Applied Artificial Neural Network for Hydrogen Sulfide Solubility in Natural Gas Purification

Prathana Nimmanterdwong, Rachaneeporn Changpun, Patipon Janthboon, Sukanya Nakrak, Hongxia Gao, Zhiwu Liang, Paitoon Tontiwachwuthikul, and Teerawat Sema*

ABSTRACT: Solubility of hydrogen sulfide (H2S) in 46 single and blended physical absorbents, amines, ionic liquids, and hybrid absorbents of amines + ionic liquids and amines + physical absorbents was successfully predicted based on artificial neural networks (ANNs). Three neural network algorithms of Levenberg–Marquardt (LM), Bayesian regularization (BR), and scaled conjugate gradient (SCG) were applied for architecting the ANN models. The results showed that both the number of hidden neurons and the prediction algorithm affected the prediction of H2S solubility. Based on the mean square error (MSE) and determination coefficient (R²), the most attractive model was the LM-ANN model with 17 hidden neurons. As a result, very satisfactory prediction performance (for the testing data set) with an MSE of 0.0014 and an R² of 0.9817 was obtained from the developed LM-ANN model. Additionally, a parity chart confirmed that the predicted solubility of H2S well aligned with the experimental data. To effectively absorb H2S and maintain high solubility of H2S, the absorbent should be well complied with the operating pressure. For a low-pressure range of less than 100 kPa, amines are very attractive. As the pressure elevated to 100−1000 kPa, amines and hybrid amine + physical absorbents are suggested. Lastly, at a high pressure over 1000 kPa, physical absorbents and ionic liquids are recommended.

1. INTRODUCTION

Natural gas is one of the most well-known and important petroleum products. Gaseous composition of natural gas can be divided into two groups: gaseous hydrocarbon (i.e., methane, ethane, propane, and butane; mostly methane) and gaseous nonhydrocarbon (including carbon dioxide (CO₂), hydrogen sulfide (H₂S), nitrogen (N₂), and water vapor (H₂O)). From the last several decades, natural gas has been used as an energy source for numerous industries and a feedstock for chemical and petrochemical industries as well as a heat/energy source for household applications. Even though natural gas contributes as the third 2019 global primary energy source (24.2%), which is just below coal (27%) and oil (33%), it is the only fossil fuel that shows an increasing demand. As a result, record-breaking natural gas consumption was observed in 2019.1,2 Typically, natural gas can be classified into four categories based on their composition and utilizations:3 First, sour gas is defined as a natural gas containing H₂S higher than 0.25 grains per 100 standard cubic feet (approximately 4 ppm). The second category of sweet gas contains less than 0.25 grains per 100 standard cubic feet of H₂S. Third, natural gas with less than 85% methane (in other words, with an appreciable portion of condensable hydrocarbons (e.g., ethane, propane, and butane)). The wet gas contains at least 0.1 gallon of condensables per 1000 cubic feet of gas. Lastly, dry gas contains less than 0.1 gallon of condensables per 1000 cubic feet of gas.

Even though H₂S is not the most challenging trace gaseous component to remove within the natural gas, it is one of the primary components to be removed from the natural gas to at least comply with pipeline specifications of 0.25−1.0 grains per 100 standard cubic feet.4 This is due to the toxicity and corrosiveness of H₂S.5 Absorption technology has been widely applied for the removal of H₂S from the gaseous stream by liquid absorbents. Advantages of this technology are maturity, a large amount of gas can be treated, and economic feasibility, while its main challenge is an effective absorbent should be used.

Kohl and Nielsen5 pointed out that the well-known gas absorption process can be typically categorized based on the interaction between gaseous absorbates and liquid absorbents. Physical process is the solubility of the absorbate into the absorbent by means of pressure without chemical reactions.
Hence, \(H_2S\) desorption can be initiated by reducing pressure. For example, \(H_2S\) absorption using dimethyl ether or ionic liquids. The reversible process is an absorption associated with the chemical reaction between an absorbate and absorbent. The reacted products in the liquid phase can be reversibly converted to the reactants by applying heat. As a result, the reversed absorbent can be recycled. Absorption—desorption of \(H_2S\) by amine solvent is a good example for this category. Lastly, the irreversible process is also associated with the chemical reaction between the absorbate and absorbent, but the products are complex and cannot revert to the reactants. The removal of \(H_2S\) by iron chelate solution to form elemental sulfur is an irreversible process. It should be mentioned that other trace gaseous components in the natural gas (e.g., carbonyl sulfide (COS) and carbonyl disulfide (CS2)) can also be removed along with \(H_2S\) by liquid absorbents by both physical and chemical mechanisms. In a practical natural gas purification, the solubility of \(H_2S\) with other trace gaseous components is found to be lower than that of individual \(H_2S\) components. This is due to the fact that the absorbent is consumed by more than one absorbate. Thus, the solubility of \(H_2S\) which is mol \(H_2S/mol\) absorbent, is reduced accordingly.

