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EFFECT OF NON-EQUILIBRIUM MASS TRANSFER IN MISCIBLE GAS RECOVERY PROCESSES

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Abstract*: The mass transfer equilibrium is a condition usually assumed to solve EOS and flash equations. However, this condition is not always true for all reservoirs, especially in regions near high-rate gas wells. For such wells, the fluids take seconds to run through a gridblock near the wellbore, and there is not enough time to achieve the equilibrium mass transfer. This paper presents a model to evaluate the non-equilibrium condition based on an empirical correlation from the literature. It takes into account the effects of diffusion coefficients and gas velocity to calculate the non-equilibrium saturations of the components. The simulation is performed in a gas-condensate reservoir, and the results are compared with the ones obtained with the local-equilibrium consideration. The simulator used was the UTCOMP compositional simulator, developed at The University of Texas at Austin.*

Keywords: *non-equilibrium, mass transfer, condensate reservoirs, EOS, UTCOMP simulator.*

1. INTRODUCTION

Most commercial oil reservoir simulators assume that hydrocarbon recovery processes occur under a thermodynamic equilibrium between the hydrocarbon phases. However, this equilibrium condition does not happen for all regions of the reservoir and throughout all simulation time. There are certain conditions which prevent this equilibrium from occurring. For example, in reservoirs with high injection gas rates, the gas velocity is so high that the gas does not have enough time to stay in the grid block in order to achieve the equilibrium condition with the oil phase. In order to consider the thermodynamic equilibrium, the simulators assume that the residence time of fluids inside the grid blocks are sufficient enough for them to reach the equilibrium condition.

Once thermodynamic equilibrium is not achieved, there is mass transfer between the interface of oil and gas phases, which must be taken into account in order to avoid erroneous calculations during reservoir simulations. Mass transfer processes change the saturation of phases and the number of moles of components in each hydrocarbon phase.

Various authors have already studied the non-equilibrium processes in reservoir simulators (Wu et al., 2000; Nghiem and Sammon, 1997) and have presented a wide variety of results showing how non-equilibrium affects the reservoir fluid dynamics. In this paper, we have implemented the model proposed by Nghiem and Sammon (1997), which considers that the mass transfer from the bulk phase to the interface between phases occurs only by molecular diffusion, while assuming that only the interfaces between phases are in thermodynamic equilibrium. We have implemented the non-equilibrium mass transfer into the UTCOMP simulator. The UTCOMP simulator was developed at the Center for Petroleum and Geosystems Engineering at The University of Texas at Austin for the simulation of enhanced recovery processes. UTCOMP is a compositional multiphase/multi-component, Implicit Pressure Explicit Composition simulator (IMPEC), which can handle the simulation of miscible gas flooding processes.

2. MODEL DESCRIPTION

In UTCOMP simulator, the variables evaluated in each time-step are the overall number of moles of each component and the pressure of the water phase. Details of the original formulation can be found in Chang et al. (1990). The implementation of the non-equilibrium model requires the calculation of the number of moles of each component in each phase. This calculation can be performed by solving the molar balance for each phase, as described by Eqs. (1) through (3).

$$\frac{\partial(\phi N_{io})}{\partial t} - \nabla\cdot\left[\xi_o\, x_{io}\, \lambda_o \overline{\overline{K}}\cdot\nabla\Phi_o\right] - \frac{q_{io}}{V_b} = \tau_i \;;\; i = 1,2,..,n_c\,, \tag{1}$$

$$\frac{\partial(\phi N_{ig})}{\partial t} - \nabla\cdot\left[\xi_g\, x_{ig}\, \lambda_g \overline{\overline{K}}\cdot\nabla\Phi_g\right] - \frac{q_{ig}}{V_b} = -\tau_i \;;\; i = 1,2,..,n_c\,, \tag{2}$$

