The four-component model approaches the dispersion-free solution much better than the 12-component model. As the numerical Peclet number increases, the effect of dispersion decreases. The break-through time predicted also increases because the gas saturation front velocities slow down. Dispersion has less effect on the four-component model as compared to the 12-component model.

Figures 3.39 and 3.40 show the simulated gas saturation velocity distribution for the 11- and five-component EOS models for different levels of dispersion. The models are more influenced by dispersion than the four-component models above. At a Peclet number of 8000, both models closely approach the dispersion-free solution whose saturations shock between zero and one. The gas saturation front velocity closely approach unity for MCM flow. This suggests that the composition path is near the critical point.

In general, the lumped models' predicted oil recoveries are not significantly affected by numerical dispersion. However, this implies that in order to match core or field recovery data, some value for dispersivity will have to be input to the numerical simulator. This also means that the numerical simulation can be made using a relatively smaller number of grid-blocks without significantly affecting the overall accuracy of the results. Simulations with less number of grid-blocks and pseudocomponents would

increase computational speed significantly. This is especially important for extensive field studies.

Figure 3.37: Twelve-component EOS model simulated gas saturation velocities for different levels of dispersion at 0.3 HCPVI, 3650 psia and 200°F.

Figure 3.38: Four-component EOS model simulated gas saturation velocities for different levels of dispersion at 0.3 HCPVI, 3650 psia and 200°F.

Figure 3.39: Eleven-component EOS model simulated gas saturation velocities for different levels of dispersion at 0.3 HCPVI, 2200 psia and 150°F.

Figure 3.40: Five-component EOS model simulated gas saturation velocities for different levels of dispersion at 0.3 HCPVI, 2200 psia and 150°F.

Chapter 4: Conclusions and Recommendations

This research was split into two parts; the development of new correlations for pure and impure CO₂ floods and an improved tuning procedure for EOS characterization. The main conclusions for each part are summarized below:

NEW CO₂ CORRELATIONS

- The new MMP correlation for pure CO₂ injection is significantly more accurate than the currently most widely used correlations.
- The new MMP correlations for impure CO₂ injection account for different fluid types, methane concentration in the gas, and reservoir temperature. The currently most widely used correlation by Sebastian *et al* (1985) is only accurate for the Levelland field.
- The MMP ratio increases as the methane content in the injection gas increases at constant temperature and decreases as the reservoir temperature is increased at constant gas composition. The MMP increase above the MMP for pure CO₂ injection is greatest for a volatile oil.
- More accurate EOS characterizations and slim-tube MMPs are needed to further increase the robustness of the correlations.
- The approach developed here using the analytical theory could also be used to develop other reliable correlations where accurate EOS characterizations are available.

IMPROVED EQUATION OF STATE FLUID CHARACTERIZATIONS

- The MMP or MME is the most important parameter to be tuned for gas compositional processes.

- Multicomponent EOS characterizations can be successfully lumped to fewer pseudocomponents by tuning the EOS to match the PVT data and the MME or MMP for the oil. For one case studied here, four pseudocomponents were sufficient.
- 1-D simulation results showed an excellent match between the multicomponent models and the reduced models tuned to fit the MMP and MME. Otherwise, the matches were poor.
- EOS models consisting of only a few pseudocomponents are less affected by numerical dispersion than the original multicomponent models.

RECOMMENDATIONS FOR FURTHER RESEARCH

The following suggestions for further research are made:

- The impure CO₂ MMP correlation can be improved further by generation of more analytical MMP data using additional EOS characterizations. Slim-tube data can be used to make the impure CO₂ correlation more robust and reduce the error margin in the prediction of slim-tube MMPs.
- The EOS characterizations were used to generate MMP data over a large temperature range. EOS characterizations are usually developed at a given temperature and may be completely unsuitable for other temperatures. The existing analytical correlation can be further improved by using only analytical MMP data generated at the temperature for which the EOS characterizations were developed.
- A correlation for impure CO₂ injection with N₂ as the major contaminant needs to be developed for projects where the nitrogen content of the injection gas stream is

- large. This will provide information for the determination of the degree of separation required for recycled CO₂ gas.
- The Sebastian correlation for impure CO₂ injection can be modified to account for reservoir temperature and oil composition. This approach would likely yield a correlation, which is applicable to any injection gas mixture. This correlation would be given as a function of the reservoir temperature, oil composition and average critical temperature of the injection gas mixture.
 - In this research, it was shown that for an example 11-component EOS characterization, the resulting lumped 5-component model gave an accurate prediction of the pressure composition data when it was tuned to the pure CO₂-MMP. It would be interesting to confirm whether this observation is consistent for other EOS characterizations.
 - The multicomponent models were successfully lumped to a few pseudocomponents. There is a need to carry out de-lumping to confirm that the resulting multicomponent model is representative of the reservoir oil. This is important for smooth transition between the multicomponent and lumped models for field scale simulations.
 - The K-values used in the Newley & Merrill approach were generated for a single composition and pressure. K-values depend on pressure and composition. The lumped model EOS properties could be calculated by using an average of K-values determined from the key tie lines along the true composition path. This would probably give more representative K-values for the displacement process.

Appendix A: Steps for MMP Calculations in PVTsim

These are the steps to calculate MMPs using the PVTsim code:

1. Open the PVTsim package and select the equation of state desired from the tools' bar.
2. Select a unit system from the options icon on the tools' bar.
3. Create a new database to store all fluid information from 'File-Create new database'.
4. From the 'Fluid' icon on the tool bar, select 'Enter new fluid' and a fluid properties spreadsheet appears as shown in Illustration A1.

Current fluid: No fluid selected

Injection gas: No injection gas selected

Enter New Fluid

Fluid: _____

Well: _____ Test: _____ Fluid: _____

Sample: _____ Text: _____

History: _____

Composition

Component	Mol %	Mol wt	Liquid Density g/cm³
N2		28.014	
CO2		44.010	
H2S		34.080	
C1		16.043	
C2		30.070	
C3		44.097	
iC4		58.124	
nC4		58.124	
iC5		72.151	
nC5		72.151	
C6		86.178	0.6640
C7		96.000	0.7380
C8		102.000	0.7650

Total %: 0.000

Options

☐ Save Char Fluid

☐ Adjust to sat point

Fluid type

☒ Plus fraction

☐ No plus fraction

☐ Characterized

Input composition in

☒ Mol%

☐ Weight%

☐ Input wax fraction

Buttons: OK, Cancel, Print, Char Options, Interact Param, PVT Data, Visc Data, Normalize, Clear, Add Comps, Mol to Weight, Complete

Illustration A1 PVTsim input menu for fluid composition and properties.

