

Phase Behavior and Properties of Gas Mixtures Relevant in Energy Transition PI: Abhijit Dandekar, Professor & Chair of Petroleum Engineering

Summary of project goals and intentions

Over the project period, the primary goal was to improve the understanding of phase behavior and properties of gas mixtures relevant in the design and operation of Carbon Capture, Utilization & Storage (CCUS) and H₂ processes through three targeted tasks: conducting a literature review and building a database, Equations of State (EOS) and fluid property modeling, and conducting selected phase behavior and fluid property experiments.

This work addressed a critical gap in decarbonization and energy transition operations: accurately predicting the thermodynamic and physical behavior of CO₂- and H₂-rich gas streams. While the literature review established a baseline across various impurity mixtures, the modeling and experimental work centered on the behavior of primary CO₂-H₂ gas mixtures. As CCUS deployment expands and hydrogen is increasingly integrated into sub-surface storage and energy supply chains, understanding the specific phase behavior and property changes of these fundamental fluid streams becomes essential. This project was undertaken to deliver reliable, calibrated models and targeted experimental data, providing the technical foundation needed to safeguard infrastructure integrity, optimize storage capacity, and ensure accurate injectivity modeling across CCUS and H₂ processes.

Reflective narrative

This project advanced the understanding of CO₂ and H₂ rich fluid systems to support decarbonization infrastructure, compressor design, and sub-surface storage modeling. As interest grows in potential CCUS and clean hydrogen developments—including regional opportunities like Alaska's Cook Inlet basin—having accurate, reliable property data for these primary gas mixtures is critical for safe and efficient operations.

Throughout execution, the project balanced comprehensive baseline modeling with real world technical adaptability. The early focus on database construction and EOS calibration established a robust thermodynamic baseline for binary CO₂ and H₂ systems. When physical testing encountered the inherent cryogenic and molecular challenges of hydrogen, the effort adapted by using literature data to anchor and tune numerical models, providing a robust framework where experimental phase behavior testing proved impractical.

Overall, this work bridges a key data gap in energy transition gas mixture behavior. By pairing targeted physical measurements with calibrated EOS modeling, the project fulfilled its core intent—delivering a validated modeling framework and a strong publication pipeline to support future energy transition research and field applications.

Thanks to the support of the Faculty Initiative Fund, this effort successfully

generated three refereed manuscripts (currently prepared for submission) to contribute back to the broader scientific community.

Lessons learned

The objectives of Tasks 1.0 and 2.0 were fully met—and in fact exceeded, as evidenced by two comprehensive manuscripts—while Task 3.0 required an adaptive approach to overcome inherent physical constraints. Measuring H₂ systems presents well-known technical challenges: H₂ is a uniquely small, leak-prone molecule, and its mixtures exhibit vapor-liquid equilibria (VLE) at extreme cryogenic temperatures. Although some density measurements were successfully performed, these extreme operational constraints made experimental phase behavior and viscosity testing extremely challenging. To address these parameters, the project pivoted to extensive tuning and calibration of the Peng-Robinson Equation of State (EOS) anchored by available data. This adapted workflow yielded meaningful results, establishing a practical modeling framework for future CCUS and H₂ applications—still accomplishing the objective, albeit through an alternative approach.

Deliverables

Three draft comprehensive manuscripts for submission to high-quality refereed journals have been produced, focusing on Tasks 1.0–3.0. As part of the first manuscript, a CO₂–H₂ Mixtures Thermophysical Properties Database was also prepared, fulfilling both Tasks 1.0 and 2.0. Because all manuscripts are extensive—spanning 50–100 pages—they are not included in full within this final report. Instead, summaries of the draft publications and the database are provided as images in **Figures 1–4**.

Phase Behavior, Thermophysical and Transport Properties of Fluid Systems

Relevant to Energy Transition: A Comprehensive Literature Review

Henry Inkum^{*}, Abhijit Dandekar[‡], Hyun Woong Jang[‡], Omid Mohammadzadeh[‡], Yin Zhang[‡]

[‡] Department of Petroleum Engineering, University of Alaska Fairbanks, Fairbanks, AK 99775, USA

^{*} Corresponding author: hinkum@alaska.edu

HIGHLIGHTS

- Reviews phase behavior and thermophysical/transport properties of CO₂–H₂ fluid systems for CCUS and UHS.
- Synthesizes eight decades of VLE, density, viscosity, and thermal conductivity data.
- Identifies critical data gaps below 273 K relevant to Arctic surface transport and to near-surface injection conditions.
- Compares EOS performance across PR, GERG-2008, EOS-CG, PC-SAFT, and SAFT-VR Mie models.
- Provides prioritized measurement recommendations and an EOS selection guide.