To date, both physical and reversible processes have been industrially used for absorbing \(H_2S\) in natural gas purification. As mentioned before, the key challenge of this technology is to use the effective solvents. To evaluate performance of the absorbent, \(H_2S\) solubility is used as a primary performance indicator, which is generally reported in mol \(H_2S/mol\) absorbent at various operating temperatures and pressures. Numbers of high potential physical solvents have been investigated and can be example as: (i) physical organic solvents of \(n\)-dodecane, sulfolane, \(N\)-methylimidazolide (NMP), and \(\gamma\)-butyrolactone (GBL) and (ii) ionic liquids of 1-butyl-3-methylimidazolium methylsulfate ([bmim][MeSO4]) and 1-ethyl-3-methylimidazolium ethylsulfate ([emim][EtSO4]).

The chemical solvents, which are typical alkanolamine solvents, include monoethanolamine (MEA), 2-amino-2-methyl-1-propanol (AMP), \(N\)-methylthiethanolamine (MDEA), and diisopropanolamine (DIPA). Additionally, combining the physical process and reversible process of blending alkanolamines with organic solvents or ionic liquids has also been considered. Examples of the hybrid solvents are MDEA + sulfolane, NMP + MEA, and MDEA + 1-butyl-3-methylimidazolium acetate [bmim][acetate].

It should be pointed out that obtaining experimental \(H_2S\) solubility is time-consuming and costly. This is because the measurement must be done at various pressures as well as repeatedly conducted until the system reaches equilibrium. Based on the experimentally measured data, several semi-empirical predictive correlations were developed to conveniently estimate the \(H_2S\) solubility for different absorbents (either physical or chemical solvents) at various operating pressures. These correlations were constructed regarding (i) physical solubility of \(H_2S\) in the absorbent, (ii) associated chemical equilibrium constants, and (iii) operating conditions. As a result, moderately good prediction performance can be obtained with average absolute deviation percentages (%AADs) of 13–33%.

Presently, artificial neural networks (ANNs) have been widely applied for complex engineering applications, especially for the prediction of highly nonlinear systems. This is due to a powerful learning ability through biological inspired neurons and synapses. Architecture of the ANN comprises three layers: input, hidden, and output layers. Each layer contains neurons, which are connected by synapses with weighted coefficients. During the learning process, the ANN model is trained by numerous inputs and outputs. As a result, weighted coefficients are adjusted regarding these data. It should be noted that a large enough data bank should be used to train the model. Thus, the trained ANN model can then be used to correctly estimate the desired outputs from the given inputs. Due to a large number of data points associated with solubility of \(H_2S\) in absorbents, ANNs have been applied for predicting the \(H_2S\) solubility at various operating conditions. However, most of the literature focused on single absorbent types either organic physical solvents, amines, or ionic liquids. The present work therefore aims to construct an ANN model from the experimental data available in the literature for predicting the solubility of \(H_2S\) for both single and blended absorbents among the abovementioned types. In addition to the highly effective ANN prediction platform, it is expected to gain more understanding on the selection criteria for properly utilizing the absorbents in \(H_2S\) removal application.

2. DATA COLLECTION AND PROCESSING

The experimental solubility of \(H_2S\) in absorbents at various operating temperatures and pressures were collected from the literature. Since several units of \(H_2S\) solubility were used, this work then converted the collected data into a single unit of mol \(H_2S/mol\) absorbent. Also, operating temperature, operating pressure, and concentration of the absorbent were reported in various units in the collected data. The present work then preliminary processed the inputs to typical units. All the operating temperature and pressure were converted into K and kPa, respectively, while the concentration of the absorbent was considered in weight fraction. As a result, \(H_2S\) solubility of 46 absorbents at various operating temperatures and pressures was processed from 37 literature studies as presented in Table S1 in the Supporting Information. The collected absorbents can be classified as amines, ionic liquids, physical organic absorbents, and hybrid absorbents (amine + physical absorbent and amine + ionic liquid).

