SPE 78481

Uses and Abuses of Equations of State

Hiroshi Kawahara, Takeshi Hiraiwa, Koichi Yoshida, Japan Oil Development Co., Ltd.
Makoto Watanabe, Japan National Oil Corporation

This paper was prepared for presentation at the 10th Abu Dhabi International Petroleum Exhibition and Conference, 13-16 October 2002.

Abstract

Equations of state (EOS) are perhaps the most abused and mis-used concept in compositional reservoir simulation. It is believed that the EOS are often need adjusting or tuning and the well-tuned EOS can capture all phase behavior in the reservoir simulation. However, the well-tuned EOS can not calculate appropriately in the reservoir simulation because the matching objectives, the existing PVT experiments, are not enough to cover all necessary pressure, temperature, and components.

An EOS for CO_2, hydrocarbon gas and sour gas injection is tuned for a reservoir fluid offshore Abu Dhabi. The universal EOS for gas injection, EOS-U8, was originally developed as EOS-H18 for hydrocarbon gas injection (both sour and sweet). After the EOS-H18 was developed, additional PVT experiments, swelling tests with CO_2 and other two hydrocarbon gases, were conducted and the EOS-U8 was tuned in order to capture the phase behavior of the reservoir fluid and all candidate injection gases. The new, tuned EOS is available for evaluating gas injection, including direct comparison between injection gases. Our tuning procedure for an EOS, including laboratory data selection, is applicable to other reservoir fluids.

The Flash calculation is compared utilizing the tuned EOS using all or selected laboratory data. Limited laboratory data may mislead the tuning process of the EOS parameters for extensive application of the EOS. The methods that gave the best match are also discussed.

Three commercial software for generating EOS parameters were compared for performance, accuracy, and ease of use. The advantages and disadvantages of three commercial EOS PVT programs are compared. The interface and function of the programs are also evaluated. Three EOS based PVT programs show different results with high concentration of CO_2 or H_2S using the tuned EOS parameters. Therefore, special cares are required for importing EOS parameters form other EOS programs. The most appropriate ways to use the EOS developed by current software products are discussed. The results from this comparison study of EOS based PVT programs are useful for selecting PVT programs.

Finally three EOS (EOS-H8, C8, U8) were compared in the compositional reservoir simulation. The tuned EOS with the selected laboratory data shows different results in the reservoir simulation using the EOS-U8. It is recommended that EOS should be tuned utilizing as much as PVT experiments.

Introduction

Equations of State (EOS) are one of the most important and sensitive factors in reservoir simulation for gas injection study. In 1998, intensive phase behavior study was conducted for a limestone reservoir in a large field of Abu Dhabi offshore. Special PVT tests were conducted using two hydrocarbon gases and one sour gas. The first EOS, EOS-H18, was developed, utilizing Software-A, in order to capture the phase behavior of the reservoir fluid with three different components of injection gases.

In the next year, additional phase behavior study was conducted for the reservoir fluid with sour gas, hydrocarbon gas and CO_2. The EOS-H18 was updated as EOS-U8 in order to capture the phase behavior of the reservoir fluid with all six gases. In this updating process, it was found that the original EOS might not be compatible with Software-B. The EOS-U8 was developed with the Software-B, which was selected because of the compatibility with the Compositional Simulation Software-D.

In this study, the matching results of EOS using all or selected data are discussed. Then, comparison results of three commercial software for generating EOS parameters are presented. Finally, influence of misused EOS is discussed in the point of the compositional reservoir simulation.

Tuning of Reference EOS

Four EOS, EOS-H18, EOS-H8, EOS-U8 and EOS-C8, were utilized in this comparison study. The EOS-H18 was the original eighteen components EOS, which was tuned with previous PVT experiments in 1998. The experiments included two swelling tests with hydrocarbon gases without H_2S and one swelling tests with sour gas. The EOS-H18 was developed by Whitson's method (Whitson, 1983) with their initial EOS parameters of Twu correlation (Twu, 1984).

The EOS-H18 was lumped to eight components EOS, EOS-H8. Omega parameters of the EOS-H8 were tuned in order to match the phase behavior calculated by the EOS-H18. Therefore, the EOS-H18 and EOS-H8 can calculate similar flash calculation in hydrocarbon gas injection.

After the EOS-H18 and the EOS-H8 were developed, additional phase behavior study was conducted including swelling test with CO_2. New eight components EOS, EOS-C8, was developed in order to capture the phase behavior of CO_2 injection and to conduct first screening study of CO_2 injection. The EOS-H8 was utilized as the initial EOS, however, the previous PVT experiments was ignored because of accelerating the tuning process and screening study. The EOS-C8 was successfully utilized for the first screening study and it is concluded that CO_2 has advantage to the hydrocarbon gas in the reservoir performance. CO_2 injection showed low GOR in the same recovery factor and high recovery factor in the same period of injection.

Finally, EOS-U8 was tuned in order to capture all phase behavior of the reservoir fluid with possible candidates of injection gases, CO_2, hydrocarbon gas and sour gas. The EOS-U8 has eight pseudo-components including H_2S and CO_2 as individual components.

In order to develop the universal EOS, EOS-U8, detailed compositional analyses were reviewed and composition of EOS-H18 was modified. In this process, instead of mole fractions, weight fractions of pseudo components in each fluid are conserved.

Molecular weights of pseudo components were determined from the detail compositional analysis up to C_{36+}. More than 30 compositional analyses up to C_{7+} show that the composition of the reservoir fluid is strongly depend on the reservoir depth in the target reservoir. Therefore, one reference composition was carefully selected and one set of molecular weight was utilized in all fluid composition.

