

Peng-Robinson Equation of State as a base for Incorporation of Polar and Ionic Effects in Broadening the Description of Various Subsurface Processes

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The introduction of the Peng-Robinson equation of state and deep knowledge of the authors on retrograde effect in natural gas systems paved the way to compute retrograde condensation in pipelines and in subsurface applications. This step was followed by description of reservoir crude oil systems by the Peng-Robinson equation of state. The fully EOS compositional reservoir simulations were then advanced. The merit of EOS compositional modeling is consistent description of various phases in the same approach to describe gravitational and non-equilibrium effects. In recent years, phase description of mixtures with polar and non-polar species and mixtures of brine with nonpolar species have become of high interest in relation to CO₂ sequestration and hydrogen storage in the subsurface. The eCPA (electrolyte cubic plus association) equation of state is being advanced to describe equilibrium in multi-salt brine and various gases. In addition to physical interactions between nonpolar species in the Peng-Robinson, other effects are accounted for. These include association between polar species, cross association between nonpolar and polar species, and ion-ion interaction in a solvent medium, and ion-solvent interactions. The framework allows for solubility of gases such as CO₂ and methane in brines with multi-salts, unusual water content in CO₂, and thermal effects.

In subsurface flow calculations, efficient and robust computation of phase split by cubic equations, CPA and eCPA equations of state are also the requirement. The concept of phase stability analysis, and numerical solution of non-linear algebraic equations combined with Gibbs free energy reduction in every computational step will facilitate robustness in the critical region and near phase boundaries.

This presentation will cover the success story of the Peng-Robinson cubic equation of state and later expansion to cover recent areas of application and integration with various concepts. Efficient computations have been achieved in geothermal energy extraction, hydrogen storage in the subsurface CO₂ sequestration in aquifers, asphalt precipitation, and multiphases (3 to 4) in high CO₂ content petroleum fluids.

Short Bio

Professor Abbas Firoozabadi is a Distinguished Research Professor at the Department of Chemical and Biomolecular Engineering at Rice University, Houston, TX, and Director of Reservoir Engineering Research Institute (RERI) in Palo Alto, CA. His published work centers on multi-component equilibrium, irreversible thermodynamics, kinetics of new phase formation, and higher-order numerical simulations of subsurface flows. His current work focuses on molecular engineering and fracturing rocks in relation to subsurface efficient energy production,

large scale numerical simulation of CO₂ sequestration in the subsurface, and stewardship of the environment. Most of his current research focuses on widespread use of CO₂ in the subsurface. He is expanding his research into geothermal energy production. He has authored two books on thermodynamics of hydrocarbon energy production published by McGraw-Hill and is author and co-author of some 300 Journal papers. His Google Scholar H index is 96.

Professor Firoozabadi has taught graduate thermodynamics at Peking University, Tokyo University, and Yale University. He has been recently appointed as honorary Professor at Tsinghua University in Beijing, China.

Professor Firoozabadi has received four major awards of the Society of Petroleum Engineers (SPE) including the Anthony Lucas Gold Medal. He is a member of the US National Academy of Engineering (NAE), and international member of the Chinese Academy of Engineering (CAE).