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Full Length Article

Thermodynamically consistent criteria for developing reliable equation of state model for compositional simulation

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ABSTRACT

Developing reliable EOS model for compositional simulation is important as replicating the composition phase behavior in Pressure – Temperature – Composition space is challenging. Current approaches for EOS model development are neither well defined nor justifiable in all cases. As a result, developing EOS model becomes subjective, and for same fluid, multiple EOS models can be developed with the same set of data used at regression step. All these EOS models have the same predictive capability at Pressure – Temperature points represented by data used at regression step, however, they have unknown reliability at other points in Pressure-Temperature-Composition space.

The objective of this paper is to develop a thermodynamically consistent criterion to select most reliable EOS models out of multiple possible EOS models for a given reservoir fluid. Thermodynamic phase equilibrium condition requires that at stable equilibrium of one or more phases, total Gibbs free energy should be minimum. However, multiple EOS models because of different set of EOS parameters result in multiple values of total Gibbs free energy at Pressure-Temperature point represented by data used in the regression. This paper shows that for a given fluid, EOS model with lowest total Gibbs free energy results into most reliable phase behavior prediction.

Total of 28 reservoir fluids have been considered in this study. On average 11 EOS models have been developed for a fluid by matching saturation pressure and saturation density data. For each of EOS model, Gibbs free energy of mixing and minimum miscibility pressure (for oils) and Gibbs free energy of mixing and CVD liquid saturation (for gas condensates) are calculated at the saturation pressure and reservoir temperature. Trends of Gibbs free energy of mixing and deviation in MMP and CVD liquid saturation predictions for all fluids confirms the criterion.

1. Introduction

Reservoir fluid characterization is an important part of hydrocarbon recovery, PVT, and phase behavior simulation. Characterization of a given reservoir fluid is achieved by developing cubic Equation of State (EOS) model. Commonly used two-parameter cubic EOSs are Peng and Robinson (PR) EOS [1,2] and Soave Redlich and Kwong (SRK) EOS [3]. These EOSs have been modified by various researchers to improve volumetric [4–9] and multiphase behavior predictions [10–18]. These two EOSs (with or without modification) are widely used for simulation in oil and gas industry.

An EOS model represents a reservoir fluid by a suitable number of pure and pseudocomponents with well-defined composition, molecular weights, critical properties, acentric factor, and binary interaction parameters (BIPs). It is expected that such an EOS model will predict reliable phase behavior for reservoir fluid in P-T-x space. The EOS model acts as input to different recovery simulation processes to simulate the phase behavior in Pressure-Temperature and composition (P-T-x) space. Such models are also used for simulating PVT relationship in Black-Oil model of reservoir simulation. Hence, the reliability of simulated results depends on the quality of the EOS model developed. Desirable qualities of an EOS model mainly include reliability, seamless applicability in P-T-x space, and uniqueness; these qualities depend on characterization methods used in developing the EOS model.

Developing a reliable EOS model particularly for processes like miscible gas injection is important as it involves reliable simulation of multiphase behavior for innumerable multicomponent mixtures resulting from non-linear mixing of injection gas and reservoir fluid at different times and spaces at isothermal pressure points. Researchers [19–21] have shown that recovery of reservoir fluid from a miscible gas injection process is a complex and implicit function of the composition of injection gas and reservoir fluids, pressure and temperature. For

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Nomenclature

AARD	average absolute relative deviation (for multiple data such as CVD liquid saturation at different pressure for a gas condensate)
ARD	absolute relative deviation (for single point data for fluid such as MMP)
BIP	binary interaction parameter
CN	carbon number of *n*-alkane
CVD	Constant Volume Depletion
EOS	equation of state
MMP	minimum miscibility pressure
PDF	probability distribution function
PnA	Perturbation from n-Alkane
P-T-x	pressure-temperature-composition
SCN	single carbon number
N_C	number of components
N_E	number of EOS models developed for a fluid
N_P	number of phases

