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Application of the Henry's law model for prediction of the vapour-liquid equilibria in impure CO₂ streams

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Abstract

The design and operation of processes involved in Carbon Capture, Utilisation and Storage, such as cryogenic separation of non-condensable components from CO₂ streams, as well as CO₂ multistage compression, liquefaction, transport and storage, require using process simulation tools that rely on accurate and robust models predicting vapour-liquid phase equilibria in impure CO₂ streams captured from power plants and industrial installations. Of particular interest are the development and validation of short-cut engineering methods that combine simplicity of the mathematical description with the accuracy of most rigorous equations of state models.

In this work, in order to describe the Vapour-Liquid Equilibrium (VLE) in binary mixtures of CO₂ with non-condensable impurity gases typically found in industrially captured CO₂ streams, a fugacity-activity method utilising Henry's law is applied. The validity of the method is assessed against predictions using reference equations of state (EoSs) for binary CO₂ mixtures with N₂, H₂, O₂, CO, Ar and CH₄. Using a simple modelling approach based on Raoult's and Dalton's laws was shown to predict the bubble- and dew-point data with low accuracy (less than *ca.* 60%), even in the infinite dilution limit and at low temperatures. To get more accurate results, a model was constructed where the solvent vapour fugacity coefficient is approximated using the truncated virial EoS and the Poynting correction is applied to the liquid solvent fugacity coefficient. The proposed model enabled predictions of the VLE phase compositions with accuracy *ca.* ±20% for CO₂ mixtures with N₂, O₂, CO, Ar and CH₄ and +10%/–60% for CO₂ - H₂, in the range of up to 10% solute mole fractions and temperatures below 273 K.

Keywords: CO₂ impurities; vapour-liquid phase equilibria; Henry constant; Carbon Capture, Utilisation and Storage; CCUS; CCS

1. Introduction

Cost-effective implementation of Carbon Capture, Utilisation and Storage (CCUS) technology relies on efficiency of the key process steps involving capture, purification, compression, liquefaction and transportation, as well as utilisation and geological storage of industrial-grade CO₂ originating from combustion units in power plants and industrial installations. Although many of these processes, especially downstream of the primary CO₂ capture units, involve processing relatively pure CO₂ carrying small amounts of impurities, the impact of these contaminant components on the physical properties of CO₂ mixtures can be substantial, and therefore should be considered in the process design.

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Nomenclature

a, b, c	Henry's law correlation parameters
B	Second virial coefficient ($\text{m}^3 \text{mol}^{-1}$)
$B_1^{(0)}, B_1^{(1)}$	Parameters in equation (12)
f_i	Fugacity of a component in a mixture (Pa)
H	Henry constant (Pa)
M	Molecular weight (kg mol^{-1})
p	Pressure (Pa)
R	Universal gas constant ($8.31446 \text{ J mol}^{-1} \text{ K}^{-1}$)
T	Temperature (K)
T_r	Reduced temperature
\bar{V}_i	Partial molar volume of component in a mixture ($\text{m}^3 \text{mol}^{-1}$)
V_i	Molar volume of pure component ($\text{m}^3 \text{mol}^{-1}$)
x	Mole fraction of liquid
y	Mole fraction of vapour
γ^H	Activity coefficient of the solute liquid phase, compatible with Henry's law
$\delta x, \delta y$	Relative deviation of the mole fraction estimates
ϕ_i	Fugacity coefficient of pure component
$\hat{\phi}_i$	Partial fugacity coefficient of component in a mixture
ω	Acentric factor

Indices:

i	Index of a component (1 – CO ₂ solvent, 2 – gas solute)
L	Liquid
V	Vapour
cr	At the critical point of CO ₂
ref	Predicted using reference Equation of State (EoS)
sat	At the CO ₂ saturated conditions
∞	At infinite dilution

Volatile impurity gases such as N₂, H₂, O₂, Ar, CH₄ and CO are typically present in CO₂ streams derived from applying carbon capture in industrial installations [1]. Accurate and robust modelling of physical properties and Vapour-Liquid Equilibria (VLE) of CO₂ mixtures with impurities is critical for development and optimisation of CO₂ purification and conditioning processes, as well as single-phase flow assurance in the design and operation of CO₂ pipeline transportation and geological injection facilities.

Although models based on the Equations of State (EoS) provide the most advanced framework for predicting VLE in CO₂ mixtures, they are relatively mathematically complex, may require using specialised software packages and include parameters that require calibration. These aspects hamper the application of EoS models in research and engineering calculations, e.g., in the conceptual and preliminary design phase or as part of CO₂ separation, transport or storage systems operation or safety monitoring, where using simpler models become more attractive, provided of course they guarantee achieving the required level of accuracy of the results.

