International Journal of Greenhouse Gas Control 39 (2015) 174–184

Contents lists available at ScienceDirect

International Journal of Greenhouse Gas Control

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

Artificial neural network models for the prediction of CO_2 solubility in aqueous amine solutions

Guangying Chen [a], Xiao Luo [a,***], Haiyan Zhang [b,**], Kaiyun Fu [a], Zhiwu Liang [a,*], Wichitpan Rongwong [a], Paitoon Tontiwachwuthikul [a], Raphael Idem [a]

[a] Joint International Center for CO_2 Capture and Storage (iCCS), Provincial Hunan Key Laboratory for Cost-effective Utilization of Fossil Fuel Aimed at Reducing Carbon-dioxide Emissions, College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, PR China
[b] Department of Petroleum and Chemical Engineering, Qinzhou University, Qinzhou, Guangxi 535000, PR China

ARTICLE INFO

Article history:
Received 5 December 2014
Received in revised form 24 April 2015
Accepted 5 May 2015
Available online 27 May 2015

Keywords:
CO_2 solubility
Amine solutions
Back-propagation neural network
Radial basis function neural network

ABSTRACT

CO_2 equilibrium solubility is an important parameter used to evaluate the performance of absorption solvents in CO_2 capture processes. Back-propagation neural networks (BPNN) and radial basis function neural networks (RBFNN) were proposed to predict the CO_2 solubility in 12 known amine solutions. Both of the models were firstly conducted in monoethanolamine, diethanolmine and methyldiethanolamine solutions to evaluate their effectiveness, and were then applied in nine other amine solutions to further verify their adaptability. The results showed that both BPNN and RBFNN models provided excellent agreements with the experimental values for all the amine solutions with average absolute relative errors and root mean square errors less than 10%. A comparison between the predicted results and those of the eight published models showed that the proposed ANN models performed better than the literature models. Furthermore, scalability analysis was carried out to evaluate the adaptability of BPNN and RBFNN models in terms of the wide input parameter ranges.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

The post-combustion capture process that uses an amine solvent is one of the most widely employed CO_2 capture technologies because of its high absorption performance and suitability for industrial applications (Rao and Rubin, 2002; Amann and Bouallou, 2009; Tontiwachwuthikul et al., 2011). As one of the most important parameters for the absorption of CO_2 in reactive chemical solvents, solubility of CO_2 in solution (i.e., equilibrium CO_2 loading) has received much attention in the process of CO_2 capture due to its crucial role in the evaluation of the absorption effectiveness of the absorbent (Liang et al., 2011; Porcheron et al., 2011).

Up to now, a variety of amine solvents have been screened and studied for the CO_2 capture process, and measurements of CO_2 solubility in these amine solutions have been performed by various researchers so far. Monoethanolamine (MEA), diethanolmine (DEA) and methyldiethanolamine (MDEA) are the mostly studied amines and have been researched for decades (Jones et al., 1959; Lawson and Garst, 1976; Jou et al., 1982; Kennard and Meisen, 1984; Shen and Li, 1992; Ermatchkov et al., 2006a; Aronu et al., 2011). Recently, some novel amine solvents (such as 2-amino-2-methyl-1-propanol (AMP), piperazine (PZ), 4-(diethylamino)-2-butanol (DEAB), and 2-(Diethylamino) ethanol (DEEA)) have been experimentally investigated (Tontiwachwuthikul et al., 1991; Kamps et al., 2003; Daneshvar et al., 2004b; Dong et al., 2010; Bougie and Iliuta, 2011; Rebolledo-Morales et al., 2011; Sema et al., 2011; Dash et al., 2012; Kumar and Kundu, 2012; Arshad et al., 2014). All of those studies determined the CO_2 solubility at various conditions such as amine concentrations (C), operation temperatures (T) and CO_2 partial pressures (P_{CO2}), and have achieved high measurement accuracies with good repeatability.

In addition to traditional experimental measurements, a number of thermodynamic models have been established to analyze and correlate the equilibrium solubility of CO_2 within different operating conditions, such as Kent-Eisenberg model (Kent and Eisenberg, 1976; Fouad and Berrouk, 2012), electrolyte-NRTL model (Chen and Evans, 1986), Deshmukh-Mather model (Deshmukh and Mather, 1981) and extended UNIQUAC model (Haghtalab and Dehghani Tafti, 2007; Aronu et al., 2011). These well-established models were developed based on the vapor–liquid equilibrium (VLE) the-

* Corresponding author. Tel.: +86 13618481627; fax: +86 73188573033.
** Corresponding author. Tel.: +86 15807770798.
*** Corresponding author. Tel.: +86 18627329998.
E-mail addresses: x_luo@hnu.edu.cn (X. Luo), zhanghyhg@163.com (H. Zhang), zwliang@hnu.edu.cn (Z. Liang).

http://dx.doi.org/10.1016/j.ijggc.2015.05.005
1750-5836/© 2015 Elsevier Ltd. All rights reserved.