5. On the left hand side of the spreadsheet, there is an option to enter the fluid description either as originally obtained from extended fluid analysis (i.e. no pseudocomponent lumping yet) or as a characterized fluid. If the fluid is characterized, then select the 'Characterized' fluid option and not the 'Plus fraction' option. It is important to have selected the appropriate EOS from step 1 because this is associated with the properties of the characterized fluid to be input.
6. Input the fluid properties and enter a name for the file in the name field for easy tracking. The software has a database of single carbon number components and their properties. Additional components can be selected from the 'Add comps' icon at the bottom of the spreadsheet. Blank input fields for pseudocomponent properties are selected by indicating the number of pseudocomponents in the characterization.
7. At the bottom right side of the same spreadsheet, select the 'Interact. Param' button and input the binary interaction parameters(K_{ij}) in the appropriate field.
8. Save the file and create another fluid file for the injection gas by following steps four to eight.
9. Make sure the same EOS is selected for the whole procedure.
10. Go back and reselect the oil created in the first steps, from 'Fluid-database' option.
11. On the tool bar, select 'Window-Simulations' option and a windows form with different simulation options will appear.
12. Select the MMP module and another interface appear.
13. Select the drive mechanism and input the temperature. Also, select the injection gas from the injection gas option on the users interface displayed.
14. Click 'Ok' on the MMP menu to make the calculation.

Illustration A.2: PVTsim input field for binary interaction parameters.

Illustration A.3: MMP simulation menu for PVTsim.

Appendix B: EOS Properties for Oils Used in the MMP Correlations

Tables B1-B12 give a summary of the EOS properties of the multicomponent EOS fluid characterizations used to develop the MMP correlations.

Table B1: Component properties for Wang and Orr (2002) EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	0.1	44.01	87.62	1071.34	1.51	0.225	0.45724	0.0778
C ₁	34.67	16.043	-116.58	667.80	1.59	0.01	0.45724	0.0778
C ₂	3.13	30.07	89.72	708.40	2.37	0.099	0.45724	0.0778
C ₃	3.96	44.097	205.82	617.40	3.25	0.152	0.45724	0.0778
C ₄	5.95	58.124	294.6	543.30	4.08	0.187	0.45724	0.0778
C ₅	4.06	72.151	366.52	475.30	4.87	0.252	0.45724	0.0778
C ₆	3.06	86.178	453.92	431.00	5.93	0.296	0.45724	0.0778
C ₇	4.95	100.205	512.92	397.00	6.92	0.351	0.45724	0.0778
C ₈₊	4.97	114.232	564.42	264.00	7.88	0.394	0.45724	0.0778
C ₁₀₊	30.11	142.285	647.62	320.00	9.66	0.491	0.45724	0.0778
C ₁₄₊	5.04	198.4	790.02	230.00	13.3	0.755	0.45724	0.0778

Table B2: Non-zero binary interaction parameters Wang and Orr (2002) EOS model.

	CO ₂	C ₁	C ₂	C ₃	C ₄	C ₅	C ₆	C ₇	C ₈₊	C ₁₀₊	C ₁₄₊
CO ₂	0.0000	0.1000	0.1300	0.1350	0.1300	0.1300	0.1400	0.1400	0.1400	0.1400	0.1400
C ₁							0.0200	0.0300	0.0350	0.0400	0.0600

Table B3: Component properties for Oil A (Yuan *et al.*, 2002) EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	0.31	44.01	87.89	1069.87	1.51	0.225	0.45724	0.0778
C ₂	5.35	30.07	90.05	708.35	2.37	0.098	0.45724	0.0778
C ₃₊	9.45	49.61	246.55	582.14	3.60	0.168	0.45724	0.0778
C ₅₊	4.46	77.77	411.32	463.69	5.39	0.265	0.45724	0.0778
C ₁ N ₂	47.92	16.07	-116.97	666.62	1.62	0.008	0.45724	0.0778
C ₇₊	19.09	128.16	694.67	332.16	9.36	0.458	0.45724	0.0778
C ₁₄₊	8.17	227.29	1109.84	222.73	17.46	0.733	0.45724	0.0778
C ₂₁₊	5.24	387.29	1494.36	177.58	25.14	1.020	0.45724	0.0778

Table B4: Binary interaction parameters for oil A (Yuan, *et al.* 2002) EOS model.

	CO ₂	C ₂	C ₃₊	C ₅₊	C ₁ N ₂	C ₇₊	C ₁₄₊	C ₂₁₊
CO ₂	0.0000							
C ₂	0.1200	0.0000						
C ₃₊	0.1200	0.0000	0.0000					
C ₅₊	0.1200	0.0000	0.0000	0.0000				
C ₁ N ₂	0.1197	0.0001	0.0002	0.0002	0.0000			
C ₇₊	0.1000	0.0000	0.0000	0.0000	0.0013	0.0000		
C ₁₄₊	0.1000	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	
C ₂₁₊	0.1000	0.0000	0.0000	0.0000	0.0013	0.0000	0.0000	0.0000

Table B5: Component properties for oil B (unpublished) EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
N ₂	0.45	28.01	-232.51	493.79	1.44	0.040	0.45724	0.0778
CO ₂	1.64	44.01	87.89	1071.34	1.51	0.228	0.45724	0.0778
C ₁	45.85	16.04	-116.59	667.20	1.59	0.008	0.45724	0.0778
C ₂	7.15	30.07	90.05	708.35	2.37	0.098	0.45724	0.0778
C ₃	6.74	44.10	205.97	615.76	3.25	0.152	0.45724	0.0778
iC ₄	0.84	58.12	274.91	529.06	4.21	0.176	0.45724	0.0778
nC ₄	3.11	58.12	305.69	551.10	4.08	0.193	0.45724	0.0778
iC ₅	1.03	72.15	369.05	490.85	4.90	0.227	0.45724	0.0778
nC ₅	1.65	72.15	385.61	489.38	4.87	0.251	0.45724	0.0778
C ₆	2.52	86.18	453.65	430.59	5.93	0.296	0.45724	0.0778
nC ₇₊	12.44	100.21	679.37	445.27	6.92	0.184	0.45724	0.0778
nC ₁₁₊	6.32	156.30	727.62	344.77	10.57	0.477	0.45724	0.0778
nC ₁₆₊	5.02	226.40	806.89	283.49	14.74	0.820	0.45724	0.0778
nC ₂₃₊	3.24	324.64	920.03	246.68	20.90	1.211	0.45724	0.0778
nC ₃₃₊	2.00	464.91	1035.23	222.35	29.71	1.372	0.45724	0.0778

Table B6: Binary interaction parameters for oil B (unpublished) EOS model.