$$N_i = N_{io} + N_{ig}\;;\; i = 1,2,..,n_c. \tag{3}$$

In Eqs. (1) through (3), the subscripts "o" and "g" refer to the oil and gas phases, respectively. N_{io} and N_{ig} are the number of moles of the *i-th* component present in oil and gas phases. The other symbols defined in Eqs. (1) and (2) are the porosity (ϕ), the molar density (ξ), the molar fraction (x) of the *i-th* component into gas or oil phase, the phase mobility (λ), the absolute permeability tensor ($\overline{\overline{K}}$), the potential of each phase (Φ), phase saturation (S), the volumetric rate of each well, and the volume of control-volume that contains a well (V_b). The right hand sides of Eqs. (1) and (2) are mole transport rates between phases and are evaluated as

$$\tau_i = \tau_{io} - \tau_{ig}\;;\; i = 1,2,...,n_c\,, \tag{4}$$

where

$$\tau_{io} = -\xi_o\left(\frac{D_{io}}{F}\right)\nabla x_{io}\;;\; i = 1,2,...,n_c\,, \tag{5}$$

$$\tau_{ig} = -\xi_g\left(\frac{D_{ig}}{F}\right)\nabla x_{ig}\;;\; i = 1,2,...,n_c. \tag{6}$$

In Eqs. (5) and (6), D_i is the diffusion coefficient of the *i-th* component and ∇x_i is the gradient of the molar fraction of the *i-th* component evaluated from the average phase volume to the phase interface.

Although the term described in Eq. (4) does not appear explicitly in most of the material balance equations, it is a key parameter for the equilibrium hypothesis. If it's null, for instance, there will be no mass transfer between phases. In this case, all components present in certain phase will remain in that phase and will be transported only by that phase. Otherwise, when the value of this parameter is very large, the system achieves equilibrium very quickly withmass transfer between phases taking place instantaneously. Finally, when the value of the mass transfer rate is between the two aforementioned limiters, the system is found in a non-equilibrium state condition.

When the non-equilibrium phenomenon is significant, the compositions must be calculated from the values obtained by the molar balance, instead of flash calculation under the equilibrium condition,

$$x_{ij} = \frac{N_{ij}}{N_j};\; i = 1,2,..,n_c \;\; j = 2,..,n_p\,, \tag{7}$$

where

$$N_j = \sum_{i=1}^{n_c} N_{ij};\; j = 2,..,n_p\,. \tag{8}$$

In Eq. (8), N_j denotes the number of moles of the *j-th* phase. The phase saturations are calculated as

$$S_j = (1 - S_1)\frac{L_j / \xi_j}{\sum_{i=1}^{n_p} L_i / \xi_i};\ j = 2,..,n_p\,. \tag{9}$$

In Eq. (9), S_1 is the water saturation, and the molar density is calculated with the new compositions in the EOS, while the molar fraction of each hydrocarbon phase is determined as

$$L_j = \frac{N_j}{\sum_{j=2}^{n_p} N_j};\ j = 2,..,n_p\,. \tag{10}$$

In Eq. (5), the diffusion coefficient for the oil phase (D_{io}) is calculated using the Wilke and Chang model (1955). This coefficient is given by

$$D_{io} = \frac{7.4\times10^{-8} T \sqrt{\dfrac{\sum_{j=1}^{n_c} x_{jo} W_j}{1 - x_{io}}}}{\mu_o v_{bi}^{0.6}}, \tag{11}$$

where V_{bi} is the molar volume of the *i-th* component in the normal boiling point, which is estimated from the critical volume by the Tyn and Calus method (1975).

$$v_{bi} = 0.285 v_{ci}^{1.048}\,. \tag{12}$$

In Eq. (6), the binary diffusion coefficient for the gas phase (D_{ig}) is calculated through a dense gas model proposed by Sigmund (1976).

$$D_{ij} = \frac{\xi_j^0 D_{ij}^0}{\xi_j}\left(0.99589 + 0.096016\xi_{jr} - 0.22035\xi_{jr}^2 + 0.032874\xi_{jr}^3\right), \tag{13}$$

where

$$\xi_{jr} = \xi_j \frac{\sum_{i=1}^{n_c} x_{ij} v_{ci}^{5/3}}{\sum_{k=1}^{n_c} x_{kj} v_{ck}^{2/3}}\,. \tag{14}$$

