



# The N<sub>2</sub>O analogy in the CO<sub>2</sub> capture context: Literature review and thermodynamic modelling considerations

Juliana G.M.-S. Monteiro, Hallvard F. Svendsen\*

Dept. of Chemical Engineering, Norwegian University of Science and Technology, N-7491 Trondheim, Norway

## HIGHLIGHTS

- The N<sub>2</sub>O analogy plays a central role in modelling CO<sub>2</sub> capture systems.
- A literature review of the solubility of CO<sub>2</sub> and N<sub>2</sub>O in water is presented.
- Thermodynamic modelling of the solubility of CO<sub>2</sub> and N<sub>2</sub>O in water is presented.
- New correlations for the N<sub>2</sub>O analogy are proposed.

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## ABSTRACT

The literature review presented in this work shows that, despite the central role of the N<sub>2</sub>O analogy, there is no sound evidence in literature that the ratios of the solubility of N<sub>2</sub>O to that of CO<sub>2</sub> in water can be used for correlating the solubilities of the two gases in the systems of industrial interest for post combustion CO<sub>2</sub> capture, for instance 5 M MEA. On the contrary, the data evaluated in this work indicates that the use of the ratio of the solubility of N<sub>2</sub>O to that of CO<sub>2</sub> in water may be restricted to systems that are much more dilute than that. The use of the ratio requires that good correlations for Henry's constants of CO<sub>2</sub> and N<sub>2</sub>O in water are available. However, we show there is a remarkable lack of VLE data on the N<sub>2</sub>O–water system in literature.

A thermodynamic modelling of Henry's constants of CO<sub>2</sub> and N<sub>2</sub>O in water is conducted, and two alternative correlations are provided: one for operations up to 1 MPa (typical of post-combustion CO<sub>2</sub> capture), and the other for operations up to 20 MPa (for natural gas sweetening process). The correlations for the ratio of the solubility of N<sub>2</sub>O to that of CO<sub>2</sub> in water are presented together with their 95% confidence bands.

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## 1. Introduction

Accurate simulations of amine based CO<sub>2</sub> capture processes is challenging, but extremely important for design and scale up of capture plants and for accurate determination of process energy requirements. As a basis for all thermodynamic models, good data and models for the solubility of molecular CO<sub>2</sub> in water and in the various amine solutions are required. Normally, the absorber is simulated using a rate-based model taking the combined mass transfer and chemical reactions into account (Al-Baghli et al., 2001), while the stripper is often simulated considering that local chemical equilibrium is reached in all the discretized column segments. This can be done by assuming that all kinetic constants are infinite (Tobiesen et al., 2008). Diffusional

resistances will nevertheless result in concentration gradients, configuring a “reaction zone”. As will be discussed in this work, Henry's constant of CO<sub>2</sub> in water and the N<sub>2</sub>O analogy have central roles in interpreting kinetics and mass transfer data, as well as in modelling and simulating the CO<sub>2</sub> absorption into and desorption from amine solutions.

When equilibrium models are developed, CO<sub>2</sub> is typically modelled in the infinite dilution reference state by using Henry's law, given in Eq. (1) in its ensemble form, also known as the Krichevsky–Ilinskaya (KI) equation (Yousef et al., 2001). The CO<sub>2</sub> activity coefficient is defined in the asymmetric reference state, according to Eqs. (2) and (3). In this framework, an apparent Henry constant of CO<sub>2</sub> in the actual solution can be given by Eq. (4) (Bishnoi and Rochelle, 2000). At infinite dilution, or under conditions in which the activities of the solvent and the solute do not differ appreciably from unity, the apparent Henry constant will coincide with the Henry constant itself.

$$p_{\text{CO}_2} \phi_{\text{CO}_2} = x_{\text{CO}_2} H_{\text{CO}_2, \text{water}}^{\infty} \gamma_{\text{CO}_2}^* \exp \int_{p_s^{\text{sat}}}^p \frac{\bar{V}_{\text{CO}_2}^{\infty}}{RT} dp \quad (1)$$

\* Correspondence to: Department of Chemical Engineering, Norwegian University of Science and Technology, Kjemi IV-402 Sem Sælands vei 6, 7491 Trondheim, Norway. Tel.: +47 73594100; fax: +47 73594080.

E-mail address: [hallvard.svendsen@chemeng.ntnu.no](mailto:hallvard.svendsen@chemeng.ntnu.no) (H.F. Svendsen).