The EOS-H18 was lumped to the eight pseudo-components. The eight pseudo-components were selected by K-value method (Li et al., 1985). CO_2 and H_2S were selected as individual components respectively because injection gas can be consist of large mole percent of these components in it. Properties of the lumped components are determined using the mole fraction weighted mixing rules.

Initial EOS was tuned of critical properties and binary interaction coefficients to match the saturation pressure of each swelling tests and then liquid saturation. S-shift parameters were tuned to match the density and critical volumes were also tuned to match the viscosity.

More detail of pseudo-components for each EOS is shown in Table 1. The PVT experiments for tuning the four EOS are shown in Table 2. All EOS adopts the three-parameter extension by Peneloux et al. for Peng-Robinson EOS and the Lohrenz-Bray-Clark correlation for viscosity.

It is noted that the EOS-H18 and the EOS-H8 were developed with the PVT Software-A and theEOS-C8 and the EOS-U8 were with the PVT Software-B. The original EOS parameters were appropriately converted from Software-A to Software-B.

Comparison of Flash Calculation Results

Typical tuning results of three eight components EOS are shown in Figures 1. The EOS-U8 and EOS-H8 shows similar results in the swelling test with hydrocarbon gas and the EOS-U8 and EOS-C8 in the swelling test with CO_2.

All three EOS shows almost identical in the original reservoir fluid without any solvent gas mixed. However, main discrepancy was observed near critical points.

The most significant discrepancy in EOS-U8 and EOS-C8 is minimum miscibility pressure (MMP), which is calculated by Jensen and Michelsen's method (1990). This is mainly due to the difference phase behavior of the dew point fluid as shown in the swelling test results. Although there are no measured data of dew point fluid, the results of EOS-U8 seems to be reliable because the MMP of EOS-U8 is matched with the measured MMP by slime tube tests.

This discrepancy is partially due to the development software, which will be discussed in the next section. All above calculation are conducted by Software-B, however the EOS-H18 and EOS-H8 were developed by the Software-A. It is noted that the saturation pressure of the EOS-H8 is smaller than that of the EOS-U8.

It is concluded that both EOS-C8 and EOS-U8 can be effective for CO_2 injection study because both EOS calculate almost identical phase behavior of swelling test with CO_2 as well as similar MMP of CO_2 injection. On the other hand, both EOS-H8 and EOS-U8 satisfied phase behavior of swelling test with the Hydrocarbon Gas 2, however, MMP of Hydrocarbon Gas 2 is different. Therefore, EOS-H8 and EOS-U8 may show some discrepancy in compositional simulation. More detail of the discrepancy will be discussed with the compositional simulation results later.

Herewith, it is recommended that as much as PVT experiments should be conducted and utilized in the tuning of EOS. Selected matching objective from PVT experiments may mislead the tuning of EOS although the EOS seems to capture the selected PVT experiments.

Comparison of three EOS based PVT programs

Three commercial software, Software-A, B and C, for generating EOS parameters were compared for performance. The EOS-H18, EOS-H8 and EOS-U8 were utilized in the comparison study.

Typical results of flash calculation are shown in Figures 2 and 3. EOS-H18 and EOS-U8 are utilized in these cases. All EOS shows similar trend as follows:

- Three programs gave quite similar results in saturation pressure, liquid saturation, and relative volume in reservoir fluid samples without any gas mixture. Therefore, it is concluded that three programs are compatible for black oil type fluid.

- The discrepancies became larger when the mixtures of the samples containing large mole percent of solvent gas. In these high GOR fluids, Software-B showed different phase behavior to the other programs. Software-A and Software-C showed similar performance except near critical point, where Software-A failed to calculate because of convergence failure. Software-B tended to recognize near critical point fluid as bubble point fluid, but the other programs as dew point fluid. Therefore, Software-B gave the lowest saturation pressure and liquid saturation in most simulation.
- Density and viscosity of Software-A were much different from the other programs as shown in Figure 4. Software-B and Software-C showed similar oil density and viscosity in most bubble point fluid as well as the mixture with CO_2. However, Software-C calculated bumpy curves of density and viscosity in the mixture with hydrocarbon gases. It was noted that Software-C could not calculate viscosity by Lohrenz-Bray-Clark correlation. Hence, Jossi-Stie-Thodos correlation was adopted in Software-C. Considering this comparison study, Software-B gives the most appropriate density and viscosity of three programs.

The regression facilities of the three PVT programs were also compared using same initial EOS, which was generated from EOS-H18 lumped to eight components. In the test case, the limited data, saturation pressure and swelling factor of five swelling tests, were selected as matching objectives.
The results are concluded as follows:

- The tuned EoS of Software-A matched the best saturation pressure of all and Software-B generated the best swelling factor of all as shown in Table 3. Software-C generated unstable EoS, which could not calculate two saturation pressure of one swelling test.
- Software-A and Software-B had stable regression facilities but Software-C sometimes stopped regression when the fluid systems requested the flash calculation near the critical point.

Software-B and Software-C had the friendly interface. Software-C had the spreadsheet output format with graph, which was easy to modify features. The graphic facilities of Software-B were also excellent with multi-window type features.
Therefore, the following judgment can be made at the moment of time. Software-A has advantage of compatibility to Software-C and disadvantage of interface. Software-B has advantage in stability and interface and disadvantage of compatibility of flash calculation to other programs. Software-C has advantage in interface and compatibility to Software-A and disadvantage in poor regression facilities.
Considering these differences in flash calculation result due to the PVT software, EOS-H18 and EOS-H8 have tendency to recognize near critical point fluid as bubble point fluid. Moreover, both EOS gave the lowest saturation pressure and liquid saturation in Software-B.