FUNDING

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors. The authors gratefully acknowledge the financial support provided by the University of Alaska Faculty Initiative Fund for this study.

Figure 1: Summary of draft manuscript based on Task 1.0.

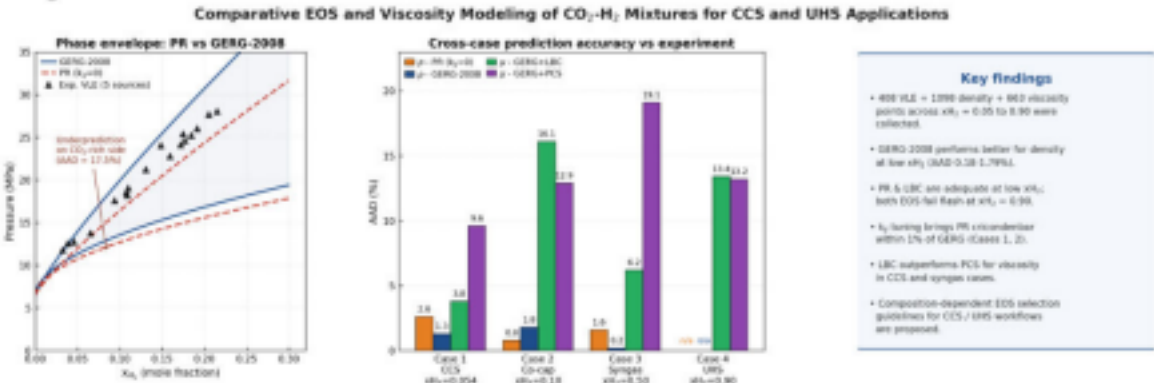
Comparative Assessment of Peng-Robinson and GERG-2008 Equations of State for CO₂-H₂ Binary Mixtures: Phase Equilibrium, Density, and Viscosity Predictions Across Carbon Capture and Hydrogen Storage Compositions

Henry Inkum*, Abhijit Dandekar, Hyun Woong Jang, Omid Mohammadzadeh and Yin Zhang
Department of Petroleum Engineering, University of Alaska Fairbanks, Fairbanks, AK 99775, USA
*Corresponding author: hinkum@alaska.edu

Highlights

- PR and GERG-2008 EOSs were compared for CO₂-H₂ mixtures across four composition cases.
- A curated database of 408 VLE, 1098 density and 663 viscosity points was assembled.
- GERG-2008 outperforms PR ($k_{ij} = 0$) for VLE but the order reverses at high H₂ concentrations.
- Density AAD remains within 1–3% for both EOSs across all four studied cases.
- LBC viscosity errors grow with H₂ content; PCS gives a smaller, more stable bias.

Graphical abstract



Funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors. The authors gratefully acknowledge the financial support provided by the University of Alaska Faculty Initiative Fund for this study.

Figure 2: Summary of draft manuscript based on Task 2.0.

CO ₂ -H ₂ Mixtures Thermophysical Properties Database					
Phase Behavior and Thermophysical Properties of Gas Mixtures Relevant to Energy Transition					
Companion to manuscript by Inkum, Dandekar, Jang, Mohammadzadeh Sharihsaz, Zhang					
Tab	Definition	Rows	References	T range (K)	P range (MPa)
CO2_H2_Binary	Binary CO ₂ -H ₂ mixtures only (exactly 2 components)	2191	19	218–1100	0.10–192.0
CO2_Mix	CO ₂ with impurities, NO H ₂ (CO ₂ +O ₂ , CO ₂ +N ₂ , CO ₂ +CH ₄ , CO ₂ +Ar, CO ₂ +SO ₂ , CO ₂ +CO, CO ₂ +H ₂ O, multi-impurity)	5245	35	213–473	0.05–152.7
H2_Mix	H ₂ with co-gases, NO CO ₂ (H ₂ +CH ₄ , H ₂ +N ₂ , H ₂ +C ₂ H ₆ , H ₂ +C ₃ H ₈ , H ₂ +CO)	1395	11	105–473	0.00–50.6