The term referring to the product between the molar density and the diffusion coefficient in a reference condition is calculated using the model found in Polling *et al.* (2001).

$$\xi_j^0 D_{ij}^0 = \frac{1.8583\times10^{-3} T^{0.5}}{\sigma_{ij}^2 \Omega_{ij} R}\left(\frac{1}{W_i} + \frac{1}{W_j}\right)^{0.5}. \tag{15}$$

In Eq. (15), R is the universal gas constant, W is the molecular weight of the component, and Ω is the collision coefficient, which is calculated using the method proposed by Neufeld *et al.* (1972).

$$\Omega_{ij} = \frac{1.06036}{(T^*)^{0.1561}} + \frac{0.193}{\exp(0.47635T^*)} + \frac{1.03587}{\exp(1.52996T^*)} + \frac{1.76474}{\exp(3.89411T^*)}, \tag{16}$$

where

$$T^* = kT / \varepsilon_{ij} \,. \tag{17}$$

Finally, the diffusion coefficient of component "*i*" in the gas mixture is calculated by the expression proposed by Nghiem and Sammon, (1997).

$$D_{ig} = \frac{1 - x_{ig}}{\sum_{j=1}^{n_c} x_{ig} D_{ij}^{-1}} \,. \tag{18}$$

2.1 Numerical discretization

The approximated molar balance equations discretized in conjunction with the finite-volume method is presented in this section. Since the UTCOMP simulator is based on an IMPEC algorithm, the explicit discretization of molar interphase transfer terms and the molar balance of components in each phase have led to serious convergence problems earlier. In order to resolve these issues, now the molar transfer term has been taken apart from the molar balance equations and has been treated using a segregated solution procedure. Equation (19) shows Eq. (1) after being integrated in time and in the control volume according Figure 1. As we can easily infer, the molar interphase transfer was removed from Eq. (1). We can also verify that an explicit procedure to physical properties at the control volume interface is used.

$$\begin{aligned}\frac{N_{P,io}^{n+1} - N_{P,io}^{n}}{\Delta t} &= \xi_o\, x_{io}\, \lambda_o\big|_{P+x/2}^{n} K_{xx} \frac{P_E^{n+1} - P_P^{n+1}}{\Delta x} \Delta y \Delta z + \xi_o\, x_{io}\, \lambda_o\big|_{P-x/2}^{n} K_{xx} \frac{P_P^{n+1} - P_W^{n+1}}{\Delta x} \Delta y \Delta z \\ &+ \xi_o\, x_{io}\, \lambda_o\big|_{P+x/2}^{n} K_{xx} \frac{P_{coE}^{\;n} - P_{coP}^{\;n}}{\Delta x} \Delta y \Delta z + \xi_o\, x_{io}\, \lambda_o\big|_{P-x/2}^{n} K_{xx} \frac{P_{coP}^{\;n} - P_{coW}^{\;n}}{\Delta x} \Delta y \Delta z \\ &+ Q_{io}^{n} \,.\end{aligned} \tag{19}$$

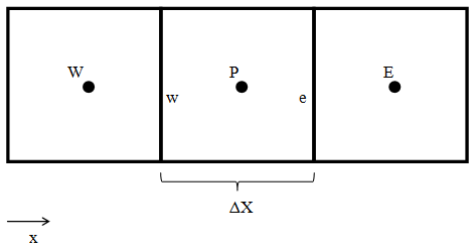


Figure 1. Control volume

After the calculation of the number of moles of each component, for each phase, considering no-mixing condition, it is necessary to correct these values by adding the molar transfer coefficient between phases. In order to have a stable approach, this procedure is carried out implicitly. Equation (20) presents the correction for the number of moles for the *i-th* component into oil phase at the center of control volume P.