Henry's law, which is widely used in environmental engineering, can provide a convenient basis for calculation of physical properties of dilute CO₂ mixtures with volatile gases. Recently, we have determined the Henry's law constants for several gases dissolved in CO₂ [2]. Given that Henry's law is a limiting law that only applies for "sufficiently dilute" solutions, it needs to be implemented in a suitable modelling framework to enable accurate VLE calculations at finite dilutions. The aim of the present study is to develop such a model and assess its ranges of validity for predicting

VLE in binary CO₂ mixtures with N₂, O₂, H₂, CO, Ar, and CH₄ at finite dilutions and various temperature and pressure conditions.

2. VLE in binary CO₂ mixtures

The thermodynamics of VLE in binary mixtures of CO₂ with non-condensable gases demands equal fugacities of the vapour (V) and liquid (L) phases, applied both to the CO₂ solvent (component 1) and the solute gas (component 2):

$$f_1^V(y_1, p, T) = f_1^L(x_1, p, T) \quad (1)$$

$$f_2^V(y_2, p, T) = f_2^L(x_2, p, T) \quad (2)$$

where p and T are respectively the total pressure and the temperature in the system, while x_i and y_i are the mole fractions of the component i ($i = 1, 2$) in the liquid and vapour phases, respectively, satisfying the component mole balances: $x_1 + x_2 = 1$ and $y_1 + y_2 = 1$.

The above conditions can be expressed using fugacity coefficients for the vapour phase and Henry's law applied to the solute [3]:

$$y_1 p \hat{\phi}_1^V(T, p) = x_1 p_{1,sat}(T) \phi_1^V(T, p_{1,sat}) \exp \int_{p_{1,sat}}^p \frac{\hat{V}_1^L dp}{RT} \quad (3)$$

$$y_2 p \hat{\phi}_2^V(T, p) = x_2 H(T, p_{1,sat}) \gamma^H(T, p, x_2) \exp \int_{p_{1,sat}}^p \frac{\hat{V}_2^L dp}{RT} \quad (4)$$

where $\hat{\phi}_i^V$ and \hat{V}_i^L are respectively the partial fugacity coefficient and the partial molar volume of the component i in the mixture, $\phi_1^V(T, p_{1,sat})$ is the vapour fugacity coefficient of pure solvent at saturation pressure, γ^H is the Henry's law compatible activity coefficient of the solute liquid phase, and H is the Henry's law constant of the solute-solvent pair defined at the solute infinite dilution ($x_2 \rightarrow 0$) [4]:

$$H = \lim_{x_2 \rightarrow 0} \frac{f_2^L}{x_2} \quad (5)$$

$$p = \frac{x_1 p_{1,sat} \phi_{1,sat}^V \exp \int_{p_{1,sat}}^p \frac{\hat{V}_1^L dp}{RT}}{\hat{\phi}_1^V} + \frac{x_2 H \gamma^H \exp \int_{p_{1,sat}}^p \frac{\hat{V}_2^L dp}{RT}}{\hat{\phi}_2^V} \quad (6)$$

For dilute binary mixtures of CO₂ with non-condensable gases, including N₂, H₂, O₂, Ar, CH₄ and CO the Henry constants can be calculated using the correlation recommended in our recent study [2]:

$$\ln \left(\frac{H}{p_{1,sat}} \right) = \frac{a}{T_r} + b \frac{(1 - T_r)^{0.355}}{T_r} + c \left(\frac{1}{T_r} - 1 \right)^{1.5} \quad (7)$$

where $p_{1,sat}$ is the CO₂ saturation pressure calculated using the correlation by Span and Wagner [5], $T_r = T / T_{1,cr}$ is the reduced temperature based on the critical temperature of CO₂ ($T_{1,cr} = 304.13$ K) and a , b and c are the solute component-specific constant parameters, for which the values are provided in Table 1.

Table 1. Values of parameters in the Henry constant equation (7) [2].

Parameter	Solute component					
	N ₂	H ₂	O ₂	Ar	CO	CH ₄
a	0.68	1.11	0.75	0.69	0.63	0.39
b	3.07	4.54	2.87	2.88	2.91	2.32
c	4.41	4.01	3.64	4.12	4.03	4.99

Dividing equations (3) and (4) by the corresponding partial vapour fugacity coefficients and then summing them together, gives an integral equation for the total pressure:

$$p = \frac{x_1 p_{1,sat} \phi_{1,sat}^V \exp \int_{p_{1,sat}}^p \frac{\hat{V}_1^L dp}{RT}}{\hat{\phi}_1^V} + \frac{x_2 H \gamma^H \exp \int_{p_{1,sat}}^p \frac{\hat{V}_2^L dp}{RT}}{\hat{\phi}_2^V} \quad (8)$$

This equation provides the basis for the bubble point calculation, and can be solved in terms of x_2 at any specific temperature and pressure, provided that suitable correlations are available to calculate the fugacity and the activity coefficients, and also the partial molar volumes \hat{V}_1^L and \hat{V}_2^L .