Comparison of Compositional Simulation Results

Total six reservoir simulation models are utilized in order to evaluate the EOS. Four cross sectional sector including one horizontal injector and one horizontal producer were selected as two-dimensional model as shown in Figure 5. Geological properties, such as porosity and permeability, were extracted from the history matched full field simulation model. No flow boundary was assumed because the existing five spot pattern water injection was well balanced to maintain the reservoir pressure.
Two types of injection gases, the Hydrocarbon Gas 2 and CO_2, are utilized. It is noted that CO_2 achieves miscible flood in this simulation conditions, however, the Hydrocarbon Gas 2 injection is immiscible.
The reservoir performances of 2 D models are shown in Figure 6. Two-dimensional simulation results show all EOS simulate almost same reservoir performance except CO_2 injection of EOS-H8. This is mainly due to that the EOS-H8 does not have individual component of CO_2.
However, three-dimensional simulation results show quite different trend. Two three-dimensional sector models were selected from the same area of the two-dimensional model. The 3D sector models included one horizontal injector in the center of the sector and four horizontal producers at the corner of the sector. The reservoir performances are shown in Figure 7.
The reservoir performances of EOS-H8 are quit different from the other two EOS. The discrepancy of reservoir performances in CO_2 injection and Hydrocarbon Gas 2 injection is relatively small in EOS-U8 and EOS-C8. However, the effects of miscible flooding are exaggerated in EOS-H8.

Conclusions

Three eight-component EOS are developed in order to capture the phase behavior of different type of injection gases. The EOS-U8 was tuned to capture the phase behavior of all possible gas injection. The EOS-H8 and EOS-C8 can capture the selected phase behavior of gas injection, however, the tuning process utilizing the selected PVT data may mislead the EOS to wrong phase behavior.
Three commercial EOS based PVT programs are compared for flash calculation as well as regression facilities. The flash calculation results show almost same in black oil, however large discrepancy was observed in high GOR fluid. Therefore, special care is required when EOS parameters are imported from the other software. Importing EOS parameters without any further tuning bring misuse of EOS and wrong phase behavior prediction and reservoir simulation.
Two-dimensional reservoir simulation results showed quite similar in the universal EOS and the EOS for the selected gas injection. However, three-dimensional simulation revealed the difference of EOS. The tuning process utilizing the selected PVT data may mislead the EOS to wrong reservoir simulation results, too. EOS should be developed utilizing as much as data available in different pressure, temperature, and components.

Acknowledgments

The authors would like to thank the management of Japan National Oil Corporation (JNOC) and Japan Oil Development Co., Ltd. (JODCO) for their support and permission to publish this paper.

References

1. Twu, C. H., “An Internally Consistent Correlation for Predicting the Critical Properties and Molecular Weight for Petroleum and Coal-Tar Liquid,” Fluid Phase Equilibria, Vol. 16, 1984, pp. 137-150.
2. Whitson, C. H., “Characterizing Hydrocarbon Plus Fractions,” Society of Petroleum Engineers Journal, August 1983, pp. 683-694.
3. Jensen, F. and Michelsen, M. L., “Calculation of First Contact and Multiple Contact Minimum Miscibility Pressures,” In Situe, Vol. 14, No. 1, 1990, pp. 1-17.
4. Li, Y. K., Nghiem, L. X., and Sie, A., “Phase Behavior Computations for Reservoir Fluids: Effects of Pseudo-Components on Phase Diagrams and Simulation Results,” J. Can. Pet. Tech., Vol. 24, No. 6, 1985, pp. 29-36.

Table 1 Pseudo Component of Reference EOS

	EOS-H18	EOS-H8	EOS-C8	EOS-U8
PSEUDO COMPONENT 1	H_2S	N_2, C1	CO_2	H_2S
PSEUDO COMPONENT 2	CO_2	CO_2, H_2S, C2	N_2, (H_2S,)* C1	CO_2
PSEUDO COMPONENT 3	N_2	C3-C4	C2-C3	N_2, C1
PSEUDO COMPONENT 4	C1	C5-C6	C4-C5	C2-C3
PSEUDO COMPONENT 5	C2	C7-C10	C6-C13	C4-C6
PSEUDO COMPONENT 6	C3	C11-C19	C14-C19	C7-C19
PSEUDO COMPONENT 7	IC4	C20-C35	C20-C35	C20-C35
PSEUDO COMPONENT 8	NC4	C36+	C36+	C36+
PSEUDO COMPONENT 9	IC5			
PSEUDO COMPONENT 10	NC5			
PSEUDO COMPONENT 11	C6			
PSEUDO COMPONENT 12	C7-C8			
PSEUDO COMPONENT 13	C9-C10			
PSEUDO COMPONENT 14	C11-C13			
PSEUDO COMPONENT 15	C14-C19			
PSEUDO COMPONENT 16	C20-C26			
PSEUDO COMPONENT 17	C27-C35			
PSEUDO COMPONENT 18	C36+			

*) H2S is not included in all fluid samples for tuning.