3. MODEL DEVELOPMENT

Neural Networks Toolbox in MATLAB with Neural Fitting Application was applied for designing the ANN model based on the collected experimental data. As discussed before, the ANN model comprises three layers: input, hidden, and output layers. In this case of predicting the solubility of \(H_2S\) in absorbents, the solubility of \(H_2S\) was considered as the output, while the absorbents and their weight fractions as well as operating temperature (K) and pressure (kPa) were considered as inputs. In case of a pure absorbent, unity weight fraction was the input as the absorbent concentration. On the other hand, for a blended absorbent, the weight fraction of each absorbent and its corresponding absorbent codename was input into the ANN model. It should also be mentioned that each absorbent was assigned an individual codename. Thus, the blend of two absorbents was input as a combination of two codenames.

From total 2526 data points, 70% (1768 data points) were randomly selected as a training data set. The remaining 30% was randomly divided into 15% (379 data points) and 15%...
(379 data points), which were considered as validation and testing data sets, respectively. A main portion of 70% of the total data points were used to train the developed ANN model. In this learning process, the architectural network adjusted the weighted coefficients regarding errors between the actual outputs and predicted outputs. After the ANN model was trained, the model was then validated with the validation data set (379 data points) to ensure that the developed model was reliable. Lastly, the remaining 379 data points were used to test the model as a testing data set to evaluate a prediction performance of the model.

According to the mentioned procedure, it can be found that designing the neural network in the training step is a key for successfully developing the ANN model. Thus, the present work studied various training algorithms of Levenberg–Marquardt (LM), Bayesian regularization (BR), and scaled conjugate gradient (SCG). In comparison with the conventional algorithms (e.g., standard back propagation (BP), radial basis function (RBF), gradient descent, conjugate gradient, and quasi-Newton algorithms), the recent robust LM, BR, and SCG algorithms show a much better prediction performance in terms of accuracy, speed, and overfitting issues.\(^{1,55}\) Thus, the three algorithms of LM, BR, and SCG were selected to construct the neural networks for predicting solubility of H\(_2\)S.

For each training algorithm, the number of hidden layers were then varied to obtain the optimum number of hidden neurons. It should be indicated that 1768 data points were used as the training data set (379 data points) to ensure that the developed model was trained, the model was then validated with the validation data set (15% of total data points) and the remaining 379 data points were used as the testing data set. To maintain the same number of data points (for training and testing data sets) with those of LM-ANN and SCG-ANN models, the BR-ANN model acquired only training and testing data sets. To determine the optimum number of hidden neurons based on both MSE and \(R^2\). Calculations of the two predictive indicators (MSE and \(R^2\)) are shown in eqs 1 and 2, respectively. Regarding the two equations, an ideal ANN model should have an MSE approaching zero and \(R^2\) converging to unity.

\[
\text{MSE} = \frac{\sum_{i=1}^{n} (\alpha_{\text{exp},i} - \alpha_{\text{pred},i})^2}{n} 
\]

\[
R^2 = 1 - \frac{\sum_{i=1}^{n} (\alpha_{\text{exp},i} - \alpha_{\text{pred},i})^2}{\sum_{i=1}^{n} (\alpha_{\text{exp},i}^2 - \alpha_{\text{pred},i}^2)} 
\]

where \(n\) is the number of data points, \(\alpha_{\text{exp},i}\) is experimental solubility of H\(_2\)S, \(\alpha_{\text{pred},i}\) is predicted solubility of H\(_2\)S, \(\alpha_{\text{exp}}\) is average experimental solubility of H\(_2\)S, and \(\alpha_{\text{pred}}\) is average predicted solubility of H\(_2\)S.