2.1. Model A: VLE using Henry's law at infinite dilution

At infinite dilution ($x_2 \rightarrow 0$), where the limits hold $\phi_{1,sat}^V \rightarrow \hat{\phi}_1^V$, $\gamma^H \rightarrow 1$, $\exp \int_{p_{1,sat}}^p \frac{\hat{V}_1^L dp}{RT} \rightarrow 1$, $\exp \int_{p_{1,sat}}^p \frac{\hat{V}_2^L dp}{RT} \rightarrow 1$, equation (6) simplifies to a form of Dalton's law with the solvent and solute components' partial pressures expressed respectively by Raoult's and Henry's laws:

$$p = x_1 p_{1,sat} + \frac{x_2 H}{\hat{\phi}_2^{V\infty}} \quad (9)$$

With the knowledge of H , $p_{1,sat}$ and $\hat{\phi}_2^{V\infty}$, this equation enables calculation of the bubble point pressure for any temperature and composition of the liquid phase at reasonably small mole fraction of the solute.

The corresponding equilibrium vapour mole fraction of the solute can be calculated using the infinite dilution form of equation (4):

$$y_2 = \frac{x_2 H}{p \hat{\phi}_2^{V\infty}} \quad (10)$$

Table 2 lists the reference EoSs adopted in the present study for resolving the VLE in CO₂ binary mixtures. For N₂, O₂, Ar, CH₄ and CO the reference EoSs are those recommended in REFPROP [6]. For CO₂-H₂ mixtures, the Peng-Robinson EoS with a single temperature-independent binary interaction parameter ($\delta_{12} = 0.6$) was fitted to describe the VLE data by Fandiño *et al.* [7]. Fig. 1 illustrates the temperature variation of the partial fugacity coefficients of the components $\hat{\phi}_i^{V\infty}$, estimated using the reference EoSs at $x_2=0.0001$.

Table 2. Reference EoSs employed for calculations of VLE in binary CO₂ mixtures with various components.

	Component					
	N ₂	H ₂	O ₂	Ar	CO	CH ₄
Reference	[8]	[9]	[10]	[11]	[12]	[8]

At finite dilutions, equation (9) is not valid and may lead to inaccurate estimates of VLE. To get more accurate results, suitable approximations for the fugacity and activity coefficients and the exponential terms in equation (6), can be developed to describe their departure from the infinite dilution limit. In any case, the ranges of validity of the model should be established by comparing its predictions with the results of simulations using more rigorous validated models (e.g. the reference EoS) or the relevant experimental data.

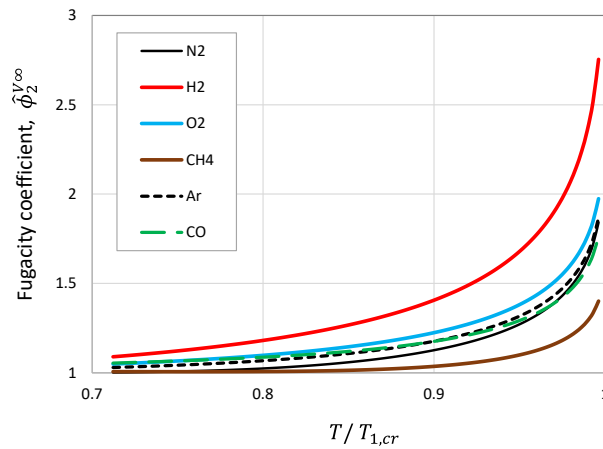


Fig. 1. Variation of the partial fugacity coefficients, $\hat{\phi}_2^{V\infty}$, with temperature for the six components at infinite dilution in saturated CO₂, estimated using the reference EoSs (Table 2).

2.2. Model B: VLE model for small dilutions

In order to use equation (6) for the bubble point calculations, the relevant fugacity and activity coefficients and the exponential terms need to be defined. Although accurate evaluation of these terms without the recourse to advanced EoS models is not possible, within certain ranges they can be estimated using simple approximations. In particular, the fugacity coefficient of solvent vapour at moderate pressures can be determined using expression developed based on the truncated virial EoS [3]:

$$\ln \phi_1^V = \frac{B_1 p}{RT} \quad (11)$$

where R is the universal gas constant and B_1 is the second virial coefficient of the solvent that can be estimated using the correlation by Van Ness and Abbott [13], as recommended in [4]:

$$B_1 = \frac{RT_{1,cr}}{p_{1,cr}} (B_1^{(0)} + \omega_1 B_1^{(1)}) \quad (12)$$

where, $B_1^{(0)} = 0.083 - 0.422 T_r^{-1.6}$ and $B_1^{(1)} = 0.139 - 0.172 T_r^{-4.2}$ are two temperature dependent parameters, while ω_1 and $p_{1,cr}$ are respectively the acentric factor and the critical pressure of the solvent component.

Furthermore, based on the truncated virial EoS, the partial fugacity coefficient of solvent vapour in a binary mixture can be approximated as [3]:

$$\ln \hat{\phi}_1^V = \frac{p}{RT} [B_1 + y_2^2 (2 B_{12} - B_1 - B_2)] \quad (13)$$

where B_2 and B_{12} are the second virial coefficient of the second component (solute gas) and the cross second virial coefficient of the binary mixture, respectively.