Table 2 Tuning Parameters and Matching Objectives

			EOS-H18***	EOS-H8	EOS-C8	EOS-U8
Tuning Parameters			BIC*, Pc, Tc, ω, s-shift	ωA, ωB	BIC, s-shift, Zc for Viscosity	Pc, Tc, BIC, s-shift, Vc
Matching Objectives	CCE		Ps, MW, ρl, γg, Zg, GOR, Vt	Ps	Ps, Vt, μl	Ps, ρl
Matching Objectives	DL		ρl, γg, Zg, GOR, Moles Produced, Vl	ρl, ρv, μl, μg, Moles Produced, γg	Bo, Rs, ρl, μl	ρl, μl, GOR, γg, Zg****
Matching Objectives	Separator Test				Bo, Rs	Bo, ρv, GOR****
Matching Objectives	Swelling Test	Hydrocarbon Gas 1**	Liquid Saturation	Ps, Liquid Saturation		Ps, Liquid Saturation
Matching Objectives	Swelling Test	Hydrocarbon Gas 2**	Liquid Saturation	Liquid Saturation		Ps, Liquid Saturation
Matching Objectives	Swelling Test	Sour Gas 1**	Liquid Saturation	Liquid Saturation		Ps, Liquid Saturation
Matching Objectives	Swelling Test	Sour Gas 2				Ps, Liquid Saturation, ρl
Matching Objectives	Swelling Test	Hydrocarbon Gas 3				Ps, Liquid Saturation
Matching Objectives	Swelling Test	CO_2			Liquid Saturation, Vt, ρl, μl	Ps, Liquid Saturation, ρl

*) BIC stands for the binary interaction coefficients.

**) These experiments include only bubble point fluid.

***) EOS-H18 has the matching objectives of the PVT experiments with the reservoir fluid in the upper formation.

****) These data are not utilized in regression facilities, however, the observed data are compared to the calculated value graphically.

Table 3 Comparison of regression facilities of Three EoS based programs.
(RMS errors before and after regression in a test case)

Test	Software	Regression	Swelling Test					Total
			Hydrocarbon Gas 1	Hydrocarbon Gas 2	Sour Gas 1	Sour Gas 2	CO_2	
Ps (psi)	A	before	695	746	740	368	2321	1316
		after	146	223	297	627	429	424
	B	before	125	73	56	1102	903	742
		after	431	417	319	793	257	508
	C	before	699	763	763	437	4129	2212
		after	677	914	1104	NA	790	756*
Swelling Factor	A	before	0.135	0.082	0.09	0.253	0.07	0.154
		after	0.082	0.042	0.059	0.088	0.029	0.064
	B	before	0.11	0.063	0.074	0.233	0.058	0.137
		after	0.046	0.022	0.04	0.071	0.019	0.046
	C	before	0.087	0.046	0.06	0.161	0.033	0.097
		after	0.075	0.039	0.057	0.408	0.012	0.215

*) RMS error is excluded the uncalculated saturation pressure data.

