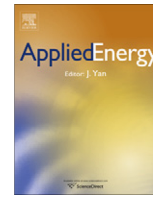
Applied Energy 88 (2011) 3567–3579

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy



PVTxy properties of CO_2 mixtures relevant for CO_2 capture, transport and storage: Review of available experimental data and theoretical models

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A R T I C L E I N F O

Article history:
Received 29 October 2010
Received in revised form 8 March 2011
Accepted 31 March 2011
Available online 11 May 2011

Keywords:
CO_2 mixtures
Thermodynamic property
VLE
Density
Equation of state
CO_2 capture and storage

A B S T R A C T

The knowledge about pressure–volume–temperature–composition (PVTxy) properties plays an important role in the design and operation of many processes involved in CO_2 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 CO_2 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 CO_2/COS and few data about the CO_2/N_2O_4 mixture. For the volume property, there are no published experimental data for CO_2/O_2, CO_2/CO, CO_2/N_2O_4, CO_2/COS and CO_2/NH_3 and the liquid volume of CO_2/H_2. The experimental data available for multi-component CO_2 mixtures are also scarce. Many equations of state are available for thermodynamic calculations of CO_2 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.

Contents

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0306-2619/$ - see front matter
doi:10.1016/j.apenergy.2011.03.052

Nomenclature

α	Helmholtz energy
k_{ij}	binary interaction parameter
ρ	density
P	pressure
R	gas constant
T	temperature
V, v	molar volume
x	mole fraction in liquid phase
X	total mole fraction
y	mole fraction in vapour phase

Abbreviation:

BWR	Benedict–Webb–Rubin
CCS	CO_2 capture and storage
Comp	compressibility
CPA	cubic plus association
EOS	equation of state
GERG	Group Européen de Recherche Gazières
HV	Huron–Vidal
ISRK	improved Soave–Redlich–Kwong
LK	Lee–Kesler
MPR	modified Peng–Robinson
MSRK	modified Soave–Redlich–Kwong
PR	Peng–Robinson
PPR	predictive-Peng–Robinson
PSRK	predictive Redlich–Kwong–Soave
PT	Patel–Teja
PVTxy	pressure–volume–temperature–composition
RK	Redlich–Kwong
SAFT	Statistical Associating Fluid Theory
SRK	Soave–Redlich–Kwong
VLE	vapour–liquid equilibrium

Subscript:

g	gas
i, j	component labels
l	liquid

1. Introduction

Currently, there are several running commercial projects about CO_2 capture, transport and storage (CCS). For example, the Snøhvit project (Northern Norway) operated by Statoil runs a 153 km off-shore pipeline transporting liquid CO_2 from an LNG plant to a sub-sea well. In the Sleipner project (North Sea) which is also operated by Statoil, the CO_2 is transported a short distance near the critical point between two connected offshore platforms. Here, the CO_2 capture unit is on one platform, while the wellhead is connected to the other [1]. From those projects, many Research & Development requests have been raised to improve the Health, Safety and Environment and reduce the costs in existing and future CCS chains.

Carbon dioxide captured from an energy conversion process always contains impurities. Previous work has revealed that the existences of impurities will clearly impact the design and operation of CCS systems [2,3]. Therefore, the knowledge of thermodynamic properties, especially the pressure–volume–temperature–composition (PVTxy) properties, is essential to the design and operation of CO_2 conditioning and transport. The knowledge of the behaviour of the mixture under the conditions of the particular process will allow (as shown in Fig. 1):

- Identification of possibly encountered problems.
- Specification of safe concentration limits for the involved impurities.
- Definition of the requirements for purification if necessary.
- Designing efficient, safe and economic processes.

A typical CO_2 capture and storage (CCS) chain normally consists of four main steps: CO_2 capture, CO_2 conditioning (dehydration, non-condensable gas separation and/or liquefaction, and compression/pumping), CO_2 transport and CO_2 storage. Fig. 2 illustrates how these steps are linked together.

The vapour–liquid-equilibrium (VLE) of CO_2 mixtures is, for example, one of the basic parameters to design the capture of CO_2 and also to design non-condensable gas separation processes. The volume property is important in the design and operation of compression, transportation and storage. It could be said that the development and technical breakthrough of new CCS systems relies on a deeper understanding of the thermodynamic properties of CO_2 mixtures. PVTxy properties can be measured directly. However, because CCS processes cover a large range of operation conditions from atmospheric pressure to supercritical states, and involve multi-component mixtures, experiments alone cannot satisfy the requirements of engineering applications. In order to exceed the limitations of the experiments, theoretical models have been developed based on the experimental data.

This work contains a review of both the experimental data and the thermodynamic models for PVTxy properties of CO_2 mixtures with impurities. The purpose of the work is to summarize and evaluate the available experimental data, identify knowledge gaps and investigate the available theoretical models that have been proposed and tested in the literature. The work will also provide suggestions for future research on the PVTxy properties of CO_2 mixtures.

2. Operating windows of CO_2 conditioning and transport

The operating windows of the process determine the relevant ranges of temperature, pressure and composition, in which experimental data are required and property models should preferably be validated to minimize the uncertainties in the design criteria of the different processes.

2.1. Temperature and pressure windows

The operating conditions of CO_2 capture, transport and storage (CCS) are estimated in Table 1 [4,5]. Some sub-processes or options for these are indicated in Table 1 as well. The table shows that the CCS chain covers pressures from ~0 MPa to 50 MPa and temperatures from 218 K to 1620 K.

2.2. Possible impurities

The type and amount of the impurities introduced into the CO_2 depend on the fuels used and the type of capture technology. The CO_2 streams captured from post-combustion with an amine solution are relatively clean, with H_2O as the main impurity. However, relative high levels of impurities are expected in the CO_2 streams captured from oxy-fuel combustion, and a more complicated composition of the CO_2 stream is expected in the cases with