At small mole fractions of the solute, where $y_2 \rightarrow 0$, the second term in the square brackets in equation (13) can be approximately neglected, so that the ratio $\phi_1^V / \hat{\phi}_1^V$ can be estimated as:

$$\frac{\phi_1^V(T, p_{1,sat})}{\hat{\phi}_1^V(T, p)} \approx \exp \left[\frac{B_1(p_{1,sat} - p)}{RT} \right] \quad (14)$$

In equation (6) the exponential terms, known as Poynting correction factors, can be expected to depart from unity at pressures above the saturation pressure of the solvent ($p > p_{1,sat}$) or near the critical point of the solvent [14]. While accurate evaluation of these terms at high pressures and close to the critical region is challenging, for practical estimations outside the vicinity of the critical point, approximations have been developed [15]. In particular, assuming \hat{V}_1^L is approximately constant within the pressure range ($p_{1,sat}, p$), the Poynting integral in the first term on the right hand side in equation (6), can be approximated as:

$$\int_{p_{1,sat}}^p \frac{\hat{V}_1^L dp}{RT} \approx \frac{\hat{V}_{1,sat}^L}{RT} (p - p_{1,sat}) \quad (15)$$

Here $\hat{V}_{1,sat}^L$ is the solvent molar volume, which can be estimated at small solute concentrations based on the liquid density of pure solvent at saturation pressure, $V_1^L = M_1 / \rho_{1,sat}^L$. In the present study $\rho_{1,sat}^L$ is calculated as function of temperature using the interpolation function from [5].

Similar approximation can be constructed for the Poynting integral in the second term on the right hand side of equation (6):

$$\int_{p_{1,sat}}^p \frac{\hat{V}_2^L dp}{RT} \approx \frac{\hat{V}_2^{L\infty}}{RT} (p - p_{1,sat}) \quad (16)$$

where $\hat{V}_2^{L\infty}$ is the partial molar volume of solute at infinite dilution, which needs to be either experimentally determined or estimated, e.g. approximated by partial molar volume of pure solute.

In the present study, assuming that both \hat{V}_2^L and $p - p_{1,sat}$ are small, the integral in equation (16) is approximately set to zero. Furthermore, the infinite dilution limit approximation is applied to the partial fugacity coefficient of the solute gas: $\hat{\phi}_2^V \approx \hat{\phi}_2^{V\infty}$, and also the activity coefficient of the solute liquid: $\gamma^H \approx 1$. Using these approximations and substituting equations (14) and (15) in equation (6) gives the following equation for the bubble point pressure:

$$p = x_1 p_{1,sat} \exp \left[\frac{(V_1^L - B_1)}{RT} (p - p_{1,sat}) \right] + \frac{x_2 H}{\hat{\phi}_2^{V\infty}} \quad (17)$$

At a given pressure and temperature this equation can easily be resolved in x_2 , while y_2 can be obtained from equation (10).

3. Results

In this section, the validity of the models for VLE calculations described in the previous section is assessed against predictions using a reference EoS fitted to experimental VLE data obtained for binary mixtures of CO₂ with non-condensable gases (N₂, H₂, O₂, Ar, CH₄ and CO) at temperatures within the interval between the triple and critical point temperatures of CO₂ (216.59 K to 304.13 K).

Fig. 2 illustrates the performance of Model A in describing the VLE for the CO₂-N₂ mixture in comparison with predictions based on the reference EoS (Table 2). In particular, Fig. 2 a shows the bubble and dew lines obtained respectively by solving equations (9) and (10) for the mole fractions x_2 and y_2 at a specific pressure and temperature. It can be seen that in the limit $x_2, y_2 \rightarrow 0$ the model predicts the saturated pressure of CO₂ in agreement with the reference EoS. Also, the slopes of the bubble and dew lines originating from $x_2, y_2 = 0$, qualitatively agree with the slopes of the curves corresponding to the reference EoS, with stronger deviations between the Model A and the reference EoS predictions observed at higher temperatures (particularly 293 K) and larger mole fractions.