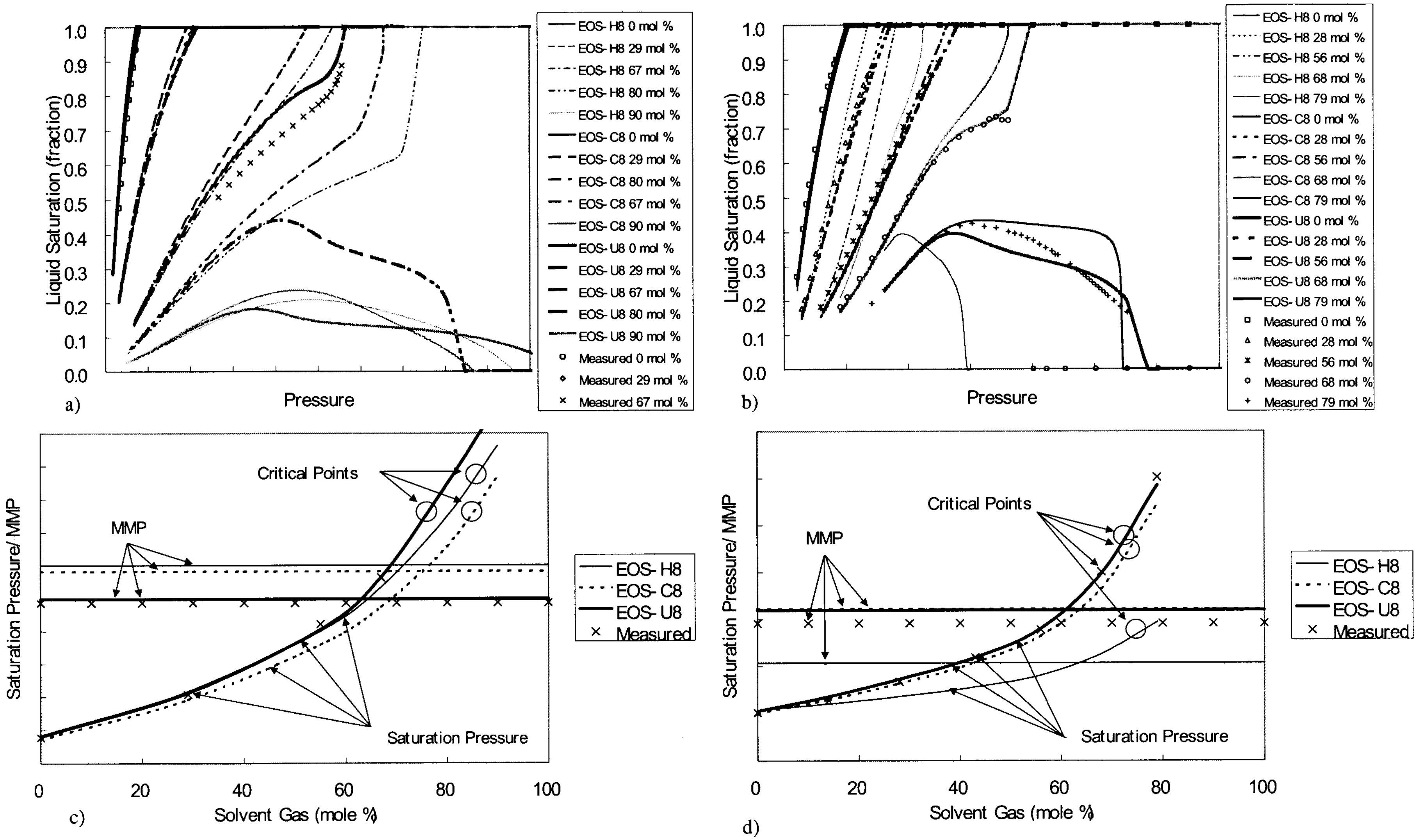

Figure 1 Matching Results of EOS-H8, EOS-C8, EOS-U8.
a) Liquid Saturation in Swelling Test with Hydrocarbon Gas 2, b) Liquid Saturation in Swelling Test with CO_2,
c) Saturation Pressure in Swelling Test and MMP with Hydrocarbon Gas 2, d) Saturation Pressure in Swelling Test and MMP with CO_2.

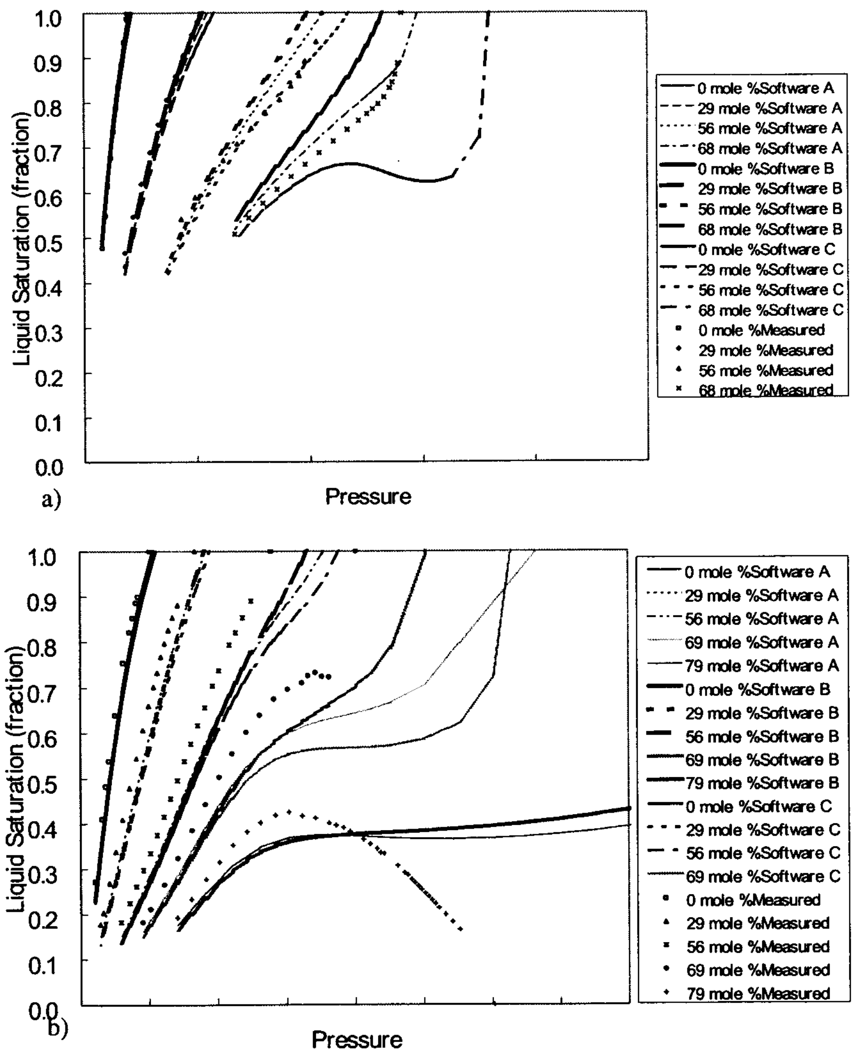

Figure 2 Comparison of EOS based PVT Programs (EOS-H18).
a) Liquid Saturation in Swelling Test with Hydrocarbon Gas 2.
b) Liquid Saturation in Swelling Test with CO_2.