	N ₂	CO ₂	NC ₇
N ₂	0.0000	0.0000	0.1441
CO ₂	-0.0170	0.0000	0.1000
C ₁	0.0311	0.1200	0.0352
C ₂	0.0515	0.1200	0.0067
C ₃	0.0852	0.1200	0.0056
iC ₄	0.1033	0.1200	0.0000
nC ₄	0.0800	0.1200	0.0033
iC ₅	0.0922	0.1200	0.0000
nC ₅	0.1000	0.1200	0.0074
C ₆	0.0800	0.1200	0.0000
nC ₁₁₊	0.0800	0.1000	0.0000
nC ₁₆₊	0.0800	0.1000	0.0000
nC ₂₃₊	0.0000	0.0000	0.0000
nC ₃₃₊	0.0000	0.0000	0.0000

Table B7: Component properties for oil C (unpublished) EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
N ₂	0.67	28.01	-232.60	493.00	1.44	0.045	0.45724	0.0778
CO ₂	1.29	44.01	87.90	1071.00	1.51	0.231	0.45724	0.0778
C ₁	74.91	16.04	-116.90	667.80	1.59	0.012	0.45724	0.0778
C ₂	7.69	30.07	89.90	707.80	2.37	0.091	0.45724	0.0778
C ₃	3.89	44.10	205.80	616.30	3.25	0.145	0.45724	0.0778
iC ₄	0.79	58.12	274.80	529.10	4.21	0.176	0.45724	0.0778
nC ₄	1.84	58.12	305.40	550.70	4.08	0.193	0.45724	0.0778
iC ₅	0.74	72.15	368.90	490.40	4.90	0.227	0.45724	0.0778
nC ₅	0.93	72.15	385.50	488.60	4.87	0.251	0.45724	0.0778
C ₆	1.11	86.18	453.50	436.90	5.93	0.296	0.45724	0.0778
nC ₇₊	3.10	100.21	612.30	390.30	6.92	0.346	0.45724	0.0778
nC ₉₊	1.59	128.26	786.10	288.70	8.78	0.514	0.45724	0.0778
nC ₁₄₊	0.88	198.40	923.10	222.30	13.30	0.691	0.45724	0.0778
C ₂₀₊	0.45	100.00	1056.40	171.90	20.78	0.908	0.45724	0.0778
C ₃₀₊	0.14	200.00	1239.50	124.60	29.19	1.270	0.45724	0.0778

Table B8: Non-zero binary interaction parameters for oil C (unpublished) EOS model.

	N ₂	CO ₂	C ₁
C ₁	0.1050	0.0250	
C ₂	0.1300	0.0100	
C ₃	0.1250	0.0900	
iC ₄	0.1200	0.0950	
nC ₄	0.1150	0.0950	
iC ₅	0.1150	0.1000	
nC ₅	0.1150	0.1100	
C ₆	0.1150	0.1100	
nC ₇₊	0.1150	0.1100	0.0351
nC ₉₊	0.1150	0.1100	0.0508
nC ₁₄₊	0.1150	0.1100	0.0638
C ₂₀₊	0.1150	0.1100	0.0768
C ₃₀₊	0.1150	0.1100	0.0945

Table B9: Component properties for oil D (Jutila, *et al.* 2001) EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
N ₂	0.57	28.01	-232.40	493.00	1.44	0.045	0.45724	0.0778
CO ₂	1.65	44.01	87.90	1070.90	1.51	0.231	0.45724	0.0778
C ₁	81.35	16.04	-116.60	667.80	1.59	0.012	0.45724	0.0778
C ₂	6.86	30.07	90.10	707.80	2.37	0.091	0.45724	0.0778
C ₃	2.80	44.10	206.00	616.30	3.25	0.145	0.45724	0.0778
nC ₄	1.49	58.12	305.70	550.70	4.08	0.193	0.45724	0.0778
nC ₅	0.77	72.15	385.70	488.60	4.87	0.251	0.45724	0.0778
C ₆	0.54	86.18	453.70	436.90	5.93	0.296	0.45724	0.0778
PS1	1.09	97.21	509.53	410	6.80	0.257	0.45724	0.0778
PS2	1.58	129.02	675.33	355	8.96	0.335	0.45724	0.0778
PS3	1.00	191.40	825.33	285	12.03	0.488	0.45724	0.0778
PS4	0.30	300	1020.33	218	16.86	0.724	0.45724	0.0778

Table B10: Non-zero binary interaction parameters for oil D (Jutila, *et al.* 2001) EOS model.

	N ₂	CO ₂	C ₁
N ₂	0.0000		
CO ₂	0.0000	0.0000	
C ₁	0.0250	0.1050	0.0000
C ₂	0.0100	0.1300	0.0000
C ₃	0.0900	0.1250	0.0000
nC ₄	0.1100	0.1150	0.0000
nC ₅	0.1100	0.1150	0.0000
C ₆	0.1100	0.1150	0.0000
PS1	0.1100	0.1150	0.0560
PS2	0.1100	0.1150	0.0749
PS3	0.1100	0.1150	0.1040
PS4	0.1100	0.1150	0.1390

Table B11: Component properties for Hong oil (1982) EOS model.

Component	Mol %	M _w	T _C (°F)	P _C (psia)	V _C (ft ³ /lb-mol)	ω	Ω _A	Ω _B
CO ₂	0.01	44.01	87.89	1069.87	1.51	0.225	0.45724	0.0778
C ₁	31.00	16.04	-116.59	667.20	1.59	0.013	0.45724	0.0778
C ₂	10.41	30.07	90.05	708.35	2.37	0.099	0.45724	0.0778
C ₃	11.87	44.10	205.97	615.76	3.25	0.152	0.45724	0.0778
C ₄	7.32	58.12	305.69	551.10	4.08	0.201	0.45724	0.0778
C ₅	4.41	72.15	385.61	489.38	4.87	0.254	0.45724	0.0778
C ₆	2.55	86.18	453.65	430.59	5.93	0.301	0.45724	0.0778
C ₇	5.71	100.21	512.69	396.79	6.92	0.348	0.45724	0.0778
C ₈	4.72	114.23	564.17	360.05	7.88	0.391	0.45724	0.0778
C ₉	2.46	128.26	610.61	335.07	8.78	0.435	0.45724	0.0778
C ₁₀	2.33	142.29	652.01	305.68	9.66	0.478	0.45724	0.0778
C ₁₁	2.12	156.30	690.17	285.10	10.57	0.521	0.45724	0.0778
C ₁₂	1.69	170.30	729.30	264.53	11.42	0.564	0.45724	0.0778
C ₁₃₊	13.40	100.00	800.33	213.09	14.36	0.800	0.45724	0.0778

Table B12: Binary interaction parameters for Hong oil (1982) EOS model.

