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The ability of artificial neural network in prediction of the acid gases solubility in different ionic liquids

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ABSTRACT

In this work, the solubility of carbon dioxide and hydrogen sulfide, in different ionic liquids (ILs) have been investigated by applying the artificial neural networks (ANNs). According to the economic benefits of CO_2 as an inexpensive, non-toxic sources of carbon, many studies have done in capturing of CO_2 from the main resources in ILs due to their specific properties such as negligible vapor pressure. Solubility is a key parameter in the phase equilibria calculations. According to the complexity of ILs structure, the phase behavior modeling for these systems is complicated. ANNs are the nonlinear mathematical models which can make a relation between the inputs and the outputs. In this paper 2930 and 664 solubility data of CO_2 and H_2S are used respectively. Network was trained, validated and tested by 70, 15 and 15 percent of total data with one hidden layer through hyperbolic tangent sigmoid transfer function. Optimum neurons are 23 and 14 for CO_2 and H_2S solubility respectively. AAD% and R^2 are 3.58 percent and 0.9947 for CO_2 and 2.07 and 0.9987 for H_2S system. In addition, the Peng–Robinson EoS with and without optimized k_{ij} and an empirical correlation with different constants are used to compare their deviations with the ANN model. Results showed that the ANN model can correlate the solubility of acid gases in ILs with a high accuracy and its error is minimum among three approaches.

1. Introduction

There is a bit uncertainty that, the conventional fuels such as coal, oil and natural gas will continue to be the major and important source of worldwide energy [1]. A rapid growing energy demand is a result of the use of faster transportation means, and like the industrialization.

This is a fact that common resources of energy release huge amount of greenhouse gases specially carbon dioxide among the last decades. Consequently this fact which is the CO_2 emission, besides the environmental effects, prepare an inexpensive, non-toxic and regenerative carbon sources, attracts researchers to explore novel procedures in order to increase CO_2 capturing [2].

CO_2 as a source of industrial production of C_1 building blocks like urea, methanol, carboxylic acid and food, change the researcher's sight of view to change the conventional techniques of CO_2 capturing to high performance techniques [3,4]. H_2S which is defined as a well-known acid gas beside the CO_2, seems to be an inexpensive sources of chemicals like sulfuric fertilizers, acids and explosive compounds which attracts the researchers to capture it from its main resources like the natural gas.

Several techniques have been investigated for CO_2 and H_2S capturing from gas mixture. Conventional strategies, with both advantages and disadvantages, such as chemical absorption in a liquid amines [5] and adsorption on the zeolite surfaces and finally membrane separation (e.g. polymeric membranes) have been developed in the last decades [6]. Chemical absorption of carbon dioxide with aqueous solution of amine has low capital cost, high absorption power and capacity. However, aqueous amine may also pose serious inherent drawbacks, including loss of solvent, corrosion of facility and high energy demand for regeneration of the absorbent [6–8].

Since both chemical and physical solvents are operating under different conditions and have certain limitations, it would be desirable to have a CO_2 capturing process that would merge their versatile advantages and depreciate intrinsic drawbacks. Thus, an ideal CO_2 and H_2S capturing sorbent should be able to provide such properties with fast adsorption and desorption kinetics, stability and regenerability. In addition, a large sorption capacity and a wide tunable range of operational conditions in order to adjust the process requirements should be realized.

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The benefits of CO_2 utilization at the industrial production of carbon-based materials, lead to this fact that CO_2 capturing technologies can be developed either by means of an improvement in the technical design of the system or by replacing the current solvent systems with new, more efficient and environmental friendly media.

Ionic liquids have been identified as a novel alternative, not only as solvents but also as candidates for other applications such as gas purifications. Thus, ionic liquids represent a new, clean and potentially green technology offering the promise of minimized waste streams, atom efficient operations and, therefore, environmental and cost benefits [9–12].

Ionic liquids are containing two ionic parts involved large cationic and small anionic parts which result in being like liquid salts at the room temperature [13,14]. The designable ability of ionic liquids allows them to be effective solvents for sour gas removal. This is mainly because of their specific chemical and physical properties which may be engineered by ionic parts replacement. These task specific components allow the researchers to use them for the improvement of the processes and products. The most attractive physical property of ionic liquids is their non-detectable vapor pressure which helps them to replace by conventional solvents in frame of "green chemistry". Highly polar, non-flammable, wide liquid range and high selectivity make the ionic liquids more attractable [15].