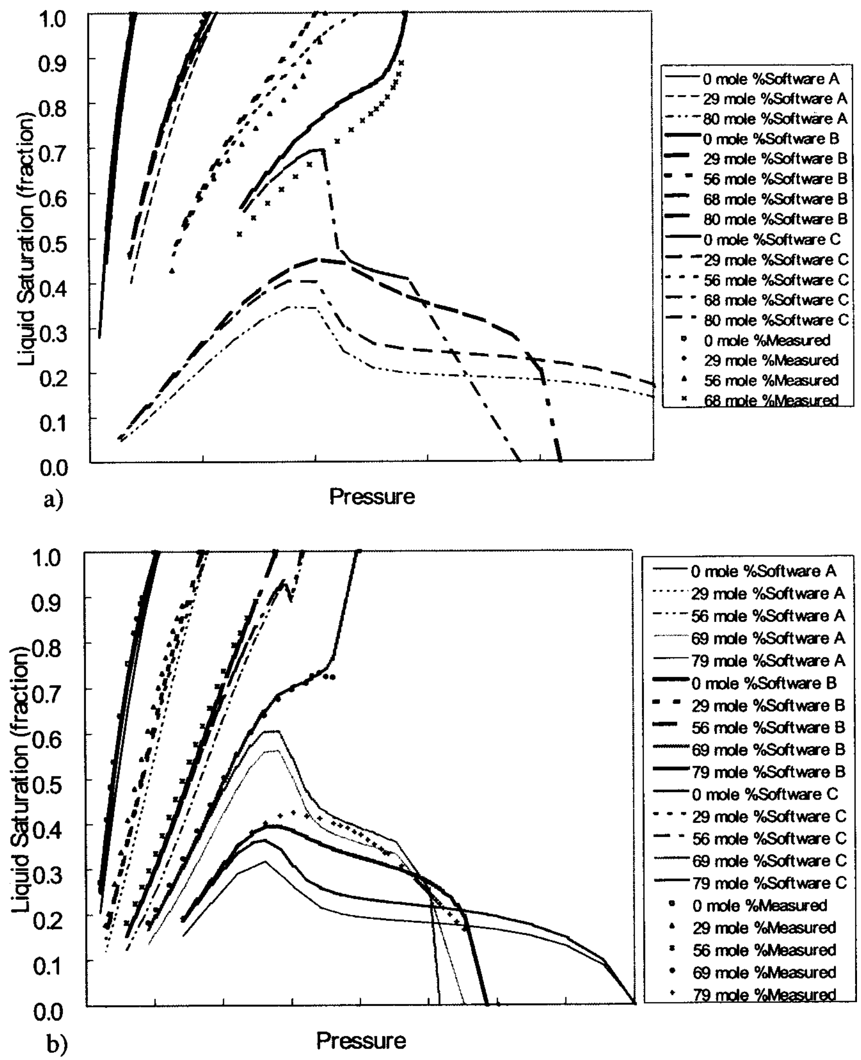

Figure 3 Comparison of EOS based PVT Programs (EOS-U8).
a) Liquid Saturation in Swelling Test with Hydrocarbon Gas 2.
b) Liquid Saturation in Swelling Test with CO_2.

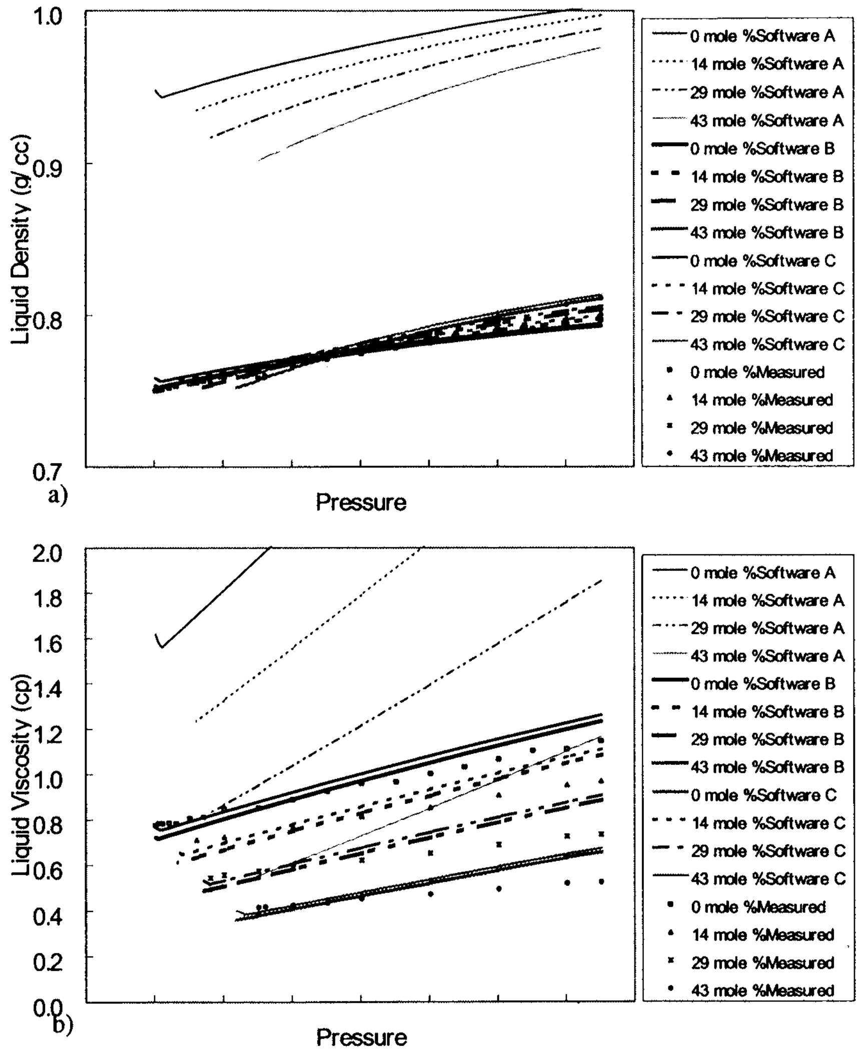

Figure 4 Comparison of EOS based PVT Programs (EOS-U8).
a) Liquid Density in Swelling Test with CO_2.
b) Liquid Viscosity in Swelling Test with CO_2.