	CO ₂	C ₁
CO ₂	0.0000	
C ₁	0.2000	0.0000
C ₂	0.1900	0.0100
C ₃	0.1800	0.0100
C ₄	0.1700	0.0100
C ₅	0.1600	0.0100
C ₆	0.1500	0.0100
C ₇	0.1400	0.0100
C ₈	0.1400	0.0500
C ₉	0.1400	0.0700
C ₁₀	0.1400	0.0800
C ₁₁	0.1400	0.1200
C ₁₂	0.1400	0.1300
C ₁₃₊	0.1400	0.1600

Appendix C: PVTSim MMP Calculation Failure

PVTSim had difficulties in the calculation of MMPs for CO₂ displacement of an 11-component oil (Wang and Orr 2002) at different temperatures. For these cases where PVTSim failed, the MMPE code was successful.

Table C1: Comparison of 11-component EOS MMP calculation results at different temperatures for displacement by pure CO₂.

Temp(°F)	MMP (psia)	
	MMPE	PVTSim
120	1536	failed
140	1768	failed
160	1982	1981.93
180	2162	2162.79
200	2308	failed
220	2422	failed

Appendix D: Computer Code for Pseudocomponent Selection

Below is a Fortran code (Johns 1992) that implements the Newley Merrill lumping scheme:

c This program forms pseudocomponents from individual components.

```
implicit double precision(a-h,o-z)
parameter(nc=12,np=4)
character gname(nc)*5
dimension mw(nc),z(nc),pc(nc),tc(nc),vc(nc),w(nc),y(nc),x(nc)
dimension xk(nc),xkm(np),bin(nc,nc),binm(np,np)
open(unit=2,file='pseudo.in')
rewind(unit=2)
open(unit=3,file='pseudo.out')
rewind(unit=3)
n1d=1
n1u=1
n2d=2
n2u=5
n3d=6
n3u=11
n4d=12
n4u=12

read(2,*)
do 1 i=1,nc
  read(2,*) gname(i),mw(i),z(i),pc(i),tc(i),vc(i),w(i),y(i),
+   x(i),xk(i)
1  continue
  do 111 i=1,nc
    do 112 j=1,nc
      bin(i,j)=0.d0
      if(i.lt.j) read(2,*) bin(i,j)
112  continue
111  continue
    do 113 i=1,nc
      do 114 j=1,nc
        if(i.eq.j) then
          bin(i,j)=0.d0
        else
          bin(j,i)=bin(i,j)
        endif
114  continue
113  continue
```

```

c Calculate effective K values of pseudo components.
  sumy=0.d0
  sumx=0.d0
  do 2 i=n1d,n1u
    sumy=sumy+y(i)
    sumx=sumx+x(i)
2  continue
  xkm(1)=sumy/sumx
  sumy=0.d0
  sumx=0.d0
  do 3 i=n2d,n2u
    sumy=sumy+y(i)
    sumx=sumx+x(i)
3  continue
  xkm(2)=sumy/sumx
  sumy=0.d0
  sumx=0.d0
  do 4 i=n3d,n3u
    sumy=sumy+y(i)
    sumx=sumx+x(i)
4  continue
  xkm(3)=sumy/sumx

  sumy=0.d0
  sumx=0.d0
  do 5 i=n4d,n4u
    sumy=sumy+y(i)
    sumx=sumx+x(i)
5  continue
  xkm(4)=sumy/sumx

c Check objective function.
  sigma=0.d0
  do 6 i=n1d,n1u
    sigma=(xkm(1)-xk(i))**2.d0/(xk(i)**2.d0)+sigma
6  continue
  do 61 i=n2d,n2u
    sigma=(xkm(2)-xk(i))**2.d0/(xk(i)**2.d0)+sigma
61 continue
  do 62 i=n3d,n3u
    sigma=(xkm(3)-xk(i))**2.d0/(xk(i)**2.d0)+sigma
62 continue
  do 63 i=n4d,n4u
    sigma=(xkm(4)-xk(i))**2.d0/(xk(i)**2.d0)+sigma
63 continue

  write(3,*) 'OBJECTIVE FUNCT. VALUE = ',sigma
  write(3,*) ' '

c Calculate pseudo component properties
c Component 1
  sum=0.d0
  sum1=0.d0
  sum2=0.d0

```

```

sum3=0.d0
sum4=0.d0
sum5=0.d0
sum6=0.d0
sum7=0.d0
sum8=0.d0
sum9=0.d0
sum10=0.d0
sum11=0.d0
do 8 i=n1d,n1u
  sum1=sum1+tc(i)*z(i)*(xk(i)**(-.5d0))
  sum2=sum2+pc(i)*z(i)*(xk(i)**(-.5d0))
  sum3=sum3+vc(i)*z(i)*(xk(i)**(-.5d0))
  sum4=sum4+w(i)*z(i)*(xk(i)**(-.5d0))
  sum5=sum5+mw(i)*z(i)*(xk(i)**(-.5d0))
  do 81 j=n2d,n2u
    sum6=sum6+bin(i,j)*z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
    sum7=sum7+z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
81  continue
  do 82 j=n3d,n3u
    sum8=sum8+bin(i,j)*z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
    sum9=sum9+z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
82  continue
  do 83 j=n4d,n4u
    sum10=sum10+bin(i,j)*z(i)*z(j)*(xk(i)**(-.5d0))*
+   (xk(j)**(-.5d0))
    sum11=sum11+z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
83  continue
  sum=sum+z(i)*(xk(i)**(-.5d0))
8  continue
binm(1,2)=sum6/sum7
binm(1,3)=sum8/sum9
binm(1,4)=sum10/sum11
write(3,*) 'PSEUDO COMPS. =',(gname(i),i=n1d,n1u)
write(3,*) 'Tc Pseudo Comp. 1 =',sum1/sum
write(3,*) 'Pc Pseudo Comp. 1 =',sum2/sum
write(3,*) 'Vc Pseudo Comp. 1 =',sum3/sum
write(3,*) 'W Pseudo Comp. 1 =',sum4/sum
write(3,*) 'Mw Pseudo Comp. 1 =',sum5/sum
write(3,*) 'K Pseudo Comp. 1 =',xkm(1)
write(3,*) ''
c Component 2
sum=0.d0
sum1=0.d0
sum2=0.d0
sum3=0.d0
sum4=0.d0
sum5=0.d0
sum6=0.d0
sum7=0.d0
sum8=0.d0
sum9=0.d0
do 9 i=n2d,n2u
  sum1=sum1+tc(i)*z(i)*(xk(i)**(-.5d0))