4. MODEL EVALUATION

4.1. Error Analysis. To evaluate a prediction performance of the developed ANN models, an error analysis through the mean square error (MSE) and determination coefficient \(R^2\) was conducted. These two parameters are typically used for indicating an error between the actual and predicted values (in this case, the experimental and the predicted solubility of H\(_2\)S). Calculations of the two predictive indicators (MSE and \(R^2\)) are shown in eqs 1 and 2, respectively. Regarding the two equations, an ideal ANN model should have an MSE approaching zero and \(R^2\) converging to unity.
The LM-ANN model showed MSE and $R^2$ in ranges of $0.0014$–$0.0502$ and $0.9468$–$0.9906$, respectively (for the three data sets), as presented in Figures 1 and 2. Even without optimizing the number of hidden neurons, these ranges of MSE and $R^2$ were reasonably good. This could be because of the great prediction ability of the LM algorithm. Additionally, it was found that as the number of hidden neurons increased, the prediction performance increased. Figures 1 and 2 show that the optimum range of hidden neurons was $16$–$19$ neurons. Within this range, MSE was low and $R^2$ approached unity for the three data sets of training, validation, and testing. To ensure that (i) the optimum value of hidden neurons was reached and (ii) the minimum number of hidden neurons was selected, the optimum number of hidden neurons was considered to be $17$ neurons in case of the LM-ANN model. It should be pointed out that at a number of hidden neurons below $16$ (below the optimum range), there were fluctuations of MSE and $R^2$. Interestingly, these fluctuations seemed to be flatter on increasing the number of hidden neurons to the optimum range. Correspondingly, the prediction performance of the model was improved in that MSE became lower and $R^2$ was getting closer to $1$. These observations were a strong confirmation that the developed LM-ANN model learned from the training data set. During the learning process, a higher number of neurons and synapses resulted in a better prediction performance. For the LM-ANN model, the optimum number of hidden neurons was selected at $17$ neurons. As a result, an impressive prediction performance ($MSE$ of $0.0014$ and $R^2$ of $0.9817$) were observed for the testing data set.

The BR-ANN model was designed based on the BR algorithm of two data sets (training and testing) as mentioned in Section 3. To determine the optimum number of hidden neurons, the hidden neurons were varied from $8$ to $21$ neurons. As a result, an overall prediction performance of the BR-ANN model can be ranged as $0.0018$–$0.0948$ and $0.8478$–$0.9948$ for MSE and $R^2$, respectively (as presented in Figures 1 and 2). Regarding the overall MSE and $R^2$, it can be seen that the BR-ANN model possessed slightly lower predictive performance than the LM-ANN model. However, a comparison between the two models should be conducted at their optimum number of hidden neurons. For the optimum range of hidden neurons for the BR-ANN model, Figures 1 and 2 show that the optimum range was $10$–$14$ neurons. This selection was done based on the results of the testing data set. It was found that in a training process, the BR-ANN model learned and was very well trained as can be seen from the satisfactory values of MSE and $R^2$. Interestingly, the predicted results from the testing data set were found to be different. For the testing data set, its prediction performance sharply increased (in other words, MSE rapidly dropped and $R^2$ increasingly approached unity) as the number of hidden neurons increased from $8$ to $10$ neurons, which was lower than the optimum range. This is due to the fact that there are more neurons and synapses to learn and be used for data fitting. After reaching the optimum range, the predictive performance dropped at a number of hidden neurons of $15$–$21$ with the poorest MSE and $R^2$ of $0.0948$ and $0.8478$, respectively (shown in Figures 1 and 2). It should be noted that within this range (higher than the optimum range), the BR-ANN model can very well fit the training data set but not the testing data set. This observation represents a model overfitting. With too many hidden neurons, the model did not learn but remembered the training data with its excess neurons and synapses. As a result, the developed BR-ANN model promisingly fitted all the training data but poorly matched the testing data. Based on prior discussion, the optimum number of hidden neurons for the BR-ANN model was selected at $11$ regarding the same criteria with those of the LM-ANN model. With $11$ hidden neurons, the optimized BR-ANN showed an MSE and $R^2$ of $0.0164$ and $0.9724$ for the testing data set.

For the third and last model of SCG-ANN, it can be seen from Figures 1 and 2 that the SCG-ANN model possessed the lowest prediction performance among the three studied models. Its overall MSE and $R^2$ were in ranges of $0.0791$–$0.2077$ and $0.7374$–$0.8646$, respectively. The results showed that the prediction performance of the SCG-ANN model increased as the number of hidden neurons increased until the optimum range ($10$–$17$ neurons) was reached, then dropped at too many hidden neurons. These represented an underfitting and an overfitting of the SCG-ANN model at a too low and too high number of hidden neurons, respectively. As a result, the SCG-ANN model was optimized at $17$ hidden neurons with an $MSE$ of $0.0791$ and an $R^2$ of $0.8626$ for the testing data set.