$$N_{p,io}^{n+1,c} = N_{p,io}^{n+1} + \Delta t \frac{\Delta x \Delta y}{\Delta z} \frac{\xi_{p,o}^{n}}{S_{p,o}^{n}} \frac{D_{p,io}^{n}}{F} \left(x_{p,io}^{n+1,c} - x_{p,io}^{n,*} \right) - \Delta t \frac{\Delta x \Delta y}{\Delta z} \frac{\xi_{p,g}^{n}}{S_{p,g}^{n}} \frac{D_{p,ig}^{n}}{F} \left(x_{p,ig}^{n+1,c} - x_{p,ig}^{n,*} \right) , \tag{20}$$

and

$$N_{p,ig}^{n+1,c} = N_{p,i}^{n+1} - N_{p,io}^{n+1,c} \,. \tag{21}$$

The superscript "*c*" in Eq. (20) and (21) represents the corrected values for the non-equilibrium condition. Eqs. (20) and (21) are implicitly solved by the Newton's method.

Presented below is the algorithm for the non-equilibrium model implemented in this work:

1. Calculate the pressure for the new time-step.
2. Calculate the total number of moles for each component in the mixture using the new pressure and compute the new global composition.

3. Calculate the number of moles of each component in oil phase and calculate the new composition of oil and gas phases considering the no-mixing hypothesis.
4. Calculate the compositions, number of moles and molar fraction of phases using Eq. (20) and (21).
5. Calculate and store the new equilibrium compositions to be used in the next-time step.
6. Update the EOS parameters with the properties calculated in step 4 and compute the new density.
7. Calculate the new saturations using the properties calculated in step 4.
8. Evaluate the all other properties for the new time-step.
9. Go back to step 1 for the next time-step.

3. RESULTS

In order to test the non-equilibrium model, a one-dimensional case was formulated based on the example given by Ngheim and Sammon (1997). The reservoir is characterized by six hydrocarbon components, and a gas injection has a high percentage of C1. The fluid flow is one-dimensional, and the contact between gas and oil is considered to be uniform with interface normal to the z-axis. This hypothesis is assumed in order to use Eq. (20). All data referring to this case study are available in Tab. 1; in-place and the injected fluid compositions are presented in Tab. 2.

Table 1. Reservoir data

Property	Values
Length, width and thickness	0.2286 m; 0.045 m; 0.045 m
Permeabilities (K_{xx}, K_{yy}, K_{zz})	$1.97x10^{-11}$ m^2; $1.97x10^{-11}$ m^2; $1.97x10^{-11}$ m^2
Porosity	0.3
Temperature	344.26 K
Inicial pressure	20.68 MPa
Inicial water saturation	0.2
Rock compressibility	$1.45x10^{-13}$ Pa^{-1}
Wellbore radius	0.003048 m; 0.003048 m
Producer BHP	20.68 MPa
Flux resistivity factor (F)	9
Grid	20x1x1

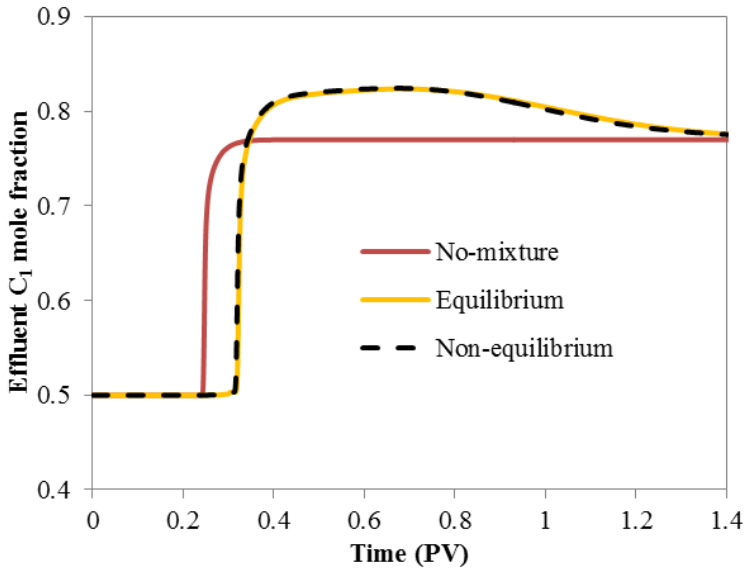
Table 2. In place and injected fluid compositions

