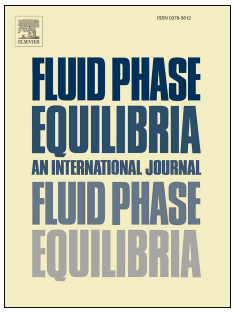

A robust procedure for three-phase equilibrium calculations of water-hydrocarbon systems using cubic equations of state

Emad Mortezazadeh, Mohammad Reza Rasaei

PII: S0378-3812(17)30274-1

DOI: 10.1016/j.fluid.2017.07.007

Reference: FLUID 11529

To appear in: *Fluid Phase Equilibria*

Received Date: 8 June 2017

Revised Date: 6 July 2017

Accepted Date: 16 July 2017

Please cite this article as: E. Mortezazadeh, M.R. Rasaei, A robust procedure for three-phase equilibrium calculations of water-hydrocarbon systems using cubic equations of state, *Fluid Phase Equilibria* (2017), doi: 10.1016/j.fluid.2017.07.007.

A robust procedure for three-phase equilibrium calculations of water-hydrocarbon systems using cubic equations of state

Emad Mortezazadeh[a], Mohammad Reza Rasaei[a,*]

[a] *Institute of Petroleum Engineering, School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, Iran*
[*] *e-mail: mrasaei@ut.ac.ir*

Abstract

Phase equilibrium calculations are one of the main steps in the compositional simulation of hydrocarbon reservoirs, well tubing, oil and gas pipelines as well as separation units. The main phases in all hydrocarbon production systems from a reservoir to a stock tank are gas, oil, and water. In most studies, the aqueous phase is considered bulk and phase equilibrium calculations are conducted only on the oil and gas phases. In some conditions such as thermal processes, the solubility of water in other phases and also hydrocarbon components in the water phase cannot be ignored. The robustness of equilibrium calculations for a wide range of compositions, temperatures, and pressures, including near critical area and saddle point curve, is essential for rapid and stable simulation studies. In this study, we propose the three-phase equilibrium calculations in detail for water, oil and gas phases. All the handling steps and strategies to establish a robust and efficient phase stability testing and flash calculation are explained. Moreover, appropriate tolerance values for decision-makings in the algorithm are defined. We successfully present the effectiveness of our algorithm for some three-phase samples covering a wide range of composition and production conditions.

Keywords: phase stability testing; flash calculations; successive substitution; Newton-Raphson method; BFGS method; phase envelop; CPU time

1. Introduction

Water and hydrocarbon components are inevitable parts of all oil and gas reservoirs. Presence of water in hydrocarbon phases and hydrocarbon components in water phase can significantly affect the results of the reservoir simulation. Studies on the real samples of the hydrocarbon reservoirs show that the presence of water in the hydrocarbon phases can result in scale formation owing to water evaporation in or near a well. Moreover, it can change the saturation curve of the phase envelop, and may have a major effect on the gas in place calculation. Meanwhile, there are some issues regarding the solubility of hydrocarbons in water, such as hydrocarbon loss in water, water pollution of aquifer in contact with the reservoir, interaction of hydrocarbon with drilling fluids leading to the risk of gas kicks, etc. [1].

Phase equilibrium analysis is one of the main parts of all compositional reservoirs and production system simulations in their initialization and all the next nonlinear iterations steps. It should be noted that the three-phase equilibrium calculations are required to model water-hydrocarbon mixtures, e.g. steam injection, in situ combustion and CO_2 sequestration [2].

Currently, the most common equations of state in petroleum industry are cubic such as Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK). Water solubility in the hydrocarbon phases is easily calculated using conventional cubic equations of state whereas these equations are deficient for predicting hydrocarbon solubility in water phase [3]. Different models of water-hydrocarbon three-phase equilibrium calculations have recently been used to overcome this deficiency. Most of the models are based upon the equality of component fugacities in all coexisting phases. Some authors like Economou and Donohue [4], Economou and Tsonopoulos [5], Oliveira et al. [6] developed the non-cubic equation of state (EoS) to calculate water-hydrocarbon equilibrium by taking into account the self-associating character of water in order to improve the accuracy of the phase envelope computation. Søreide and Whitson [7] used the cubic EoS with two modifications to predict the brine-hydrocarbon systems' behavior at high pressures and temperatures. In the first modification, a specific temperature dependency of α parameter in the EoS for water component is employed, resulting in improving the prediction accuracy of the water vapor pressure