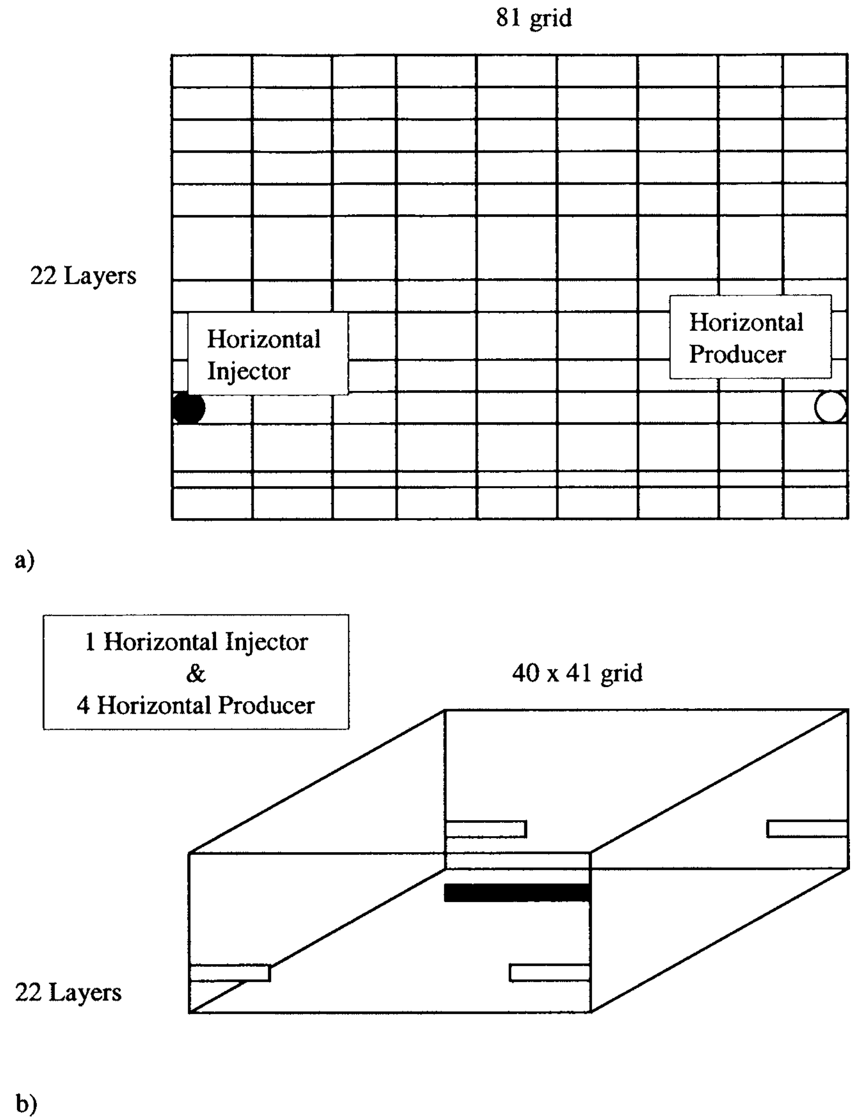

Figure 5 Compositional Simulation Model.
a) 2D cross sectional model.
b) 3D Sector Model.