```

```

sum2=sum2+pc(i)*z(i)*(xk(i)**(-.5d0))
sum3=sum3+vc(i)*z(i)*(xk(i)**(-.5d0))
sum4=sum4+w(i)*z(i)*(xk(i)**(-.5d0))
sum5=sum5+mw(i)*z(i)*(xk(i)**(-.5d0))
do 84 j=n3d,n3u
    sum6=sum6+bin(i,j)*z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
    sum7=sum7+z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
84  continue
do 85 j=n4d,n4u
    sum8=sum8+bin(i,j)*z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
    sum9=sum9+z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
85  continue
sum=sum+z(i)*(xk(i)**(-.5d0))
9  continue
binm(2,3)=sum6/sum7
binm(2,4)=sum8/sum9
write(3,*) 'PSEUDO COMPS. =',(gname(i),i=n2d,n2u)
write(3,*) 'Tc Pseudo Comp. 2 =',sum1/sum
write(3,*) 'Pc Pseudo Comp. 2 =',sum2/sum
write(3,*) 'Vc Pseudo Comp. 2 =',sum3/sum
write(3,*) 'W Pseudo Comp. 2 =',sum4/sum
write(3,*) 'MW Pseudo Comp. 2 =',sum5/sum
write(3,*) 'K Pseudo Comp. 2 =',xkm(2)
write(3,*) ''
c Component 3
sum=0.d0
sum1=0.d0
sum2=0.d0
sum3=0.d0
sum4=0.d0
sum5=0.d0
sum6=0.d0
sum7=0.d0
do 10 i=n3d,n3u
    sum1=sum1+tc(i)*z(i)*(xk(i)**(-.5d0))
    sum2=sum2+pc(i)*z(i)*(xk(i)**(-.5d0))
    sum3=sum3+vc(i)*z(i)*(xk(i)**(-.5d0))
    sum4=sum4+w(i)*z(i)*(xk(i)**(-.5d0))
    sum5=sum5+mw(i)*z(i)*(xk(i)**(-.5d0))
do 86 j=n4d,n4u
    sum6=sum6+bin(i,j)*z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
    sum7=sum7+z(i)*z(j)*(xk(i)**(-.5d0))*(xk(j)**(-.5d0))
86  continue
sum=sum+z(i)*(xk(i)**(-.5d0))
10 continue
binm(3,4)=sum6/sum7
write(3,*) 'PSEUDO COMPS. =',(gname(i),i=n3d,n3u)
write(3,*) 'Tc Pseudo Comp. 3 =',sum1/sum
write(3,*) 'Pc Pseudo Comp. 3 =',sum2/sum
write(3,*) 'Vc Pseudo Comp. 3 =',sum3/sum
write(3,*) 'W Pseudo Comp. 3 =',sum4/sum
write(3,*) 'MW Pseudo Comp. 3 =',sum5/sum
write(3,*) 'K Pseudo Comp. 3 =',xkm(3)
write(3,*) ''

```

```

c Component 4
sum=0.d0
sum1=0.d0
sum2=0.d0
sum3=0.d0
sum4=0.d0
sum5=0.d0
do 11 i=n4d,n4u
sum1=sum1+tc(i)*z(i)*(xk(i)**(-.5d0))
sum2=sum2+pc(i)*z(i)*(xk(i)**(-.5d0))
sum3=sum3+vc(i)*z(i)*(xk(i)**(-.5d0))
sum4=sum4+w(i)*z(i)*(xk(i)**(-.5d0))
sum5=sum5+mw(i)*z(i)*(xk(i)**(-.5d0))
sum=sum+z(i)*(xk(i)**(-.5d0))
11 continue
write(3,*) 'PSEUDO COMPS. =',(gname(i),i=n4d,n4u)
write(3,*) 'Tc Pseudo Comp. 4 =',sum1/sum
write(3,*) 'Pc Pseudo Comp. 4 =',sum2/sum
write(3,*) 'Vc Pseudo Comp. 4 =',sum3/sum
write(3,*) 'W Pseudo Comp. 4 =',sum4/sum
write(3,*) 'MW Pseudo Comp. 4 =',sum5/sum
write(3,*) 'K Pseudo Comp. 4 =',xkm(4)
c Write binary interaction parameters
write(3,*) ''
write(3,*) 'Binary Interaction Parameters'
write(3,*) ''
write(3,*) 'PC1-PC2 =',binm(1,2)
write(3,*) 'PC1-PC3 =',binm(1,3)
write(3,*) 'PC1-PC4 =',binm(1,4)
write(3,*) 'PC2-PC3 =',binm(2,3)
write(3,*) 'PC2-PC4 =',binm(2,4)
write(3,*) 'PC3-PC4 =',binm(3,4)
stop
end

```

The Fortran input file for 12-component lumping is:

Name	Mw	Zi	PC	TC	VC	ω	Yi	Xi	Ki
'CH4N2'	16	0.334049	671.17	-117.07	1.585	0.013	0.354462	0.215487	1.644934
'C02'	44	0.18311	1071.34	87.56	1.504	0.225	0.192117	0.130798	1.468809
'C2'	30	0.17497	708.35	89.72	2.366	0.098	0.178641	0.153651	1.162639
'C3'	44	0.191844	617.38	205.82	3.252	0.1524	0.196351	0.165668	1.18521
'C4'	58	0.037154	543.31	294.58	4.085	0.187	0.036738	0.03957	0.928426
'C5'	72	0.001342	475.28	366.46	4.87	0.2523	0.001261	0.001798	0.701545
'C6'	86	0.001936	419.54	439.41	5.981	0.3138	0.001746	0.003041	0.574184
'C7+'	108	0.014033	417.69	584.35	7.029	0.3739	0.011345	0.029643	0.382731

'C10+'	152	0.017121	407.14	670.78	8.106	0.5489	0.011896	0.047472	0.25058
'C14+'	213	0.017174	314.34	808.24	12.208	0.755	0.008597	0.066991	0.128334
'C20+'	312	0.01392	205.28	954.6	21.739	0.875	0.006082	0.059445	0.102319
'C30+'	451	0.013347	171.07	1136.59	30.644	1.0259	7.64E-04	0.086436	8.84E-03

0.1
 0
 0
 0
 0
 0.02
 0.03
 0.04
 0.06
 -0.0239
 0.2
 0.13
 0.135
 0.13
 0.125
 0.12
 0.12
 0.12
 0.12
 0.225
 0.225
 0
 0
 0
 0.03
 0.03
 0.03
 0.03
 0.03
 0.04
 0.04
 0
 0
 0.03
 0.03
 0.03
 0.03
 -0.0175
 0.1417
 0
 0.03
 0.03

[illegible]

Example output file for the 12-component lumped to 4 pseudocomponents is:

