



PVTxy properties of CO₂ mixtures relevant for CO₂ capture, transport and storage: Review of available experimental data and theoretical models

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ABSTRACT

The knowledge about pressure–volume–temperature–composition (PVTxy) properties plays an important role in the design and operation of many processes involved in CO₂ capture and storage (CCS) systems. A literature survey was conducted on both the available experimental data and the theoretical models associated with the thermodynamic properties of CO₂ mixtures within the operation window of CCS. Some gaps were identified between available experimental data and requirements of the system design and operation. The major concerns are: for the vapour–liquid equilibrium, there are no data about CO₂/COS and few data about the CO₂/N₂O₄ mixture. For the volume property, there are no published experimental data for CO₂/O₂, CO₂/CO, CO₂/N₂O₄, CO₂/COS and CO₂/NH₃ and the liquid volume of CO₂/H₂. The experimental data available for multi-component CO₂ mixtures are also scarce. Many equations of state are available for thermodynamic calculations of CO₂ mixtures. The cubic equations of state have the simplest structure and are capable of giving reasonable results for the PVTxy properties. More complex equations of state such as Lee–Kesler, SAFT and GERG typically give better results for the volume property, but not necessarily for the vapour–liquid equilibrium. None of the equations of state evaluated in the literature show any clear advantage in CCS applications for the calculation of all PVTxy properties. A reference equation of state for CCS should, thus, be a future goal.

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Contents

1. Introduction	3568
2. Operating windows of CO ₂ conditioning and transport	3568
2.1. Temperature and pressure windows	3568
2.2. Possible impurities	3568
3. Available experimental data	3570
3.1. Summary of measurements	3570
3.2. Knowledge gaps	3570
3.3. The precision, consistency and reliability of the experimental data	3570
4. Existing models	3573
4.1. Cubic EOS	3573
4.2. Benedict–Webb–Rubin (BWR) EOS [79]	3575
4.3. Statistical Associating Fluid Theory EOS	3576
4.4. Predictive EOS	3577
4.5. The GERG equation [92]	3577
5. Discussion	3577
6. Conclusions	3578
Acknowledgement	3578
References	3578

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