Component	Reservoir composition	Injection fluid composition
C_1	0.5	0.77
C_3	0.03	0.20
C_6	0.07	0.03
C_{10}	0.2	-
C_{15}	0.15	-
C_{20}	0.05	-

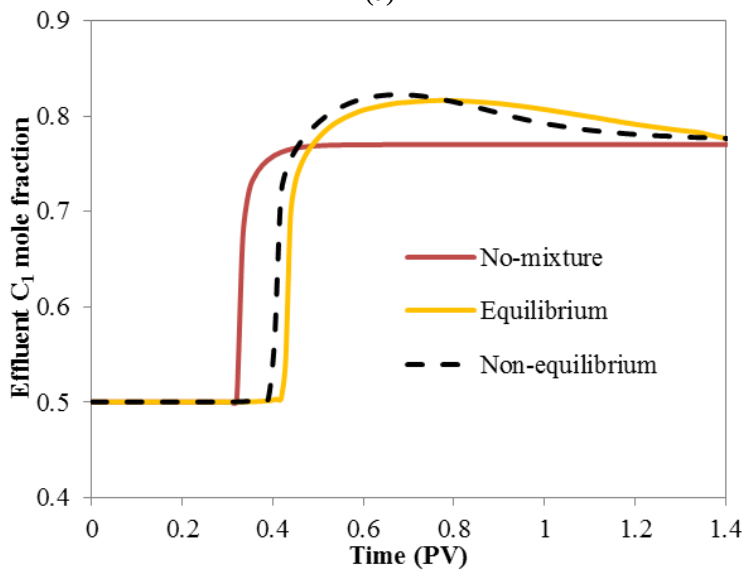
The relative permeabilities and capillary pressure data were obtained from the 5th SPE comparative study (Killough and Kossack, 1987).

The analysis of the non-equilibrium effect was performed for three different gas injection rates: $1.71x10^{-9}$ m^3/s, $1.71x10^{-8}$ m^3/s, and $4.03x10^{-8}$ m^3/s.

Figure 2 shows the concentration curves of C_1 versus time in the producer well, for each one of the injection rates mentioned above. For a better comparison, time is expressed in terms of the injected pore volume (PV). From this figure, one can easily see that the no-mixture hypothesis anticipates an early gas breakthrough compared to the equilibrium solution. We can also see from Fig. 2 that when the injection rate is increased the non-equilibrium model goes toward the non-mixture curves. On the other hand, for low injection rates, the curves of non-equilibrium are close to the ones considering the equilibrium condition.



(a)