5.2. Model Selection. Three algorithms of LM, BR, and SCG were used to construct the ANN models for predicting solubility of H$_2S$. Their prediction performance was evaluated in terms of MSE and $R^2$ at various numbers of hidden neurons. It was found that the optimized number of hidden neurons for the three ANN models were different depending on the algorithm. For the LM-ANN model, $17$ hidden neurons were considered to be the optimum number. Additionally, the remaining two models of BR-ANN and SCG-ANN were optimized at numbers of hidden neurons of $11$ and $17$, respectively. Even though, both LM-ANN and SCG-ANN models required the same optimum number of hidden neurons of $17$, the prediction performance of the LM-ANN model was much better than that of the SCG-ANN model as shown in Figures 1 and 2. The results also showed that LM-ANN and BR-ANN models were much more attractive than SCG-ANN. To specifically compare the prediction performance among the three developed ANN models, MSE and $R^2$ (as performance indicators) for the testing data set were considered in the present work. As mentioned before, the MSE should be minimized with an ideal value of zero, while the $R^2$ should approach unity with a promising value of one. The optimized SCG-ANN with $17$ hidden neurons showed reasonably good

![Figure 2. $R^2$ of the three developed ANN models at various numbers of hidden neurons.](image-url)
prediction performance with an MSE of 0.0791 and an $R^2$ of 0.8626 (for the testing data set). However, a much better prediction performance can be obtained from the optimized LM-ANN (17 neurons) and BR-ANN (11 neurons) with an MSE and $R^2$ for the testing data set of 0.0014 and 0.9817 (LM-ANN) and 0.0164 and 0.9724 (BR-ANN), respectively. Since the LM algorithm is much simpler than the BR algorithm, the optimized number of hidden neurons of LM-ANN (17 neurons) was found to be higher than that of the BR-ANN model (11 neurons). Table 1 summarizes MSE and $R^2$ as well as the number of hidden neurons of the three optimized ANN models.

Table 1. MSE, $R^2$, and the Number of Hidden Neurons of the Three Optimized ANN Models

| ANN model | number of hidden neurons | MSE for the testing data set | $R^2$ for the testing data set |
|-----------|--------------------------|-------------------------------|------------------------------|
| LM-ANN    | 17                       | 0.0014                        | 0.9817                       |
| BR-ANN    | 11                       | 0.0164                        | 0.9724                       |
| SCG-ANN   | 17                       | 0.0791                        | 0.8626                       |

As shown in Figures 1 and 2 and Table 1, the optimized LM-ANN model provided a better satisfactory prediction result than the optimized BR-ANN and SCG-ANN models, respectively. Even though the BR-ANN model required a smaller number of hidden neurons, the LM-ANN model was chosen in this study because (i) the optimized LM-ANN model possessed the most attractive prediction performance in terms of MSE and $R^2$ (shown in Table 1) and (ii) overall prediction performance of the LM-ANN model was more consistent than that of the remaining two models (presented in Figures 1 and 2).

Typically, the SCG-ANN model is developed based on conjugate directions and a scaling of step size. This makes the SCG-ANN model suitable for highly nonlinear large-scale prediction of several thousand data points. On the other hand, the LM-ANN model is constructed by means of nonlinear optimization and minimization of prediction errors. As a result, a complex medium-scale problem is suggested for the LM-ANN model. Lastly, the BR-ANN model is formulated by minimizing weighted coefficient and avoids cross validation. Thus, a small validation data set is recommended for BR-ANN model. For the present study with a couple thousand data points, a relatively poor prediction performance of SCG-ANN was therefore observed in comparison with the remaining two models.

To further evaluate the prediction performance of the selected LM-ANN model with 17 hidden neurons, a parity plot was applied. Figure 3a–d shows parity plots comparing the experimental H$_2$S solubility data (in the $x$-axis) and the predicted data (in the $y$-axis) for training, validation, testing, and all data sets, respectively. It can be seen that the data distributions were well located along the diagonal line of $y = x$ for the three data sets (training, validation, and testing) and all the data. This observation very well corresponded to the error analysis of MSE and $R^2$ for the testing data set (presented in Table 1) in that the MSE was considerably low (0.0014) and $R^2$ was satisfactory close to unity (0.9817). Both error analysis and the parity plot confirmed that the LM-ANN model (with a number of hidden neurons of 17) was very convinced for predicting the solubility of H$_2$S in 46 different absorbents. The developed LM-ANN model was very attractive regarding its promising prediction performance and flexibility to estimate the solubility data. Additionally, the optimized LM-ANN model (MSE of 0.0014 and $R^2$ of 0.9817) showed a better prediction performance than the conventional simpler models: adaptive boosting (MSE of 0.02 and $R^2$ of 0.960), quasi-Newton BP ANN ($R^2$ of 0.8704), gradient decent ANN ($R^2$ of 0.9233), and response surface methodology or RSM ($R^2$ of 0.946).