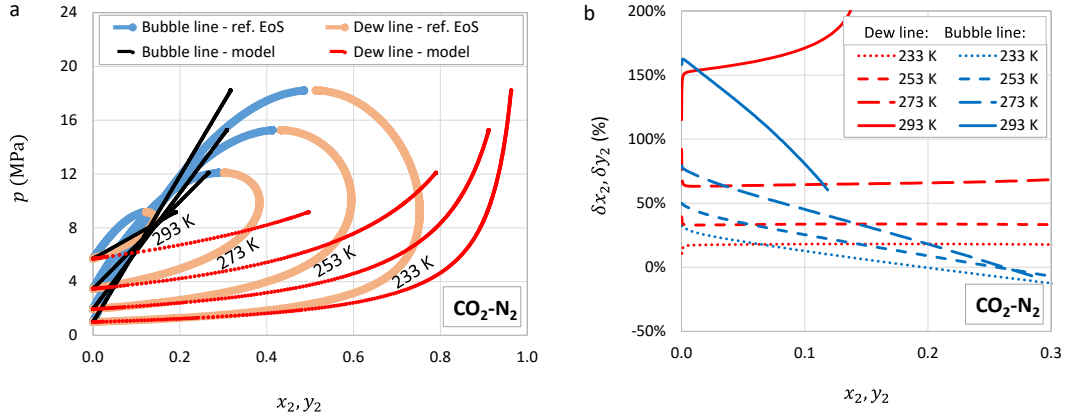


Fig. 2. The bubble and dew lines of CO₂-N₂ mixture constructed at 233 K, 253 K, 273 K and 293 K using Model A and the reference EoS (Table 2) (a), and the corresponding relative deviations between the Model A and the reference EoS predictions (b).

Corresponding to Fig. 2 a, Fig. 2 b illustrates the relative accuracy of the Model A predictions as compared with the reference EoS. The relative deviations between predictions by the model and the reference EoS, are calculated as:

$$\delta x_2 = \frac{x_2 - x_{2,ref}}{x_{2,ref}} \quad (18)$$

$$\delta y_2 = \frac{y_2 - y_{2,\text{ref}}}{y_{2,\text{ref}}} \quad (19)$$

The figure clearly shows that Model A is not accurate, with the deviations from the reference EoS being more than 60% at 273 K, and in excess of 100% at 293 K, even at very small mole fractions of the solute component. As such, Model A cannot be recommended for reliable estimates of the VLE in CO₂-N₂ mixture. This conclusion was also reached for CO₂ binary mixtures with H₂, O₂, Ar, CH₄ and CO, although for the sake of brevity, the results of VLE calculations are not presented here.

Fig. 3 and Fig. 4 show respectively the results of calculations of the VLE boundaries (the bubble and dew lines predicted using Model B and the reference EoS), and the corresponding errors of the Model B predictions, for the six mixture component gases and various temperatures.

In particular, as can be seen in Fig. 3 a and Fig. 4 a for the CO₂-N₂ mixture, Model B enables a more accurate predictions of the VLE boundaries, especially at low concentrations ($x_2, y_2 < 0.1$), at the four temperatures studied. As can be seen in Fig. 4a, Model B predicts x_2 and y_2 along the dew and bubble lines with the accuracy better than +20% / -10% at temperatures below 273 K and *ca.* +50%/ -10% at 293 K. This is a significant improvement in comparison with much less accurate predictions by Model A (Fig. 2 b).

In Fig. 3 and Fig. 4, the subplots b-f show respectively the results for the binary mixtures of CO₂ with H₂, Ar, O₂, CO and CH₄ gases. For all the mixtures, apart from the CO₂-H₂, at temperatures below 273 K, Model B predicts the vapour and liquid mole fractions at the VLE boundary (the dew and bubble lines) with the deviations from the reference EoS data less than *ca.* ±20%, while at 293 K, the deviations reach *ca.* 50% for x_2, y_2 of 0.1. In the case of CO₂-H₂ mixture (Fig. 3 b and Fig. 4 b), the model predicts fairly well the dew line data (+10% at $y_2 < 0.3$), while the mole fractions x_2 along the bubble line are predicted less accurately (with the deviations from the reference EoS of *ca.* 60% at $x_2 = 0.1$).

Although the accuracy of the VLE predictions by Model B (*ca.* 20% at small dilutions $x_2 < 0.1$) is less than what can be achieved using some commonly used EoSs (typically 2-14% for the Peng-Robinson, SRK, BWR, GERG-2008 and SAFT EoSs [16]), it can be sufficient for practical calculations that require using simple correlations, e.g. in the preliminary design of CO₂ conditioning and transportation steps of the CCUS process chain.