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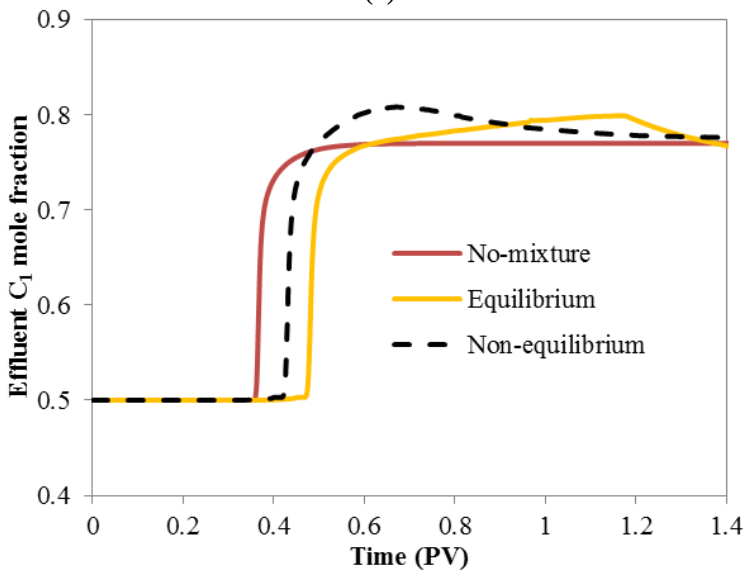
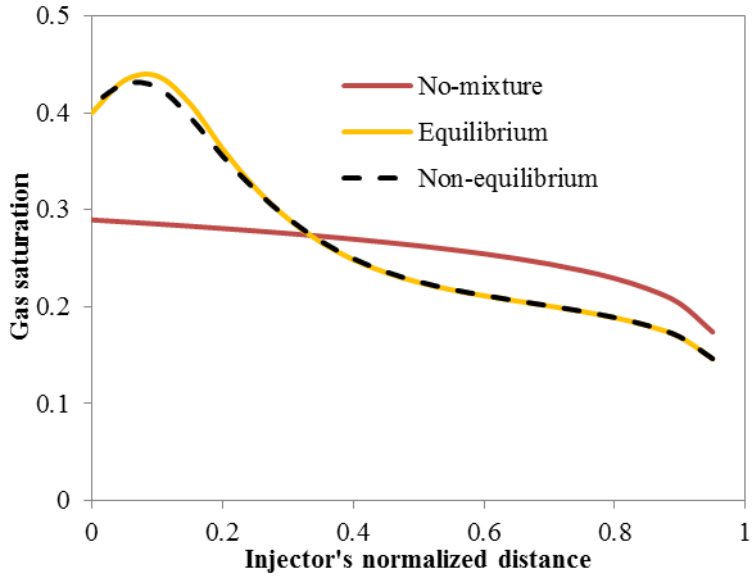


(c)

Figure 2. C_1 Concentration in the producer well for injection rates of : a) 1.71×10^{-9} m^3/s, b) 1.71×10^{-8} m^3/s, and c) 4.03×10^{-8} m^3/s.

Figure 3 shows gas saturation for each case at 0.4 PV (pore volume). The profile is plotted in terms of the normalized distance from the injector to the producer well. In this figure, we can observe a similar behavior already presented for the C_1 composition. The gas saturation profile is more uniform for the no-mixture, and the breakthrough occurs early as before. For the equilibrium case, the breakthrough is delayed when the injection rate is increased for the same PV. We also can observe that the non-equilibrium model produces approximately the same saturation profile for small injection rates. However, when the injection rate is increased, the non-equilibrium case becomes closer to the results obtained by considering no-mass transfer between the phases.



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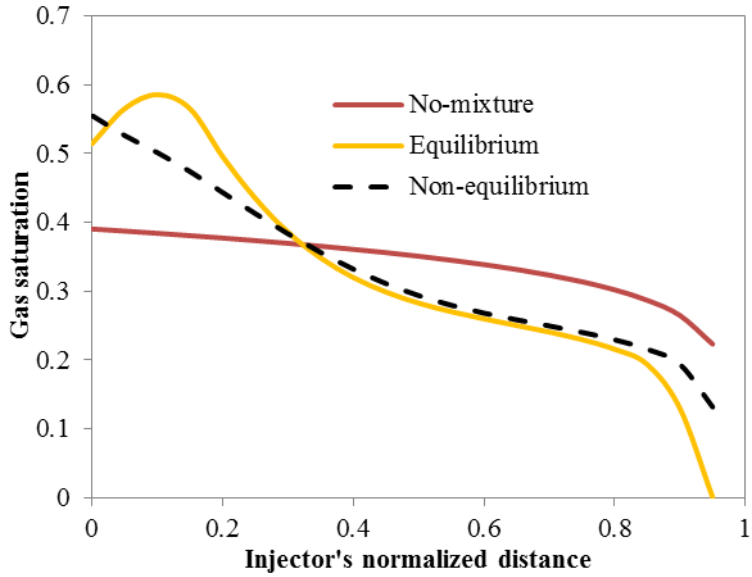