OBJECTIVE FUNCT. VALUE = 2.50065550419702

PSEUDO COMPS. = CH4N2

Tc Pseudo Comp. 1 = -117.070000000000

Pc Pseudo Comp. 1 = 671.170000000000

Vc Pseudo Comp. 1 = 1.58500000000000

W Pseudo Comp. 1 = 1.3000000000000000E-002

Mw Pseudo Comp. 1 = 16.00000000000000

K Pseudo Comp. 1 = 1.64493433865379

PSEUDO COMPS. = C02 C2 C3 C4

Tc Pseudo Comp. 2 = 142.796957035988

Pc Pseudo Comp. 2 = 769.790430980971

Vc Pseudo Comp. 2 = 2.54052949390466

W Pseudo Comp. 2 = 0.158980852374447

MW Pseudo Comp. 2 = 40.7206179225850

K Pseudo Comp. 2 = 1.23312872746389

PSEUDO COMPS. = C5 C6 C7+ C10+ C14+ C20+

Tc Pseudo Comp. 3 = 775.053316546237

Pc Pseudo Comp. 3 = 322.857602567702

Vc Pseudo Comp. 3 = 13.0560109504973

W Pseudo Comp. 3 = 0.673660648933066

MW Pseudo Comp. 3 = 208.342560039309

K Pseudo Comp. 3 = 0.196399413891622

PSEUDO COMPS. = C30+

Tc Pseudo Comp. 4 = 1136.590000000000

Pc Pseudo Comp. 4 = 171.070000000000

Vc Pseudo Comp. 4 = 30.6440000000000

W Pseudo Comp. 4 = 1.02590000000000

MW Pseudo Comp. 4 = 451.000000000000

K Pseudo Comp. 4 = 8.838886807457022E-003

Binary Interaction Parameters

$$\text{PC1-PC2} = 2.860771792480373\text{E-}002$$

$$\text{PC1-PC3} = 2.581008572811162\text{E-}002$$

$$\text{PC1-PC4} = 0.2000000000000000$$

$$\text{PC2-PC3} = 6.067108614431680\text{E-}002$$

$$\text{PC2-PC4} = 0.126857513116071$$

$$\text{PC3-PC4} = 0.0000000000000000\text{E+}000$$

Appendix E: PVTsim EOS Tuning Module

The regression tool menu showing the different options available for tuning an EOS characterization is given below:

Illustration D.1: PVT data selection menu for PVTsim regression tool.

Regression

Crit T Crit P Ac fac Crit V Cpen Om A Om B kij 1 kij 2 kij 3 kij 4 kij 5

CO2											
CO2											
C2+											
C5+											
C14+											
C21+											

Max adj % 20.00 20.00 20.00 20.00 20.00 20.00 20.00 20.00 20.00

Viscosity
CSP correction factors ☐ 1st ☐ 2nd

Illustration D.2: Menu of EOS parameters for regression.

Appendix F: Compositional Simulation Sample Input and Output

The GEM (2003) simulation input file for the 12-component model is shown below:

```
RESULTS SIMULATOR GEM
RESULTS SECTION INOUT
*TITLE1 '12 comp'
*CASEID '12-1'
*INUNIT *FIELD

*INTERRUPT *INTERACTIVE
*RANGECHECK *ON
*XDR *ON
*MAXERROR 20
*WPRN *WELL *TIME
*WPRN *GRID *TIME
*WPRN *ITER *NONE
*WSRF *WELL *TIME
*WSRF *GRID *TIME
*OUTPRN *WELL *PSPLIT
*OUTPRN *GRID FRG KRG SG Z 'C10+' Z 'C14+' Z 'C1N2' Z 'C2' Z 'C20+' Z 'C3'
      Z 'c30+' Z 'C6' Z 'C7+' Z 'CO2' Z 'nC4' Z 'nC5' KRO SO PRES TSO
      KRW SW

*OUTPRN *RES *NONE
*OUTSRF *WELL *PSPLIT
*OUTSRF *WELL      *WKRO 'Producer' 400 1 1
      *WKRG 'Producer' 400 1 1
      *WKRW 'Producer' 400 1 1
      *ZWEL 'CO2' 'Producer'
      *XWEL 'CO2' 'Producer'
      *YWEL 'CO2' 'Producer'
      *ZWEL 'C1N2' 'Producer'
      *XWEL 'C1N2' 'Producer'
      *YWEL 'C1N2' 'Producer'
      *ZWEL 'C2' 'Producer'
      *XWEL 'C2' 'Producer'
      *YWEL 'C2' 'Producer'
      *ZWEL 'C3' 'Producer'
      *XWEL 'C3' 'Producer'
      *YWEL 'C3' 'Producer'
      *ZWEL 'nC4' 'Producer'
      *XWEL 'nC4' 'Producer'
      *YWEL 'nC4' 'Producer'
      *ZWEL 'nC5' 'Producer'
      *XWEL 'nC5' 'Producer'
      *YWEL 'nC5' 'Producer'
      *ZWEL 'C6' 'Producer'
      *XWEL 'C6' 'Producer'
```

```

*YWEL 'C6' 'Producer'
*ZWEL 'C7+' 'Producer'
*XWEL 'C7+' 'Producer'
*YWEL 'C7+' 'Producer'
*ZWEL 'C10+' 'Producer'
*XWEL 'C10+' 'Producer'
*YWEL 'C10+' 'Producer'
*ZWEL 'C14+' 'Producer'
*XWEL 'C14+' 'Producer'
*YWEL 'C14+' 'Producer'
*ZWEL 'C20+' 'Producer'
*XWEL 'C20+' 'Producer'
*ZWEL 'c30+' 'Producer'
*XWEL 'c30+' 'Producer'
*YWEL 'c30+' 'Producer'
*PAVG
*MOIP
*MGIP
*MWIP
*RECO
*RECI
*RECG
*WKRO 'gas injector' 1 1 1
*WKRK 'gas injector' 1 1 1
*WKRW 'gas injector' 1 1 1

*OUTSRF *GRID KRG SG Z 'C10+' Z 'C14+' Z 'C1N2' Z 'C2' Z 'C20+' Z 'C3'
      Z 'c30+' Z 'C6' Z 'C7+' Z 'CO2' Z 'nC4' Z 'nC5' KRO SO PRES TSO
      VELOCRC KRW SW

*OUTSRF *RES *NONE

RESULTS XOFFSET 0.
RESULTS YOFFSET 0.
RESULTS ROTATION 0
RESULTS AXES-DIRECTIONS 1. -1. 1.

GRID VARI 400 1 1
KDIR DOWN
DI CON 2.5

DJ CON 800.

DK CON 20.
PAYDEPTH ALL
      400*7010.