Nomenclature

a	Output value of the neuron
a_i	The prediction value of the ith input data
A_j	The matrix of output values of the jth layer (j = 1–3)
AARE	Average absolute relative error
ARE	Absolute relative error
AMP	2-Amino-2-methyl-1-propanol
ANN	Artificial neural network
b	Bias
B_j	Bias matrix of the jth layer (j = 1–3)
BPNN	Back-propagation neural network
C	Amine concentration
C_1, C_2, C_3, C_4	Regression coefficient
DEA	Diethanolmine
DEAB	4-(Diethylamino)-2-butanol
DEEA	2-(Diethylamino)-ethanol
f_i	Transfer function of the jth layer (j = 1–3)
g	The momentum factor
H_{CO2}	Henry's constant for CO_2
k	Current training iteration
k_i	Equilibrium constants
MAE	Methyl amino ethanol
MAPA	3-(Methylamino)-propylamine
MDEA	Methyldiethanolamine
MEA	Monoethanolamine
MIPA	1-Amino-2-propanol
MPA	Monoproanolamine
n	The number of inputs
p_{min}	The minimum value among all the $p_i$variable
p_{max}	The maximum value among all the p_i variables
$p_{n,i}$	The normalized value of input variable p_i
P_{CO2}	CO_2 partial pressure
P	Input vector
PZ	Piperazine
R	Correlation coefficient
RBFNN	Radial basis function neural network
RMSE	Root mean square error
$[RR'NH]_0$	The initial amine concentration
t_i	The target value of the ith input data
T	Operation temperature
TIPA	Triisopropanolamine
w_i	The weight of the ith input parameter p_i
W	The weight vector related to P
W_j	Weights matrix of the jth layer (j = 1–3)

Greek symbols

α	Equilibrium CO_2 loading
γ	Learning rate
δ_i	Radius or width of the ith hidden neuron
$\|p_i - \mu_i\|$	Euclidean distance between p_i and μ_i
μ_i	The center vector of the i hidden neuron

ory, and reflected the thermodynamic properties of the CO_2-amine systems. However, there are still some limitations on the accuracy and range on those prediction models, which sometimes are only suitable for the specific amine solutions. For example, Benamor and Aroua (Benamor and Aroua, 2005) applied the Deshmukh-Mather model to determine the CO_2 solubility in DEA and MDEA solutions as well as their mixtures at various conditions of amine concentrations (2–4 M), temperatures (30–50 °C) and CO_2 partial pressures (0.09–100 kPa). Although the average absolute relative errors (AAREs) for DEA and MDEA were barely acceptable (4.84% and 10.72%, respectively), the lack of studied amines (only two) and the narrow ranges of concentration and temperature still hindered its subsequent applicability.

Artificial neural network (ANN) is an artificial intelligence method that mimics human brain's operation and computation performance, and processes information using certain mathematical principles. ANNs have powerful and effective nonlinear regression ability, and can reflect the system's complexity and the input-output data groups' inherent relationship with high confidence and precision (Hagan et al., 1996). These special capabilities have made them applicable in many areas such as machine automation, environmental science and engineering, petroleum engineering, and chemical engineering (Ozcan et al., 2006; Benardos and Vosniakos, 2007; Feng et al., 2011; Chen et al., 2014; Fu et al., 2014).

In this study, two types of ANN models (i.e., back-propagation neural network (BPNN) and radial basic function neural network (RBFNN)) are proposed to predict CO_2 solubility in 12 amine solutions for wide ranges of amine concentrations, temperatures and CO_2 partial pressures. The amines used in this work mainly include: (i) three typical amines, i.e., MEA, DEA, and MDEA, and (ii) nine other novel amines, i.e., 2-amino-2-methyl-1-propanol (AMP), piperazine (PZ), triisopropanolamine (TIPA), monoproanolamine (MPA), 1-amino-2-propanol (MIPA), 4-(diethylamino)-2-butanol (DEAB), methyl amino ethanol (MAE), 2-(Diethylamino)- ethanol (DEEA) and 3-(Methylamino)-propylamine (MAPA). As these 12 amines covered all the three amine categories (i.e., primary, secondary and tertiary), accurate predictions of the CO_2 solubility by using ANN models can be considered to overcome the limitations of theoretical models that may only be applicable to specific amines. Therefore, this study will show the applicability of ANN models for the prediction of CO_2 solubility in all amine types. The study involved initially setting and training the adjustable configuration parameters of the BPNN and RBFNN models during the training processes to obtain optimized network models. The performances of these well-established models were then evaluated by comparing their prediction results with experimental data as well as the predicted results of eight numerical models proposed in the literature. In addition, scalability analysis was performed to evaluate the adaptability of BPNN and RBFNN models for predicting the CO_2 solubility in various amine solutions in terms of the wide input parameter ranges.

2. Theory

2.1. Reaction mechanisms of CO_2 solubility in aqueous amine solutions

As is well known, CO_2 absorption into an amine solution combines both physical and chemical absorptions. In order to obtain the CO_2 equilibrium solubility, the concentration of CO_2 in the aqueous solution needs to be calculated.

The reaction of CO_2 with primary and secondary amines can be explained by the zwitterion mechanism (Caplow, 1968) as expressed in the following equilibrium equations:

Amine deprotonation reaction:

$$RR'NH_2^+ \overset{K_1}{\leftrightarrow} RR'NH + H^+ \quad (1)$$

Carbamate hydrolysis reaction:

$$RR'NCOO^- + H_2O \overset{K_2}{\leftrightarrow} RR'NH + HCO_3^- \quad (2)$$

Bicarbonate formation reaction:

$$CO_2 + H_2O \overset{K_3}{\leftrightarrow} HCO_3^- + H^+ \quad (3)$$

دریافت فوری ← متن کامل مقاله

ISIArticles
مرجع مقالات تخصصی ایران

✓ امکان دانلود نسخه تمام متن مقالات انگلیسی
✓ امکان دانلود نسخه ترجمه شده مقالات
✓ پذیرش سفارش ترجمه تخصصی
✓ امکان جستجو در آرشیو جامعی از صدها موضوع و هزاران مقاله
✓ امکان دانلود رایگان ۲ صفحه اول هر مقاله
✓ امکان پرداخت اینترنتی با کلیه کارت های عضو شتاب
✓ دانلود فوری مقاله پس از پرداخت آنلاین
✓ پشتیبانی کامل خرید با بهره مندی از سیستم هوشمند رهگیری سفارشات