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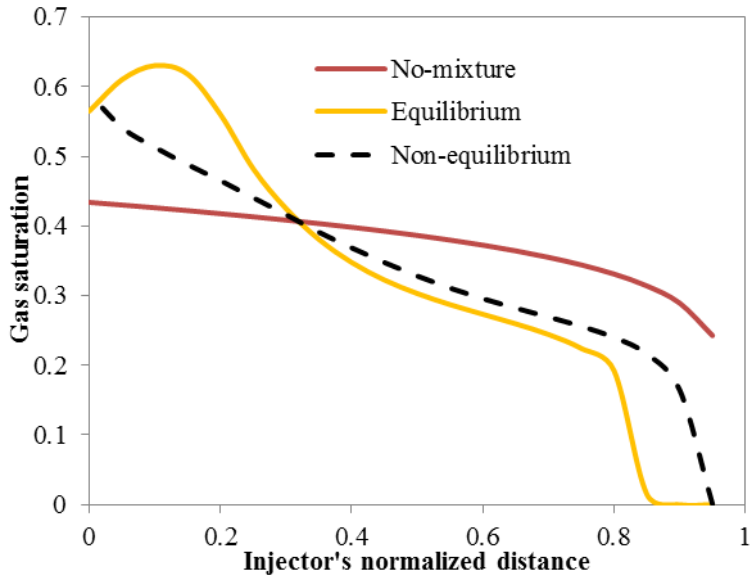

(c)

Figure 3. Gas saturation profile at 0.4 PV for injection rates of: a) 1.71×10^{-9} m^3/s, b) 1.71×10^{-8} m^3/s, and c) 4.03×10^{-8} m^3/s.

4. CONCLUSIONS

This paper presents a non-equilibrium mass-transfer and a no-mixing reservoir simulator with an IMPEC formulation. The formulation is discretized for Cartesian grids in one dimension using the finite-volume method.

The results show that the no-mixing model advances the gas breakthrough, compared to the equilibrium solution. On the other hand, the non-equilibrium solution is generally in between equilibrium and no-mixing solutions. However, when a low injection rates is used, the usual premise of thermodynamic equilibrium constitutes a sound approach to address the problem. For a high injection rate, the equilibrium phase behavior cannot accurately predict the reservoir fluid flow.

5. ACKNOWLEDGEMENTS

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6. REFERENCES

Chang, Y. B., Pope, G.A., Sepehrnoori, K., 1990. “A higher-order finite difference compositional simulator”. *Journal of Petroleum Science and Engineering*, Vol. 5, p. 35–50.

Killough, J. E., Kossack, C. A., 1987. “Fifth Comparative Solution Project: Evaluation of Miscible Flood Simulators”. In *Proceedings of the 9th Symposium on Reservoir Simulation*, San Antonio, USA.

Neufeld, P. D., Janzen, A. R., Aziz, R. A., 1972. “Empirical Equations to Calculate 16 of the Transport Collision Integrals Ω for the Lennard-Jones Potential”. *Journal of Chemical Physics*, Vol. 57, p. 1100-1102.

Nghiem, L. X., Sammon, P. H., 1997. “A Non-Equilibrium Equation-of-State Compositional Simulator”, In *proceedings of the SPE Reservoir Simulation Symposium 1997*, Dallas, USA.

Polling, B. E., Prausnitz, J. M., O’Connell, J. P., 2001. *The Properties of Gases and Liquids*. McGraw-Hill, 5th Edition.

Sigmund, P. M., 1976. “Prediction of Molecular Diffusion at Reservoir Conditions. Part I – Measurement and Predicition of Binary Dense Gas Diffusion Coefficients”. *The Journal of Canadian Petroleum Technology*, Vol. 15, p. 48-57.

Tyn, M. T., Calus, W. F., 1975. “Estimating Molal Volume”. *Processing*, Vol. 21, p. 16-17.

Wilke, C. R., Chang, P., 1955. “Correlation of Diffusion Coefficients in Dilute Solutions”. *AlChE Journal*, Vol. 1, p. 264-270.

Wu, W.-J., Wang, P., Delshad, M., Wang, C., Pope, G. A., Sharma, M. M., 2000. “Modelling Non-Equilibrium Mass-Transfer Effects for a Gas Condensate Field”. *In Situ*, Vol. 24, p. 139-162.

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