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AI Modeling of CO_2 and H_2S Pure Gas and Their Mixture Solubility in Water and NaCl Brine

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Summary

Accurate determination of CO_2 and H_2S solubility in water and brine at subsurface temperature and pressure conditions is important for many applications such as reservoir souring, CO_2 sequestration, CO_2-EOR, thermal recovery/SAGD via aquathermolysis, and corrosion-related issues in sour gas fields. Experiment is the most common method to measure gas solubility, but its application is limited because of the cost, extensive duration of laboratory testing, and their cumbersome implementation. The toxic and corrosive nature of H_2S is also an important safety concern for laboratory work. In this study, we firstly compile a large database with experimental and theoretical modeling data based on literature, and then apply AI methods on the CO_2 and H_2S pure gas and their mixture solubility prediction for a better performance with wider ranges of subsurface temperatures and pressure.

Method

It is well-established in the literature that the solubility of CO_2 and H_2S in water and saline solutions is a function of pressure, temperature, and salinity as shown in:

$$\text{Solubility}=f(P,T,S,xH_2S) \tag{1}$$

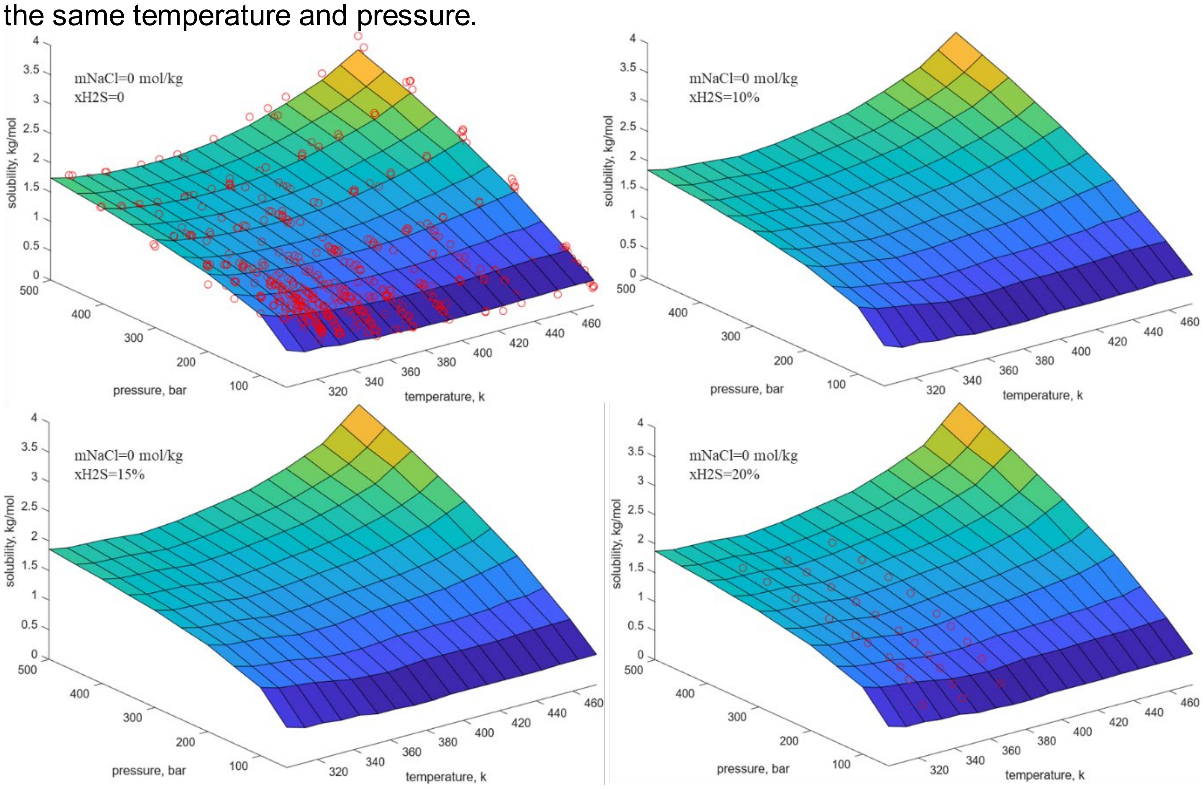
where P is pressure (bar), T is temperature (K), S is salinity (m NaCl, mol/kg), and xH_2S is the proportion of H_2S in the total gas.

It means that gas solubility in water and brine can be treated as a non-linear regression prediction problem with four input parameters (independent variables) and one output parameter (dependent variable). In this study, three ML models, including backpropagation neural networks (BPNN), generalized regression neural network (GRNN), and XGBoost, were chosen to predict gas solubility.

Firstly, we compiled a large database of nearly 3000 experimental and 400 theoretical modeling data points. The total data was divided into two sets: the training set (80% of the total data), and the testing set (20% of the total data). Secondly, the three ML models were developed with the training set and validated with the testing set, and the final modeling parameters were adjusted based on two statistical criteria RMSE and adjusted R^2). Thirdly, we built a new ML-based fusion model by stacking the BPNN, GRNN, and XGBoost models for better prediction performance. Stacking is the practice of employing multiple ML models, subjecting them to K-fold cross-validation to generate prediction results. Subsequently, the prediction outcomes from each model are combined into new features, and a new fusion model is trained using these features. The key advantage of the fusion modeling is that it can combine the predictions of multiple ML models to generate more accurate predictions than an individual model alone, reducing the risk of overfitting or underfitting the data and improving generalizability and robustness (Anifowose et a., 2015).