```

```

**$ RESULTS PROP NULL Units: Dimensionless
**$ RESULTS PROP Minimum Value: 1 Maximum Value: 1
**$ 0 = NULL block, 1 = Active block
NULL CON 1.

**$ RESULTS PROP PINCHOUTARRAY Units: Dimensionless
**$ RESULTS PROP Minimum Value: 1 Maximum Value: 1
**$ 0 = PINCHED block, 1 = Active block
PINCHOUTARRAY CON 1.
RESULTS SECTION GRID

RESULTS SPEC 'Grid Thickness'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 20
RESULTS SPEC STOP

RESULTS SPEC 'Grid Top'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 7000
RESULTS SPEC STOP

RESULTS SPEC 'NULL Blocks'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 1
RESULTS SPEC STOP
RESULTS PINCHOUT-VAL 0.0002 'ft'
RESULTS SECTION NETPAY

RESULTS SPEC 'Net Pay'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 20
RESULTS SPEC STOP

**$ RESULTS PROP NETPAY Units: ft
**$ RESULTS PROP Minimum Value: 20 Maximum Value: 20
NETPAY CON 20.
RESULTS SECTION NETGROSS

```


RESULTS SECTION POR

RESULTS SPEC 'Porosity'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 0.2195
RESULTS SPEC STOP

***\$ RESULTS PROP POR Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.2195 Maximum Value: 0.2195
POR CON 0.2195
RESULTS SECTION PERMS

RESULTS SPEC 'Permeability K'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 1200
RESULTS SPEC STOP

RESULTS SPEC 'Permeability I'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 1200
RESULTS SPEC STOP

RESULTS SPEC 'Permeability J'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 1200
RESULTS SPEC STOP

***\$ RESULTS PROP PERMI Units: md
***\$ RESULTS PROP Minimum Value: 1200 Maximum Value: 1200
PERMI CON 1200.

***\$ RESULTS PROP PERMJ Units: md
***\$ RESULTS PROP Minimum Value: 1200 Maximum Value: 1200
PERMJ CON 1200.

***\$ RESULTS PROP PERMK Units: md
***\$ RESULTS PROP Minimum Value: 1200 Maximum Value: 1200
PERMK CON 1200.

RESULTS SECTION TRANS
 RESULTS SECTION FRACS
 RESULTS SECTION GRIDNONARRAYS
 CPOR MATRIX 3.E-06
 PRPOR MATRIX 4100.

RESULTS SECTION VOLMOD
 RESULTS SECTION SECTORLEASE

RESULTS SECTION ROCKCOMPACTION
 RESULTS SECTION GRIDOTHER
 RESULTS SECTION MODEL

```

*MODEL      *PR
*NC          12 12
*COMPNAME    'CO2'   'C1N2'   'C2'   'C3'   'nC4'
              'nC5'   'C6'     'C7+'   'C10+'  'C14+'
              'C20+'  'c30+'
*HCFLAG      0       0       0       0       0
              0       0       0       0       0
              0       0
*TRES        200.
*PCRIT        72.900000 45.670000 48.200000 42.010000 36.970000
              32.340000 28.550000 28.420000 27.700000 21.390000
              13.970000 11.640000
*TCRIT        304.01700 190.33300 305.21700 369.71700 419.02800
              458.96100 499.48900 580.01100 628.02800 704.39500
              785.70600 886.81100
*AC           0.225000 0.013000 0.098600 0.152400 0.187000
              0.252300 0.313800 0.373900 0.548900 0.755000
              0.875000 1.025900
*VCRIT        0.093900 0.098900 0.148000 0.203000 0.255000
              0.304000 0.373000 0.439000 0.506000 0.762000
              1.360000 1.910000
*MW           44.01000 16.00000 30.07000 44.09700 58.12400
              72.15100 86.17800 108.00000 152.00000 213.00000
              312.00000 451.00000
*PCHOR        78.00000 96.90000 108.90000 151.90000 191.70000
              233.90000 271.00000 312.00000 415.00000 557.70000
              789.40000 1114.60000
*TB           -109.30000 -258.39400 -127.39000 -43.69000 31.19000
              85.02700 155.75000 258.63500 348.28900 497.36200
              661.21200 842.86600
*VSHIFT       0.000000 0.000000 0.000000 0.000000 0.000000
              0.000000 0.000000 0.000000 0.000000 0.000000
              0.000000 0.000000
*OMEGA        .457240000 .457240000 .457240000 .457240000 .457240000
              .457240000 .457240000 .457240000 .457240000 .457240000
              .457240000 .457240000
*OMEGB        .077800000 .077800000 .077800000 .077800000 .077800000
              .077800000 .077800000 .077800000 .077800000 .077800000
              .077800000 .077800000
*BIN
              0.1
              0.13    0.0
  
```

0.135	0.0	0.0			
0.13	0.0	0.0	0.0		
0.125	0.0	0.0	0.0	0.0	
0.12	0.02	0.03	0.03	0.03	0.0
0.12	0.03	0.03	0.03	0.03	0.0
0.0					
0.12	0.04	0.03	0.03	0.03	0.0
0.0	0.0				
0.12	0.06	0.03	0.03	0.03	0.0
0.0	0.0	0.0			
0.225	-0.0239	0.04	-0.0175	0.04	0.0
0.0	0.0	0.0	0.0		
0.255	0.2	0.04	0.1417	0.04	0.0
0.0	0.0	0.0	0.0	0.0	

*PHASEID *DEN
 *RHOW 1572.605
 *CW 3.E-06
 *REFPW 4100.
 *VISW 0.34

RESULTS SECTION MODELARRAYS RESULTS SECTION ROCKFLUID

*ROCKFLUID

*RPT 1 *DRAINAGE

*SWT

0.000000	0.000000	0.640000	0.000000
0.050000	0.002500	0.562500	0.000000
0.100000	0.010000	0.490000	0.000000
0.150000	0.022500	0.422500	0.000000
0.200000	0.040000	0.360000	0.000000
0.250000	0.062500	0.302500	0.000000
0.300000	0.090000	0.250000	0.000000
0.350000	0.122500	0.202500	0.000000
0.400000	0.160000	0.160000	0.000000
0.450000	0.202500	0.122500	0.000000
0.500000	0.250000	0.090000	0.000000
0.550000	0.302500	0.062500	0.000000
0.600000	0.360000	0.040000	0.000000
0.650000	0.422500	0.022500	0.000000
0.700000	0.490000	0.010000	0.000000
0.750000	0.562500	0.002500	0.000000
0.800000	0.640000	0.000000	0.000000

*SGT

0.000000	0.000000	0.640000	0.000000
0.050000	0.002500	0.562500	0.000000
0.100000	0.010000	0.490000	0.000000
0.150000	0.022500	0.422500	0.000000
0.200000	0.040000	0.360000	0.000000
0.250000	0.062500	0.302500	0.000000

RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 0
RESULTS SPEC STOP

RESULTS SPEC 'Endpoint Saturation: Residual Oil for Gas-Liquid Table'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 0.2
RESULTS SPEC STOP

RESULTS SPEC 'Endpoint Saturation: Residual Oil for Water-Oil Table'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 0.2
RESULTS SPEC STOP

**\$ RESULTS PROP SORM Units: Dimensionless
**\$ RESULTS PROP Minimum Value: 0 Maximum Value: 0
SORM CON 0

**\$ RESULTS PROP SORW Units: Dimensionless
**\$ RESULTS PROP Minimum Value: 0.2 Maximum Value: 0.2
SORW CON 0.2

**\$ RESULTS PROP SORG Units: Dimensionless
**\$ RESULTS PROP Minimum Value: 0.2 Maximum Value: 0.2
SORG CON 0.2

RESULTS SECTION INIT
*INITIAL
*USER_INPUT
*DATUMDEPTH 7000. *INITIAL
*NREGIONS 1
*INJECTOR-P 3650.
*INJECTOR-T 200.
*INJECTOR-EOS 1