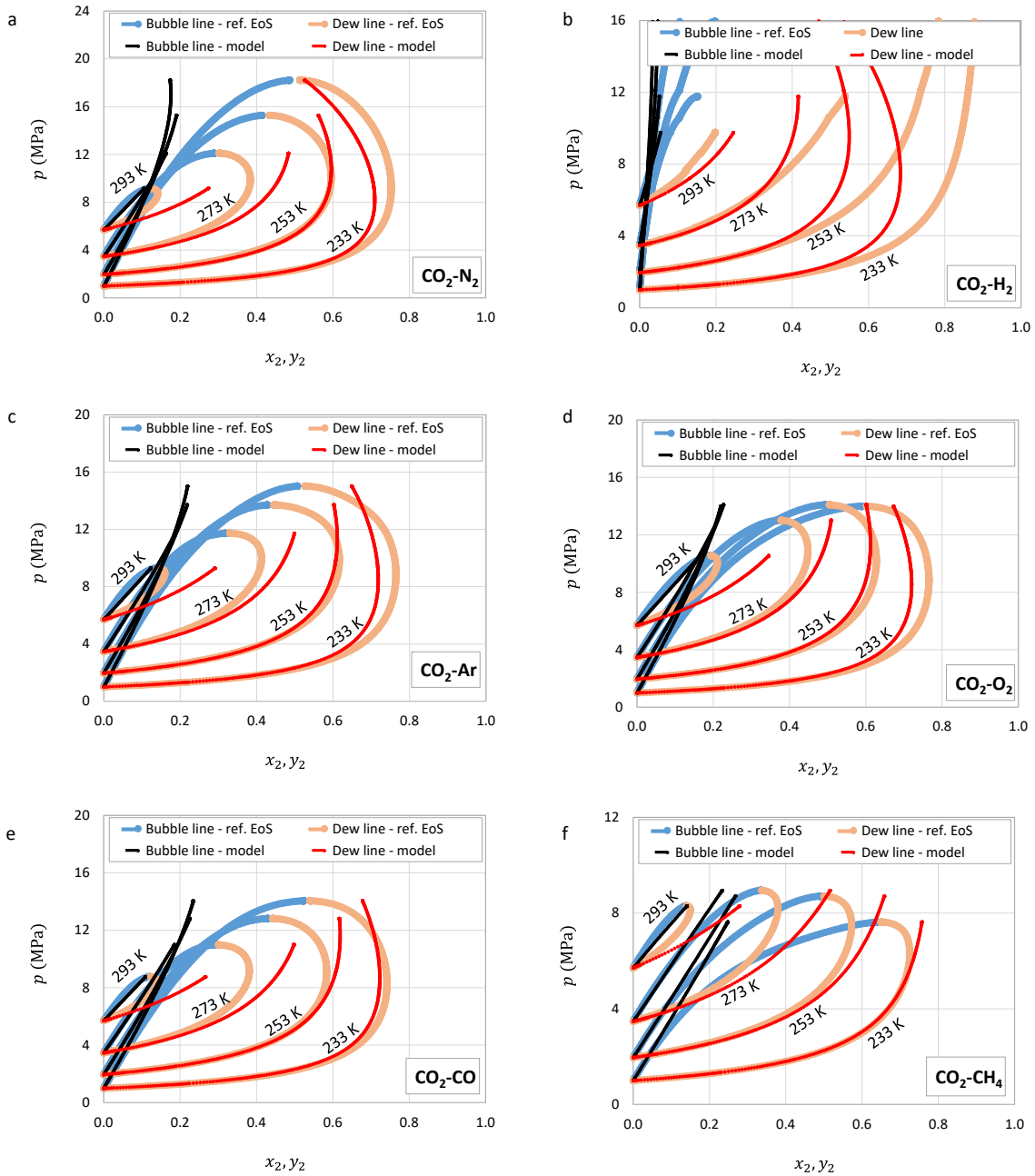


Fig. 3. The bubble and dew lines of binary CO₂ mixtures with various components (a – CO₂-N₂, b – CO₂-H₂, c – CO₂-Ar, d – CO₂-O₂, e – CO₂-CO, f – CO₂-CH₄) at 233 K, 253 K, 273 K and 293 K, predicted using Model B and the reference EoS (Table 2).