Results, Observations, Conclusions

The models were trained and validated with a database of experimental data with a wide range of temperature, pressure, NaCl salinity, and initial H_2S gas ratio (xH_2S). The results from the four models are highly consistent and agree well with the experimental data. Among these models, XGBoost and the fusion model have the best performance among the four models with the lowest RMSE (both of 0.027) and the highest adjusted R2 (both of 0.999).
Figure 1 summarizes the trends of solubility in CO_2-NaCl-H2O and CO_2-H_2S-NaCL-H2O systems as increased temperature, pressure, and their difference in water and brine. Results show that the gas solubility increases with increasing pressure, which changes rapidly in the low-pressure zone and slowly in the high-pressure zone. However, the gas solubility decreases firstly at the low-temperature zone and then increases with the increase of temperature, and increases rapidly at the high-temperature zone (higher than 420 K). The gas solubility in the water is higher than that in the brine at the same temperature and pressure ranges. For the impacts of the inclusion of H_2S, the CO_2-H_2S solubility is slightly higher than pure CO_2 solubility in the water or brine at the same temperature and pressure.



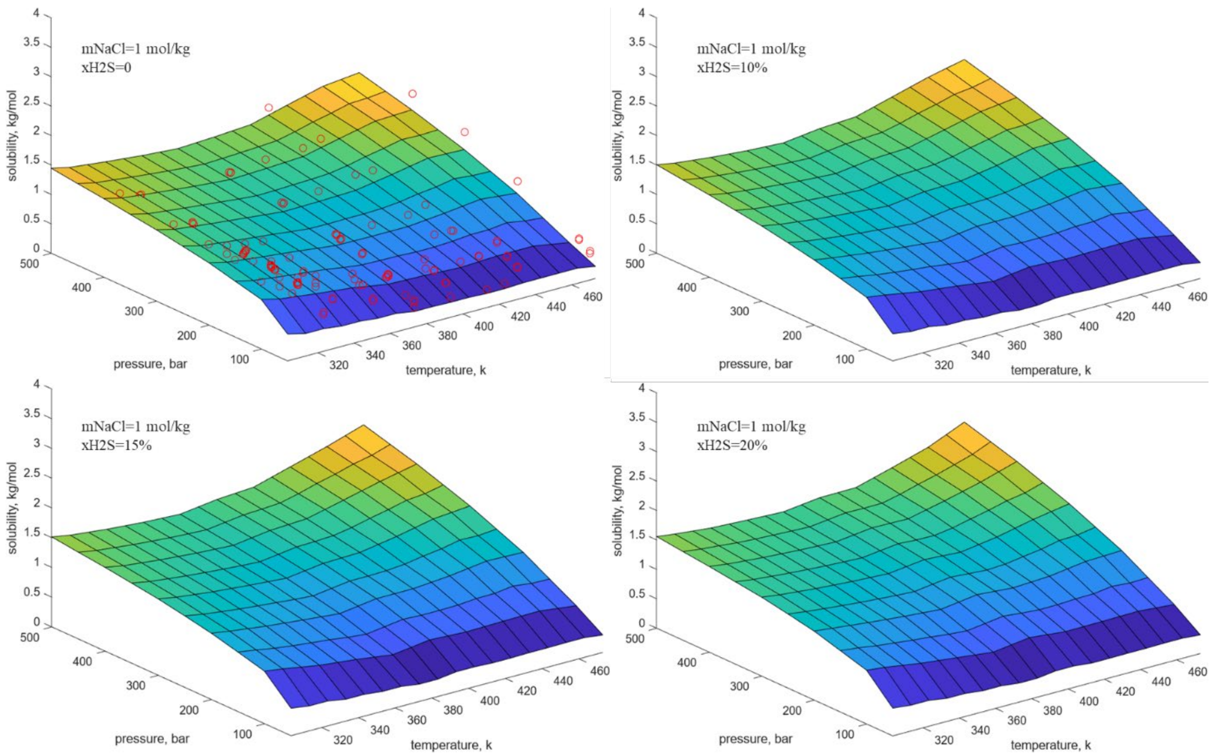


Fig. 1 The modeling results under typical temperature, pressure, and salinity ranges for petroleum reservoirs

Sensitivity analyses show that pressure and temperature are the most sensitive parameters. The gas solubility in water and brine increases monotonically with temperature, but logarithmically with increasing pressure. The solubility of CO_2-H_2S mixture is higher than that of pure CO_2. Salinity has an inhibitory effect on the solubility; at high salinity, the increase of solubility with the increasing pressure or temperature is less than that in the low salinity.

Novel/Additive Information

(1) The modeling prediction from this study is reliable, showing good performance and consistency with the experimental data. Meanwhile, the modeling prediction is more efficient compared to the existing empirical equation (Sun et al., 2021), thermodynamic models (Duan and Sun, 2003; Duan et al, 2006, 2007; Ju and Zhu, 2012, 2013) and ML models (Amar, 2020; Menad et al., 2019), with better performance, a larger amount of modeling data and wider ranges of conditional parameters.
(2) The prediction of the gas mixture in water and brine with wide ranges of reservoir temperature (298.15-623.15 K), pressure (0-2000 bar), salinity (0-6 m NaCl), and the proportion of H_2S in the total gas (0-100%). The experimental data are abundant in some conditions (e.g., around room temperature and at atmospheric pressure), but are almost inexistent in other conditions. This is because experiments are difficult to carry out under extreme conditions of pressure and temperature and in view of the corrosivity and toxicity of the fluids. In addition, measurements have large uncertainties when small concentrations are encountered.

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