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Evolving machine learning models to predict hydrogen sulfide solubility in the presence of various ionic liquids

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ABSTRACT

Substituting conventional solvents for gas sweetening with ionic liquids (ILs) is an interesting way to specify superior design from energy consumption in regeneration and reduction solvent loss. In this study, based on the critical temperature (T_c), critical pressure (Pc), and molecular weight (Mw) of pure ionic liquids, a feed forward Multi-Layer Perceptron Artificial Neural Network (MLP-ANN), an Adaptive Neuro-Fuzzy Inference System (ANFIS) and a Radial Basis Function Artificial Neural Network (RBF-ANN) were developed to predict solubility of Hydrogen Sulfide in the presence of various ILs over wide ranges of temperature, pressure and concentration. To develop the aforementioned methods, 664 experimental data points collected from the literatures were employed. Moreover, to investigate the Hydrogen Sulfide solubility in ternary mixture containing Carbon Dioxide, Hydrogen Sulfide and ILs, MLP-ANN model was proposed. To propose MLP-ANN method for estimating H_2S solubility in ternary mixture, 89 experimental data points collected from the previous published works were employed. To examine the ability of the methods suggested in this study different statistical criteria including R-Squared (R^2), Mean Squared Error (MSE), Standard Deviation (STD) and Mean Absolute Relative Error (MARE) were used. The values of R^2 and MSE achieved for the MLP-ANN model are 0.9951 and 0.000117 respectively. Furthermore, the values of R^2 and MSE for both ANFIS and RBF-ANN methods obtained 0.901, 0.002268 and 0.9679, 0.000787 respectively. In addition, R^2 and MSE of the MLP-ANN model for ternary mixtures are 0.9955 and 0.000082 correspondingly. Therefore, the ability and acceptable performance of using the MLP-ANN as an accurate model for estimating Hydrogen Sulfide solubility in ILs was showed versus other computational intelligence models.

1. Introduction

In lots of oil and gas fields, the acid gases, i.e. Hydrogen sulfide and Carbon Dioxide are produced along with methane and light hydrocarbons. Treatment processes to separate Hydrogen sulfide and Carbon Dioxide are required for production of natural gas. Because of toxicity of Hydrogen sulfide and releasing of it to the atmosphere during combustion, it must be removed [1].

The gas–liquid absorption in amine based solvents is one of the most commonly used processes in industrial natural gas treatment and sweetening plants among various treatment methods have been reported for the removal of acid gases and purify natural gases [2–10].

Recently, a new class of non-aqueous and environmentally friendly innovating fluids which excited both the chemical industries and academia is the class of ionic liquids (ILs). Because of interesting characteristics of ILs for reducing application of hazardous and polluting organic solvents, they can take part in the various new syntheses [11]. In the literature, the earliest type of ILs was created for nuclear warheads batteries in 1970s [12]. Substituting ionic liquids with solvents which are very high in term of volatile that leads to producing new materials with effectiveness conducting heat, high capability of them for purification of gases and removal of metal ions are several applications of ILs that have been studied by researchers [12].

ILs are molten salts which are liquid at room temperature. They are made of positive and negative charged ions which their structures are similar to the table salt such as sodium chloride and tend to have a bulky cation group [13].

Capability of ILs for dissolving numerous organic, inorganic and organometallic compounds, having high thermal conductivity, being highly polar and non-aqueous polar alternatives and the most important feature meaning to have very low vapor pressures are the several remarkable advantages of ILs against conventional organic solvents which make them clean [14–20]. In the gas sweetening, negligibly

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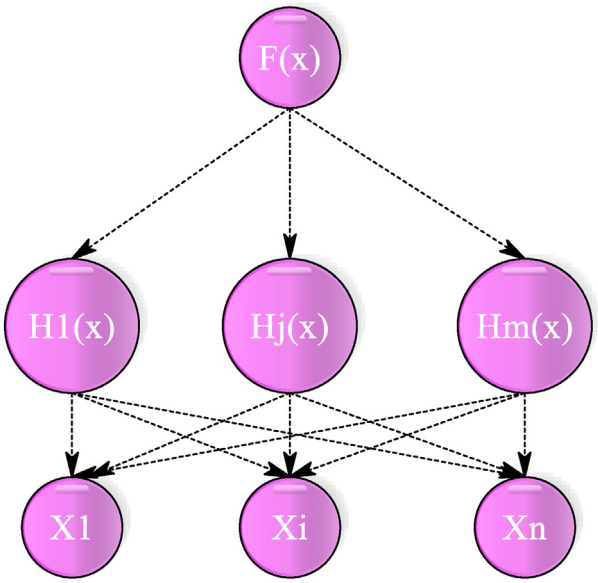

Fig. 1. Structure of radial basis artificial neural network.

small vapor pressure of ILs is one of the greatest remarkable features which allows them to be regenerated and recycled to absorbing section with no significant losses into the gas stream results in negligible solvent make-up requirements [21].