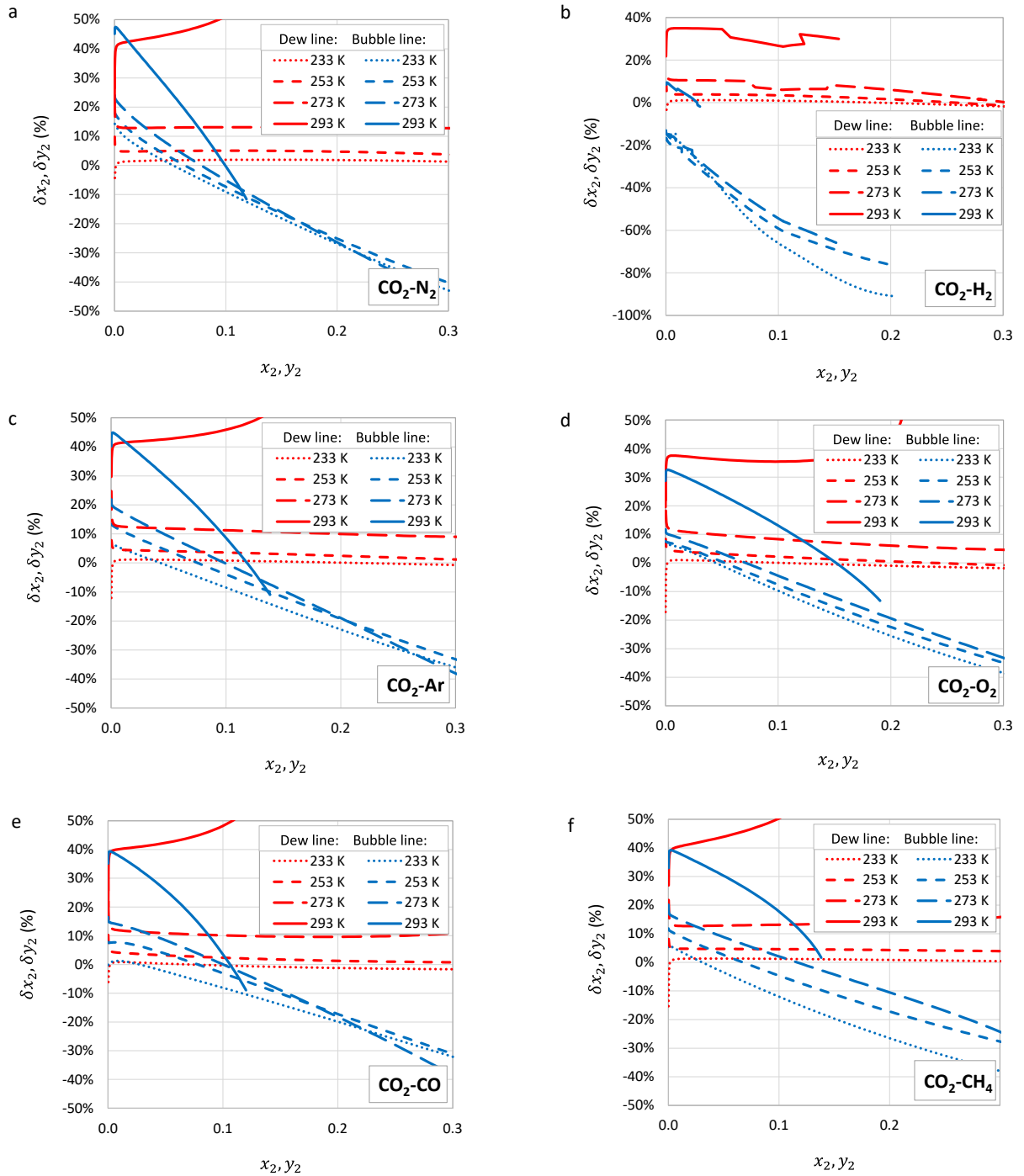


Fig. 4. Relative errors of the Model B predictions of the mole fractions at the bubble (δx_2) and dew (δy_2) lines (see Fig. 3) for binary mixtures of CO_2 with various components at 233 K, 253 K, 273 K and 293 K (a – $\text{CO}_2\text{-N}_2$, b – $\text{CO}_2\text{-H}_2$, c – $\text{CO}_2\text{-Ar}$, d – $\text{CO}_2\text{-O}_2$, e – $\text{CO}_2\text{-CO}$, f – $\text{CO}_2\text{-CH}_4$).

4. Conclusions

The present study describes a simple engineering (short-cut) model based on fugacity-activity method utilising Henry's law for calculation of VLE in CO₂ mixtures with non-condensable gases, including N₂, H₂, O₂, CO, Ar and CH₄, which are typically present in CO₂ streams captured from power plants and industrial installations as part of the CCUS scheme.

To achieve most accurate predictions, the model was constructed incorporating the Poynting correction for the liquid solvent fugacity and the solvent vapour fugacity coefficient approximated using the truncated virial equation of state (EoS). The model was validated by comparing its predictions with the results obtained using most reliable reference EoSs at temperatures between 233 K and 293 K and the solute concentrations up to 30 mol%.

The study showed that at small dilutions (the solute mole fractions below 10 mol%) and temperatures below 273 K the model predicts the phase composition with the accuracy of *ca.* ±20% for CO₂ mixtures with N₂, O₂, CO, Ar and CH₄ and +10% / -60% for CO₂ mixture with H₂, providing competitive alternative to using EoSs models predicting the VLE data with the 2-14% accuracy [16].

At the solute concentrations above 10% and temperatures above 293 K (i.e. closer to the critical point of the CO₂, 304.13 K), the simple approximations used in the model for evaluation of the Poynting integral, the solute and the solvent vapour fugacity coefficients and the Henry's law activity coefficient ($\gamma^H = 1$) lose their validity, resulting in large deviations between the predictions and the reference EoS-based data. To improve the accuracy of predictions at finite solute concentrations, the method can potentially be further extended to account for the effect of composition on the solute liquid activity coefficient. Where the VLE predictions at large solute concentrations or temperatures above 293 K are of interest, using the EoS approach can be recommended.

The main advantage of the proposed method is that it enables (a) very simple calculations of VLE without the recourse to EoSs and (b) predicts the phase composition with the accuracy (*ca.* 20%), which is sufficient for many practical applications where CO₂ contains relatively small amount of non-condensable components, as e.g. in post-capture steps of CO₂ processing steps in CCUS chain. In this context, the method can become useful in the design and optimisation of separation processes and units removing non-condensable components from CO₂ streams, along with flow assurance calculations and safety assessment of CO₂ transport and storage systems. In some of these applications, the VLE models may need to be complemented by suitable correlations predicting thermodynamic and transport properties of CO₂ mixtures in the subcooled liquid and superheated vapour states [4].

