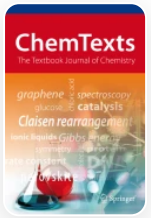
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Understanding high-pressure CO_2–H_2S phase equilibria using Aspen Plus and the Peng–Robinson equation of state

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Abstract

Teaching vapor–liquid equilibrium in real fluid systems is often difficult because students must connect abstract thermodynamic relations with numerical calculations and engineering interpretation. This study presents a computational teaching case based on the binary CO_2–H_2S system to illustrate how fugacity-based equilibrium can be analyzed using the Peng–Robinson equation of state (EOS) in a commercial process simulator. The purpose of the work is not to generate new experimental thermodynamic data but to provide an instructional bridge between textbook thermodynamics and simulation-based engineering analysis. The methodology was applied as a guided modeling exercise for third-year undergraduate chemical technology students within the course *Modeling of Chemical Technological Processes*. By combining phase equilibrium theory, fugacity relations, and pressure-dependent flash calculations, the approach enables learners to interpret non-ideal vapor–liquid behavior in terms of equilibrium criteria, vapor fraction, and p–x–y relations, rather than treating simulator outputs as black-box results. The results show that the proposed framework can be used to explain how pressure influences phase splitting and composition in an acid gas mixture while preserving the thermodynamic meaning of the calculations. Instructor-based classroom observations indicated improved student engagement when the topic was taught through an industrially relevant simulation case instead of theory and hand calculations alone. Limited classroom performance data also suggested improved student outcomes after implementation of the simulator-based activity, although the present work does not constitute a full controlled educational study. Overall, the study shows that industrially relevant simulation exercises can support conceptual understanding of real-fluid thermodynamics and provide an effective pedagogical link between equilibrium theory and engineering practice.

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Availability of data and materials

The data used in this study were compiled from publicly available literature sources. The curated dataset and processed data supporting the findings of this work are available from the corresponding author upon reasonable request.

Abbreviations

CO_2: Carbon dioxide

H_2S: Hydrogen sulfide

VLE: Vapor–liquid equilibrium

EOS: Equation of state

PR: Peng–Robinson

$p-x-y$: Pressure–liquid composition–vapor composition diagram

$T-x-y$: Temperature–liquid composition–vapor composition diagram

Aspen Plus: Aspen Plus process simulation software

p: Pressure

T: Temperature

${V}_{\text{m}}$: Molar volume

R: Universal gas constant

${\widehat{f}}_{i}$: Fugacity of component i

${\widehat{\phi }}_{i}$: Fugacity coefficient of component i in a mixture

x_i: Mole fraction of component i in the liquid phase

y_i: Mole fraction of component i in the vapor phase

z_i: Overall mole fraction of component i

μ_i: Chemical potential of component i

a: Attraction parameter in the EOS

b: Co-volume parameter in the EOS

a_{m}: Mixture attraction parameter

b_{m}: Mixture co-volume parameter

a_{ij}: Cross-interaction attraction parameter between components i and j

k_{ij}: Binary interaction parameter

T_{c}: Critical temperature

$\({p}_{\text{c}}\)$: Critical pressure

$\(\omega\)$: Acentric factor

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Contributions

Adham Norkobilov contributed to the conceptualization of the study, development of the methodology, supervision of the work, and preparation of the original draft, as well as review and editing of the manuscript. Sanjar Ergashev was responsible for the software work, formal analysis, data curation, and visualization. Feruza Bobokulova contributed to the investigation, validation, and manuscript review and editing. Malika Kiyamova contributed to the investigation, literature review, data interpretation, and manuscript review and editing. Fazliddin Meylikov contributed to methodology development, validation, and manuscript review and editing. Oybek Valiev contributed to formal analysis, visualization, and manuscript review and editing. All authors have read and agreed to the published version of the manuscript.

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Ethics declarations

Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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