There are several investigation conducted on solubility of Carbon Dioxide in the presence of various ILs [22–29], data points of solubility for Hydrogen sulfide in ILs are limited and have been not investigated extensively [30–40]. Solubility data of Carbon Dioxide in different ionic liquids are the most often found in the literature. Also, investigations about phase behavior of ternary mixture containing $CO_2 + H_2S +$ ILs are more limited than $H_2S +$ ILs/$CO_2 +$ ILs systems [33,34,40].

Several studies and investigations have been made to model the solubility of gas in ILs by thermodynamic laws and also artificial neural network approaches, besides lots of studies that have been made about experimentally measurement of the gas solubility in ILs [41–45].

Artificial Neural Network (ANN) is the most important category of computational intelligence methods that is a non-parametric statistical modeling tool which does not need any pre-assumption of the input–output relationship. Perceptron, adaptive linear element (ADALINE), brain state in a box (BSB), hopfield network, radial basis function network, multi-layer feed forward network, recurrent network and ART network are the common categories of ANNs [46]. Therefore ANN technology can be employed for gas solubility and phase equilibrium modeling [47,48].

Other embranchment of computational intelligence paradigms is Fuzzy Logic System (FLS) that is conceptually easy to understand owing to very simple mathematical concepts. Also, it is able to model the nonlinear complicated functions [49].

By coupling of learning abilities from the artificial neural networks (ANNs) [50–52] with the knowledge of Fuzzy Logic [53,54], other embranchment of computational intelligence called "ANFIS" method is created. ANFIS is an abbreviation of Adaptive Neuro-Fuzzy Inference System.

There are different mathematical optimization methods to create optimum configuration of ANNs or ANFIS parameters including weights and biases. Back Propagation (BP) [43], Genetic Algorithm [55], Particle Swarm Optimization (PSO) [56,57], Hybrid Particle Swarm Optimization and Genetic Algorithm (HPSOGA) [58], Unified Particle Swarm Optimization (UPSO) [50], Imperialist Competitive Algorithm (ICA) [59], and Pruning Algorithm are optimization methods which have been employed in previous studies.

In the present paper, a couple of particle swarm optimization algorithm with the ANFIS, MLP-ANN, and RBF-ANN models were employed to predict Hydrogen Sulfide solubility in [emim][eFAP], [hemim][BF4], [emim][EtSO4], [omim][PF6], [omim][Tf2N], [emim][PF6], [emim][Tf2N], [bmim][PF6], [bmim][BF4], [bmim][Tf2N], [hmim][PF6], [hmim][BF4] and, [hmim][Tf2N] over wide ranges of temperature, concentration and pressure [30–39]. Moreover, solubility of Hydrogen Sulfide in ternary mixture of Carbon Dioxide and Hydrogen Sulfide in [omim][PF6],

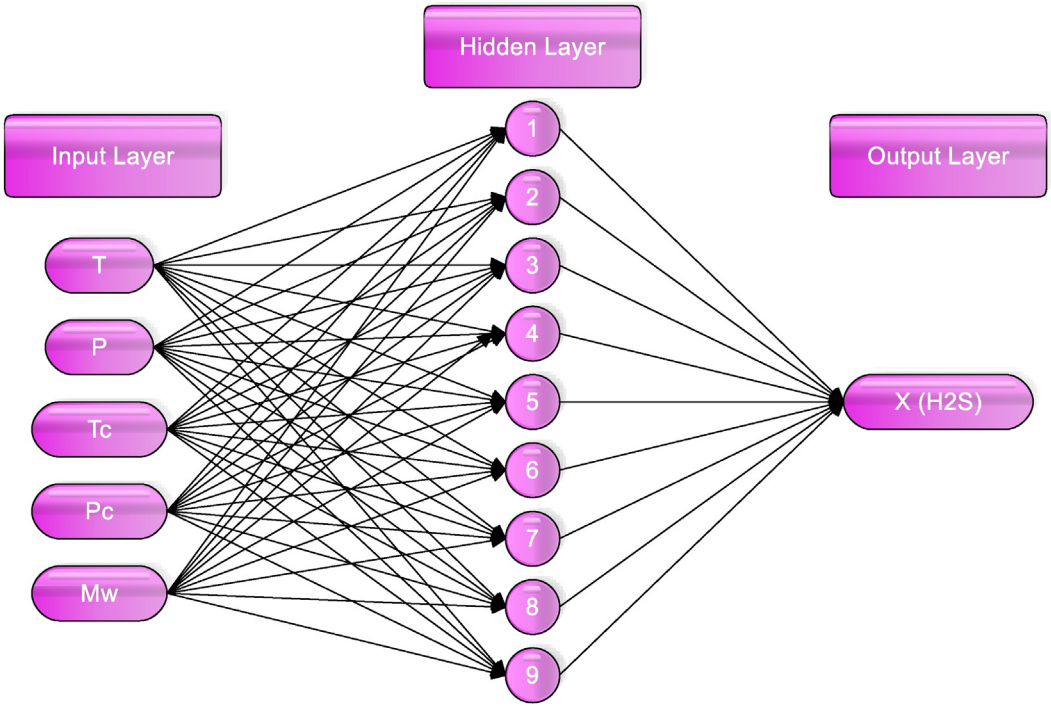

Fig. 2. Structure of multi-layer perceptron artificial neural network in the current work.