Multicomponent	Mixtures containing BOTH CO ₂ AND H ₂ plus 21 other component	333	8 233-939	0.60-152.0
TOTAL		9162	67	
• Source: existing CO ₂ -H ₂ literature review database				
Quality flag legend				
A	Primary experimental, uncertainty declared in source paper			
B	Experimental from secondary source (e.g., digitized from figure) or thesis with limited validation			
C	Older data or theses where method may be less rigorous; included for coverage			

Figure 3:

Summary page of the Thermophysical Properties Database (companion to manuscript based on Task 1.0).

Composition-Dependent Peng–Robinson Binary Interaction Parameters for CO₂–H₂ Mixtures: Bubble-Point, Dew-Point, and Two-Phase Property Predictions

Henry Inkum^{1*}, Abhijit Y. Dandekar¹, Hyun Woong Jang¹, Omid Mohammadzadeh¹, Yin Zhang¹

¹ Department of Petroleum Engineering, University of Alaska Fairbanks, Fairbanks, Alaska 99775-5880, USA

*Corresponding author: hinkum@alaska.edu

Highlights

- Composition-specific Peng–Robinson binary interaction parameters tuned independently at three CO₂–H₂ compositions
- k_{ij} ladder of 0.20, 0.30, and 0.15 spans x_{H_2} from 0.054 to 0.50 (non-monotonic in composition)
- 138 literature bubble- and dew-point pressures from five independent laboratories used as tuning targets (112 converged and physical for AAD reporting)
- Two-phase liquid density predicted with tuned Peng–Robinson to 4.42% mean absolute deviation against REFPROP 9.0 GERG-2008
- LBC and Pedersen viscosity correlations compared for two-phase liquid across the same composition range; LBC recommended (4.11% overall AAD)

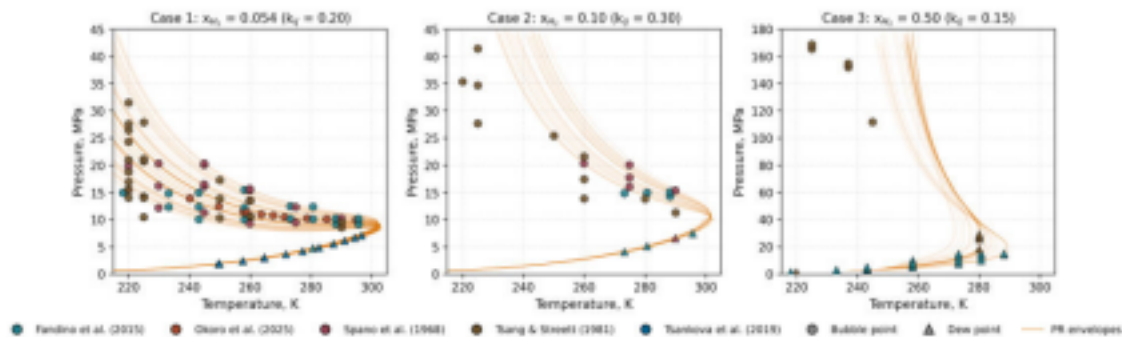


Figure 2. Three-panel P–T saturation envelopes for Case 1 ($x_{H_2} = 0.054$, $k_{ij} = 0.20$, left), Case 2 ($x_{H_2} = 0.10$, $k_{ij} = 0.30$, center) and Case 3 ($x_{H_2} = 0.50$, $k_{ij} = 0.15$, right). Solid orange curves are the composition-specific PR predictions; open circles are the experimental saturation-pressure measurements color-coded by source (Spano et al., 1968; Tsang & Streett, 1981; Fandiño et al., 2015; Tsankova et al., 2019; Okoro et al., 2025). Bubble and dew branches share the same envelope curve within each panel.

Funding

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors. The authors gratefully acknowledge the financial support provided by the University of Alaska Faculty Initiative Fund for this study.

Figure 4: Summary of draft manuscript based on Task 3.0.