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A Novel Approach for Phase Equilibrium Calculations for Geological Sequestration

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Abstract

Due to excessive amount of anthropogenic CO_2 emissions, scientists have been trying to develop some reasonable solutions to this problem (greenhouse gases). One of the most reasonable short-term solutions for removing greenhouse gases (mainly CO_2) is to sequester them in underground formations including seabed as well as geological formations. In this regards, in order to have an exact prediction of the capacity of the mentioned areas to sequester, we must have a clear understanding about CO_2-brine thermodynamic equilibrium meaning that we must have a precise mathematical model with ability to predict the latter calculations. In this paper, artificial neural network technique as data processing tool was applied to CO_2-Brine tertiary system and consequently was used as our model. In this regards, a feed-forward network architecture was used and later optimized in regards of the number of hidden layers and neurons in each layer by using sensitivity analysis on our target variables. Finally, our model was verified by experimental data acquired from the literature. The results show that our model predictions are in close agreement with the experimental data having a regression coefficient – R2 – of about 0.997. Also they represent that in some cases, the neural network – based models can be more accurate than equation of state – based ones which makes it reliable for substituting classic methods in the near future.

Keywords: global warming, greenhouse gases, CO_2 sequestration, neural networks.

1. INTRODUCTION

Excessive amount of anthropogenic CO_2 production in the 20th century has caused several critical issues such as global warming and air pollution. Thus, controlling the amount of CO_2 emissions has become a serious problem. Several mitigation methods have been introduced which can be divided into two main categories. **(a)** Reducing the use of fossil fuels, and **(b)** storing the excess CO_2 in some storage sites such as geological formations and deep sea sediments. Since fossil fuels are the source of about 88% of the total world energy consumption, it seems that method **(a)** is not applicable at least for short-term reduction purposes [1]. This leaves us with the second solution; geological sequestration. One of the most efficient geological sequestration methods which has been applied to several sites (such as "The Sleipner project" in Norway and "The Weyburn EOR project" in Canada) is solubility trapping [2]. It can be inferred from the experimental CO_2 solubility data in the literature that the aqueous CO_2 solution could be slightly denser than that of pure water. Consequently, aqueous CO_2 will be hydro-dynamically stable in the saline aquifer [3]. Therefore, accurate description of CO_2 solubility in brine (formation water) is important for evaluating the capacity of saline aquifers to sequester CO_2 by this mechanism. In addition, CO_2 injection for EOR purposes also requires accurate phase equilibrium calculations. In this study, we have modelled CO_2 solubility in brine using artificial neural networks and the results are compared to the experimental data.

2. METHODOLOGY

Artificial neural networks are data processing tools that can recognize highly complicated patterns. As can be seen in Fig. 1, the network model used in this study has three inputs (Pressure, temperature, salt molality in brine) and one output (CO_2 mole percent in brine).