Greek symbols

α	parameter defining shape of curve in Gamma Distribution
β	molar phase fraction
μ	chemical potential
$\bar{\phi}$	fugacity coefficient of a component in mixture
Φ	fugacity coefficient of pure component
$\boldsymbol{\delta}$	set of ARD values for a reservoir fluid
Γ	Gamma function
γ	specific gravity
ψ	parameter defined by a/b^2, where a and b are attraction and covolume parameters
ω	Acentric factor
$\boldsymbol{\omega}$	set of acentric factors of components in EOS model
χ	parameter in Gamma Distribution model

Roman symbols

a	attraction parameter in PR EOS
b	covolume parameter in PR EOS
f	fugacity
G	Gibbs free energy
$\mathbf{g}$	set of g values for reservoir fluid calculated at P_{SAT} and T_{RES}
g	Gibbs free energy in dimensionless form $\frac{\Delta_{mix}G}{RT}$
$\mathbf{K}$	binary interaction parameter matrix for EOS model
M	molecular weight
n	number of moles
P	pressure, bara
P_C	critical pressure, bara
$\mathbf{P_C}$	set of critical pressure of components in EOS model
P_{SAT}	saturation pressure
R	universal gas constant
T	temperature, K
T_b	boiling point
T_{br}	ratio of T_b and T_C
T_C	critical temperature, K
T_{RES}	reservoir temperature
T_b	boiling point
$\mathbf{T_C}$	set of critical temperature of components in EOS model
x	mole fraction
V	partial molar volume
$\bar{z}$	overall composition of reservoir fluid

Subscripts

C	critical
C_7^+	heptane plus fraction
EXP	experimentally measured
i	component index
j	phase index
k	index used for component and phase
mix	for mixture
SAT	saturation

example, generally oil recovery decreases with increasing methane content in the injection gas, however, researchers such as [19–21] observed non-monotonic recovery behavior of oil with increasing methane content in injection gas. Their experimental results show that with increasing methane content in injection gas, recovery decreases up to certain methane concentration and for higher concentration than this specific concentration recovery starts increasing. Explaining such behavior is not possible without EOS model with capability of reliable multiphase behavior prediction [21] in composition space.

Over the years, various researchers used conventional fluid characterization approach [22] to develop EOS models for different types of reservoir fluids such as Gas condensates [23–27], Volatile oils [28], Near-critical fluids [29,30], and Heavy oils [31,32]. Conventional characterization methods have been used by various researchers [19,21,33–40] to develop EOS models to predict three-phase behavior for solvent injection cases for numerical simulation of hydrocarbon recovery. Kumar and Okuno [41–44] developed Perturbation from n-Alkane (PnA) approach and successfully characterized all major reservoir fluid types with a single approach.

A typical conventional approach can be represented by following four steps process (Pedersen and Christensen [22]):

Step 1. Splitting of Plus Fraction: At this step, plus fraction (usually heptane plus) is split into several single carbon number fractions by applying Probability Distribution Functions (PDFs).

Step 2. Estimation of EOS Parameters: Properties for the detailed components at Step 1 such as critical temperature (T_C), critical pressure (P_C), acentric factor (ω), and volume-shift parameters are estimated using correlations.

Step 3. Lumping of SCN Fractions: SCN fractions at Step 1 and their estimated properties at Step 2 are lumped to achieve fewer pseudocomponents with known mole fraction, molecular weight, T_C, P_C, and ω. BIPs are also estimated at this step. At this stage, a default EOS model is ready for testing and further improvement.

Step 4. Regression of Pseudocomponents' Properties: Predicted phase behavior from default EOS model at previous step usually does not match with the phase behavior represented by saturation pressure and density data. Hence, adjustable parameters such as T_C, P_C, and ω for pseudocomponents are regressed to match the saturation pressure, and density data is matched by adjusting volume shift parameters [4].

In the PnA based approaches of fluid characterization, default EOS model is found by assuming pseudocomponents to be n-alkanes and accordingly pseudocomponents are assigned T_C, P_C, and ω estimated using correlations. Though there are many correlations such as Ambrose [45], Magoulos and Tassios [6], Tsonopoulos and Tan [46], Constantinou and Gani [47], Riazi and Al-shhaf [48], Gao et al. [49],