Although the proposed method of VLE calculations was demonstrated for binary mixtures, it can potentially be extended to multi-component mixtures. Further research is needed to explore using short-cut engineering methods for calculation of VLE in realistic multicomponent CO₂ streams carrying other components, including e.g. hydrocarbons, H₂O and acid gases, such as NO_x, H₂S and SO_x.

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References

- [1] R. Porter, M. Fairweather, M. Pourkashanian, and R. M. Woolley, "The range and level of impurities in CO₂ streams from different carbon capture sources," *Int. J. Greenh. Gas Control*, vol. 36, pp. 161–174, 2015, doi: 10.1016/j.ijggc.2015.02.016.
- [2] S. B. Martynov, R. T. J. J. Porter, and H. Mahgerefteh, "Henry's law constants and vapor-liquid distribution coefficients of volatile gases dissolved in carbon dioxide," *ACS Omega*, vol. 7, no. 10, pp. 8777–8788, 2022, doi: 10.1021/acsomega.1c07044.
- [3] I. Tosun, *The Thermodynamics of Phase and Reaction Equilibria*. London, UK: Elsevier B.V., 2013.
- [4] R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids*, 5th ed. NY, USA: McGraw-Hill, 2001.
- [5] R. Span and W. Wagner, "A new equation of state for carbon dioxide covering the fluid region from the triple point temperature to 1100 K at pressures up to 800 MPa," *J. Phys. Chem. B*, vol. 25, pp. 1509–1596, 1996.
- [6] E. W. Lemmon, I. H. Bell, M. L. Huber, and M. O. McLinden, "REFPROP Documentation, Release 10.0." NIST, p. 135, 2018.
- [7] O. Fandiño, J. P. M. M. Trusler, and D. Vega-Maza, "Phase behavior of (CO₂+H₂) and (CO₂+N₂) at temperatures between (218.15 and 303.15)K at pressures up to 15MPa," *Int. J. Greenh. Gas Control*, vol. 36, pp. 78–92, 2015, doi: 10.1016/j.ijggc.2015.02.018.
- [8] O. Kunz and W. Wagner, "The GERG-2008 wide-range equation of state for natural gases and other mixtures: An expansion of GERG-2004," *J. Chem. Eng. Data*, vol. 57, no. 11, pp. 3032–3091, 2012, doi: 10.1021/je300655b.
- [9] D.-Y. Peng and D. B. Robinson, "A New Two-Constant Equation of State," *Ind. Eng. Chem. Fundam.*, vol. 15, no. 1, pp. 59–64, Feb. 1976, doi: 10.1021/i160057a011.
- [10] J. Gernert and R. Span, "EOS-CG: A Helmholtz energy mixture model for humid gases and CCS mixtures," *J. Chem. Thermodyn.*, vol. 93, pp. 274–293, 2016, doi: 10.1016/j.jct.2015.05.015.
- [11] S. W. Løvseth et al., "Thermodynamics of the carbon dioxide plus argon (CO₂ + Ar) system: An improved reference mixture model and measurements of vapor-liquid, vapor-solid, liquid-solid and vapor-liquid-solid phase equilibrium data at the temperatures 213–299 K and pressures up," *Fluid Phase Equilib.*, vol. 466, pp. 48–78, Jun. 2018, doi: 10.1016/j.fluid.2018.02.009.
- [12] L. F. S. Souza, S. Herrig, R. Span, and J. P. M. Trusler, "Experimental density and an improved Helmholtz-energy-explicit mixture model for (CO₂ + CO)," *Appl. Energy*, vol. 251, no. June, p. 113398, 2019, doi: 10.1016/j.apenergy.2019.113398.
- [13] H. C. Van Ness and M. M. Abbott, *Classical Thermodynamics of Non Electrolyte Solutions*. McGraw-Hill, New York, 1982.
- [14] E. Wilhelm, "Solubilities, fugacities and all that in solution chemistry," *J. Solution Chem.*, vol. 44, no. 5, pp. 1004–1061, 2015, doi: 10.1007/s10953-014-0279-8.
- [15] E. Wilhelm and R. Battino, "Partial Molar Volumes of Gases Dissolved in Liquids," in *Volume Properties: Liquids, Solutions and Vapours*, The Royal Society of Chemistry, 2015, pp. 273–306.
- [16] H. Li, J. P. Jakobsen, Ø. Wilhelmsen, and J. Yan, "PVTxy properties of CO₂ mixtures relevant for CO₂ capture, transport and storage: Review of available experimental data and theoretical models," *Appl. Energy*, vol. 88, no. 11, pp. 3567–3579, Nov. 2011, doi: 10.1016/j.apenergy.2011.03.052.