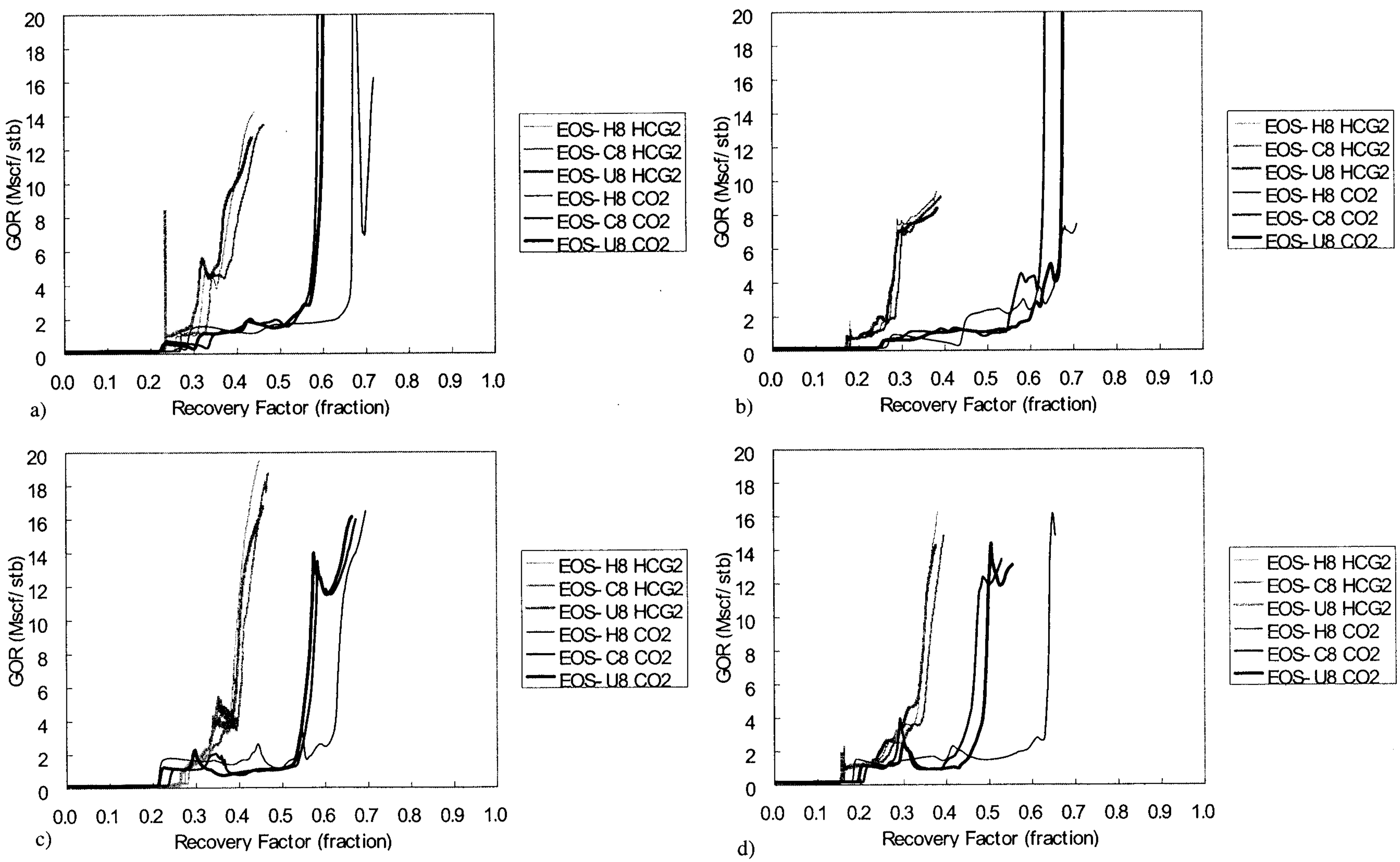

Figure 6 Simulation Results of 2D Cross Sectional Model (GOR vs. Recovery Factor).
a) WELL-A, b) WELL-B, c) WELL-D, d) WELL-D.

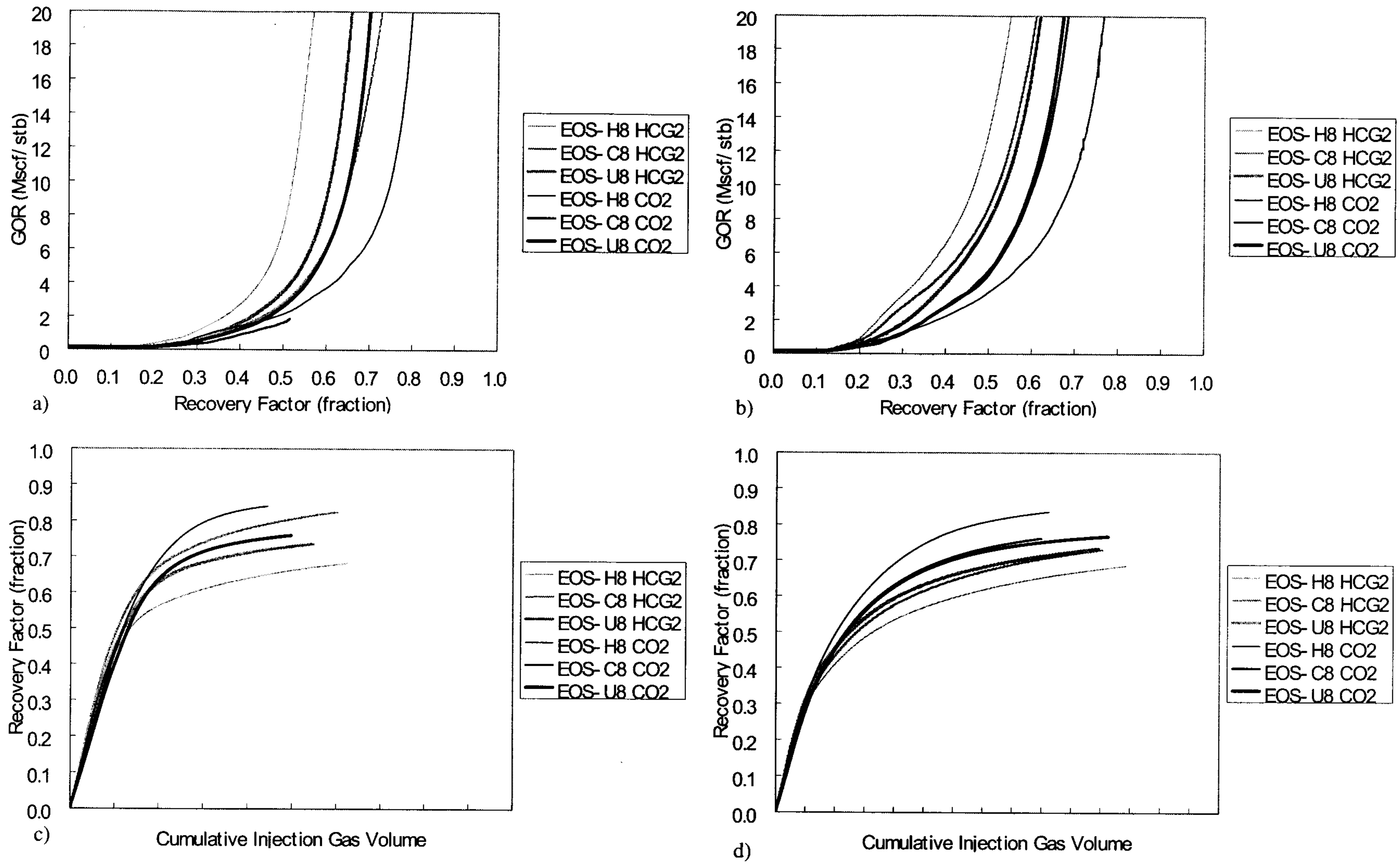

Figure 7 Simulation Results of 3D Sector Model .

a) GOR vs. Recovery Factor (WELL-C), b) GOR vs. Recovery Factor (WELL-D),

c) Recovery Factor vs. Gas Injection Volume (WELL-C), d) Recovery Factor vs. Gas Injection Volume (WELL-D).