Within 46 absorbents collected in this study, five groups of absorbents can be categorized. They are physical absorbents, amines, ionic liquids, amines + ionic liquids, and amines + physical absorbents (hybrid absorbents) as presented in Table 2. It can be found that each categorized absorbent differently performed regarding its physical–chemical interaction with H$_2$S and operating pressure. Thus, their performance (in terms of solubility of H$_2$S) was analyzed over three ranges of operating pressures including a low operating pressure of less than 100 kPa, a medium operating pressure of 100–1000 kPa, and a high operating pressure above 1000 kPa.

As tabulated in Table 2, amine is recommended for low-pressure operation. Its solubility of H$_2$S is much higher than the others. This is due to the fact that at low-pressure operation, there is small driving force for H$_2$S in the gas phase to be soluble into the liquid absorbent. Thus, the reversible chemical reaction between H$_2$S and amines then plays a key role in enhancing the solubility of H$_2$S. Since the experimental H$_2$S solubility data of physical absorbents are not available in the literature, the developed LM-ANN model was applied. The predicted results are given in Table 2. It can be seen that at a low-pressure range of less than 100 kPa, H$_2$S solubility of the physical absorbent is comparable with that of ionic liquids but much lower than that of amines.
For the medium range of operating pressure, H$_2$S solubility of the five categorized absorbents increase to be higher than that of the low-pressure range. It is because there is enough pressure to largely initiate physical solubility of H$_2$S at an operating pressure of 100–1000 kPa. Typically, there are both physical and chemical solubility of H$_2$S in the absorbent, but the chemical mechanism dominates the absorption process at a low range of pressure. However, at a medium-pressure range, the pressure driving force is not high enough for H$_2$S to be soluble solely by physical mechanism. Hence, chemical absorption by amines is still convinced. As a result, both amines and the amine + physical absorbent seem to be the most attractive absorbents. Regarding a satisfactory solubility performance of the amine + physical absorbent at medium operating pressure, physical solvent has then been blended with amines as a nonaqueous absorbent to be used in substitution of the conventional aqueous amine absorbent. Since the physical absorbent is typically more viscous than water, the amine + physical absorbent then has higher viscosity than the conventional aqueous amine absorbent. Thus, a mass transfer limitation due to a high absorbent viscosity should be considered in case of the amine + physical absorbent.

With high operating pressure above 1000 kPa, physical absorbents and ionic liquids show very promising solubility of H$_2$S as presented in Table 2. This confirms that there is high enough pressure to physically drive the solubility of H$_2$S. At this point, the chemical reaction plays a minor role while pressure dominates the absorption process. Unfortunately, the hybrid absorbent of amines + ionic liquids does not provide a convincing solubility of H$_2$S in both low and high ranges of operating pressure. Since ionic liquids can very well perform at high operating pressure, it is therefore believed that H$_2$S solubility of the amine + ionic liquid at a high-pressure range will be greater than that at medium and low-pressure ranges. Due to the fact that contribution of amines at high-pressure operation is quite small, H$_2$S solubility of the hybrid amine + ionic liquid is expected to be poorer than that of the physical absorbent and ionic liquid. These hypotheses can be confirmed by the ANN-predicted H$_2$S solubility of the hybrid amine + ionic liquid at high pressure (as shown in Table 2).

Regarding the collected experimental H$_2$S solubility data, it can be summarized that to reach high solubility of H$_2$S, the absorbent should be properly selected based on the operating pressure. At a low range of pressure (less than 100 kPa), amines are suggested. For medium operating pressure (100–1000 kPa), amines and hybrid amine + physical absorbents should well be considered. Lastly, physical absorbents and ionic liquids are recommended for high-pressure operation (over 1000 kPa).