The more focused application of ILs is in the supercritical processes. Due to the high solubility of different gases in ILs in comparison with the low solubility of ILs in the gas phases, there are several papers which investigate the solubility of CO_2 and H_2S in ILs at high pressures [3]. Besides the environmental effects of CO_2 capturing in ILs, other applications such as organic chemical extraction with supercritical CO_2 with or without ILs, liquid-liquid extraction in the presence of a mixture of CO_2 and ILs, homogenous catalysis reaction and fatty acid esters and vegetable oils extraction are attracting the large amounts of research papers [15,16].

According to the limitations of experimental researches to measure the solubility of CO_2 and H_2S in ILs such as highly toxic and hazardous nature of H_2S and costly nature of ILs, it is recommended to propose a model with the ability to predict the solubility of these gases in ILs. Regarding to complexity of ILs, large cation besides small anion, simple models like SRK and PR equation of states by assuming the unique molecular structure for each anion, instead of separation of the cation and anion, reveals more deviation form experimental data in comparison with complex models like Statistical Associating Fluid Theory (SAFT EOS) and its revisions such as PC-SAFT, SAFT-γ, EPC-SAFT and TPC-PSAFT [17]. Some researches include CO_2 and H_2S solubility prediction in the ILs mixture by activity coefficients approach with different Gibbs energy models such as UNIQUAC, NRTL, Wilson, UNIFAC associated with group contribution method and finally some papers published recently based on the simple algebraic models with large number of constants to predict the solubility of sour gases in IL systems [13,18].

All above models predict the thermodynamic solubility of CO_2 and H_2S, but according to long chain with non-spherical species exerting repulsive, Columbus force and dispersive ionic parts in IL structure and high pressure in supercritical conditions, all of the mentioned methods have been developed for a certain IL–gas system separately, and there is no any general predictive model to forecast the solubility of sour gases in IL, simple models such as equation of states or empirical equations need too many constants or many binary interaction fitting parameters, consequently complex models such as associating and activity models by complex interacting terms and coefficients should be used.

Recently, artificial neural networks (ANNs) are widely used in many technical fields due to their simplicity, flexibility and ability in the modeling of linear and nonlinear systems [19]. ANNs have also been used by many scientists in the phase equilibrium calculations. The advantage of the ANNs methods is highlighted when a large experimental database in the wide ranges of variables is available. Zeinolabedini Hezave et al. [20], used the ANNs method to correlate the bubble points of ternary systems involving nine solvents and two ionic liquids. Mehdizadeh and Movagharnejad [21] compared between neural network method and semi

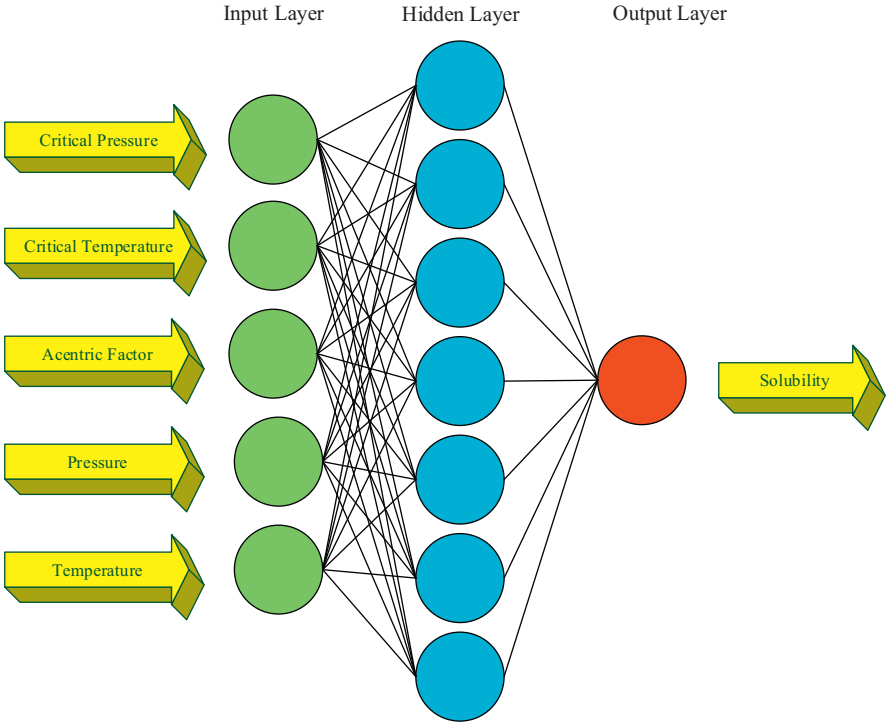

Fig. 1. Schematic diagram of artificial neural network.