RESULTS SECTION INITARRAYS

RESULTS SPEC 'Pressure'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 3650
RESULTS SPEC STOP

RESULTS SPEC 'Water Saturation'
RESULTS SPEC SPECNOTCALCVAL 0
RESULTS SPEC REGION 'All Layers (Whole Grid)'
RESULTS SPEC REGIONTYPE 0
RESULTS SPEC LAYERNUMB 0
RESULTS SPEC PORTYPE 1
RESULTS SPEC CON 0
RESULTS SPEC STOP

***\$ RESULTS PROP SW Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0 Maximum Value: 0
SW CON 0

***\$ RESULTS PROP PRES Units: psi
***\$ RESULTS PROP Minimum Value: 3650 Maximum Value: 3650
PRES CON 3650.

***\$ RESULTS PROP ZGLOBALC 'CO2' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.04484 Maximum Value: 0.04484
ZGLOBALC 'CO2' CON 0.04484

***\$ RESULTS PROP ZGLOBALC 'C1N2' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.36918 Maximum Value: 0.36918
ZGLOBALC 'C1N2' CON 0.36918

***\$ RESULTS PROP ZGLOBALC 'C2' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.03205 Maximum Value: 0.03205
ZGLOBALC 'C2' CON 0.03205

***\$ RESULTS PROP ZGLOBALC 'C3' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.02333 Maximum Value: 0.02333
ZGLOBALC 'C3' CON 0.02333

***\$ RESULTS PROP ZGLOBALC 'nC4' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.01532 Maximum Value: 0.01532
ZGLOBALC 'nC4' CON 0.01532

***\$ RESULTS PROP ZGLOBALC 'nC5' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.00877 Maximum Value: 0.00877
ZGLOBALC 'nC5' CON 0.00877

***\$ RESULTS PROP ZGLOBALC 'C6' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.01265 Maximum Value: 0.01265
ZGLOBALC 'C6' CON 0.01265

***\$ RESULTS PROP ZGLOBALC 'C7+' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.09168 Maximum Value: 0.09168
ZGLOBALC 'C7+' CON 0.09168

***\$ RESULTS PROP ZGLOBALC 'C10+' Units: Dimensionless
***\$ RESULTS PROP Minimum Value: 0.11185 Maximum Value: 0.11185
ZGLOBALC 'C10+' CON 0.11185

***\$ RESULTS PROP ZGLOBALC 'C14+' Units: Dimensionless

**\$ RESULTS PROP Minimum Value: 0.1122 Maximum Value: 0.1122
 ZGLOBALC 'C14+' CON 0.1122

**\$ RESULTS PROP ZGLOBALC 'C20+' Units: Dimensionless
 **\$ RESULTS PROP Minimum Value: 0.09094 Maximum Value: 0.09094
 ZGLOBALC 'C20+' CON 0.09094

**\$ RESULTS PROP ZGLOBALC 'c30+' Units: Dimensionless
 **\$ RESULTS PROP Minimum Value: 0.08719 Maximum Value: 0.08719
 ZGLOBALC 'c30+' CON 0.08719
 RESULTS SECTION NUMERICAL
 *NUMERICAL
 *MAXSTEPS 300000000
 *DTMAX 20.
 *DTMIN 0.0001
 *SORDER *NATURAL
 *NORM *PRESS 200.
 *NORM *GMOLAR 0.0001
 *NORM *SATUR 0.002
 *MAXCHANGE *PRESS 200.377
 *MAXCHANGE *GMOLAR 0.0001
 *MAXCHANGE *SATUR 0.02
 *CONVERGE *PRESS 0.514884

RESULTS SECTION NUMARRAYS
 RESULTS SECTION GBKEYWORDS
 RUN

DATE 2004 06 25

DTWELL 0.0001

*INJECTOR-T 200.

*INJECTOR-EOS 1

*DTMAX 20.

*DTMIN 0.0001

*WPRN *WELL *TIME
 *WPRN *GRID *TIME
 *WPRN *ITER *NONE
 *WSRF *WELL *TIME
 *WSRF *GRID *TIME

WELL 1 'gas injector'
 INJECTOR 'gas injector'
 INCOMP SOLVENT 0.2081 0.3277 0.2008 0.2223 0.0411 0 0 0 0 0 0
 OPERATE MAX BHG 151.14 CONT
 OPERATE MAX BHP 5000. STOP

Nomenclature

$a_1 - a_{10}$	=	Parameters given in Eq. 2.1 & 2.3
k	=	Key tie-line number
K_i	=	Equilibrium constant of component i
B_o	=	Oil formation volume factor
B_g	=	Gas formation volume factor
CH_4N_2	=	Pseudocomponent formed by lumping methane and nitrogen
Cum.	=	Cumulative component or oil recovery
δ_{ij}	=	Binary interaction parameter between components i and j
EOS	=	Equation of state
GOR	=	Total gas- oil ratio
HCPVI	=	Hydrocarbon pore volume injected
L	=	Liquid phase mole fraction
M_w	=	Molecular weight
$M_{C_{5+}}$	=	Molar weight of C_5 plus fraction
$M_{C_{7+}}$	=	Molar weight of C_7 plus fraction
MMP_{pure}	=	Minimum miscibility pressure for pure CO_2 injection, psia
MMP_{imp}	=	Minimum miscibility pressure for impure CO_2 injection, psia
nc	=	Number of components
$nc - 1$	=	Number of key tie lines
$nc - 3$	=	Number of crossover tie lines
ϕ	=	Fugacity coefficient
P_{CO_2}	=	Molar percentage CO_2 in the injection gas
$P_{C_{2-6}}$	=	Molar percentage of $C_2 - C_6$
P_c	=	Critical pressure
PV	=	Pore volume
PVT	=	Pressure volume and temperature
Rec.	=	Recovery
R_s	=	Solution gas-oil ratio
SVP	=	Saturation vapor pressure
S_g	=	Solution gas-oil ratio
T	=	Reservoir temperature, °F
T_c	=	Critical temperature
td	=	Dimensionless time in pore volume
V	=	Vapor phase mole fraction
V_c	=	Critical volume

V_b	=	<i>Volume of oil at the bubble point pressure</i>
ω	=	<i>Accentric factor</i>
x_i	=	<i>Equilibrium mole fraction of component i in the liquid phase</i>
y_i	=	<i>Equilibrium mole fraction of component i in the vapor phase</i>
Z_i	=	<i>Overall mole fraction of component i in the fluid mixture</i>

References

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