6. CONCLUSIONS

Solubility of H$_2$S in single and blended absorbents including physical absorbents, amines, ionic liquids, and hybrid absorbents (amine + ionic liquid and amine + physical absorbent) were collected from the experimental work reported in the literature. To predict these solubility data, the ANN models with three algorithms of LM, BR, and SCG were constructed and evaluated for their prediction performance at various numbers of hidden neurons. The results showed that both the algorithms and the number of hidden neurons affected the prediction performance. Based on two performance indicators of MSE and $R^2$, the optimized numbers of hidden neurons for the three algorithms were obtained as follows: 17 neurons for LM-ANN, 11 neurons for BR-ANN, and 17 neurons for SCG-ANN. The results clearly indicated that the LM-ANN model with 17 hidden neurons showed the most attractive prediction performance of H$_2$S solubility with an MSE of 0.0014 and an $R^2$ of 0.9817 (for the testing data set). Additionally, the collected data showed that each categorized absorbent behaved differently at various operating pressures. To maintain high solubility of H$_2$S, the absorbent should be well complied with the operating pressure. At operating pressure below 100 kPa, amine is suggested. For a higher operating pressure of 100–1000 kPa, amines and the hybrid amine + physical absorbent are recommended. Lastly, at a high operating pressure of greater than 1000 kPa, physical absorbents and ionic liquids should be used.

ASSOCIATED CONTENT

Supporting Information
The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.1c05169. H$_2$S solubility data at various operating conditions used for developing the ANN models (PDF)

AUTHOR INFORMATION

Corresponding Author
Teerawat Sema — Department of Chemical Technology, Faculty of Science and Center of Excellence on Petrochemical and Materials Technology, Chulalongkorn University, Bangkok 10330, Thailand; orcid.org/0000-0002-1390-3992; Email: teerawat.se@chula.ac.th

Authors
Prathana Nimmatnerdpong — Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand
Rachaneeporn Changpun — Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Table 2. H$_2$S Solubility of Various Absorbents over Ranges of Operating Pressure Collected from the Literature

| Operating pressure (kPa) | Physical absorbent | Ionic liquid | Amine + Ionic liquid | Amine + Physical absorbent | Amine |
|-------------------------|--------------------|--------------|----------------------|-----------------------------|-------|
| Low (<100)              | (0.0015–0.0519)$^a$| 0.0019–0.0925| 0.0302–0.2724         | 0.0032–0.5364               | 0.0014–1.1924 |
| Medium (100–1000)       | 0.0067–0.6000      | 0.0122–1.5590| 0.1854–0.3908         | 0.0352–3.1120                | 0.0972–2.9991 |
| High (>1000)            | 0.1905–9.2041      | 0.0753–7.0000| (0.5315–5.1003)$^a$  | 0.1930–3.5750                | 0.4054–3.3485 |

$^a$Predicted data obtained from the developed LM-ANN model (up to 5000 kPa for the high-pressure range).
Patipon Janthboon — Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Sukanya Nakrak — Department of Chemical Technology, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand

Hongxia Gao — Joint International Center for CO₂ Capture and Storage (iCCS), Provincial Hunan Key Laboratory for Cost-effective Utilization of Fossil Fuel Aided at Reducing CO₂ Emissions, College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, PR China

Zhiwu Liang — Joint International Center for CO₂ Capture and Storage (iCCS), Provincial Hunan Key Laboratory for Cost-effective Utilization of Fossil Fuel Aided at Reducing CO₂ Emissions, College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, PR China; orcid.org/0000-0003-1935-0759

Paitoon Tontiwachwuthikul — Clean Energy Technologies Research Institute (CETRI), Faculty of Engineering and Applied Science, University of Regina, Regina, Saskatchewan S4S0A2, Canada

Complete contact information is available at: https://pubs.acs.org/10.1021/acsomega.1c05169

Notes

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NOMENCLATURE

\( a_{\text{exp}} \) tabexperimental solubility of H₂S (mol H₂S/mol absorvent)
\( a_{\text{avg}} \) tabaverage experimental solubility of H₂S (mol H₂S/mol absorvent)
\( a_{\text{pred}, \text{tab}} \) predicted solubility of H₂S (mol H₂S/mol absorvent)
\( a_{\text{avg}, \text{tab}} \) average predicted solubility of H₂S (mol H₂S/mol absorvent)
\( \bar{R} \) tabdetermination coefficient
\( n \) tabnumber of data points

Abbreviation

ADDtaverage absolute deviation
ANNtabartificial neural network
BRtabBayesian regularization
LMtabLevenberg–Marquardt
MSEtabmean square error
RStabresponse surface methodology
SCGtabscaled conjugate gradient

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