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Revisiting the Kinetic of Polymerization of Silicic Acid: AI-Assisted Prediction of Polymerization and Adsorption Behavior of Silicic Acid

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ABSTRACT

Scaling remains as the major hurdle in the utilization and development of geothermal energy in addition to corrosion. This is because scaling can occur in almost all locations in geothermal power plants, i.e., in production well, on surface facilities, in reinjection well, and even in the geologic formation around the reinjection well. Despite the vast studies, there are no single and universal mitigation method to date. This is likely due to the unique characteristics of each geothermal water and, consequently, the complexity of scale formation. However, the current understanding suggests that silica scale formation is generally controlled by the interaction between dissolved silicic acid and the metal surface (initiation), and the interaction between silicic acid and the surface of silica scale (growth). This study aims to better understand and quantify silica scaling with the help of artificial intelligence (AI). As training data, the behavior of polymerization of silicic acid in geothermal water and its adsorption on silica gel (model surface material of silica scale) were considered in addition with physicochemical properties of geothermal water. First, geochemical results of various geothermal waters were collected. The data was used to calculate the saturation index of minerals. Both data were used as input parameters. In addition, batch polymerization and adsorption experiments were also conducted onsite each corresponding geothermal power plants at similar temperature condition to quantify the polymerization and adsorption rates of silicic acid. As a preliminary AI calculation, the data were then used as output parameters. Here, we used a supervised type of machine learning, which produce several prediction models. The produced models have percent root mean square error (%RMSE) values ranging from 2.7 to 15.7, suggesting the acceptability and applicability of the models. In addition, factor analysis using the produced model suggest that total concentration of silicic acid contribute the most to the polymerization rate of silicic acid, aligned with the classical understanding. Interestingly, iron concentration of geothermal water gives significantly higher contribution than other species despite its low concentration in geothermal water. This study provides a preliminary result of AI modelling for polymerization and adsorption behavior of silicic acid, as well as proposes its AI modelling procedure. Further, the established AI models need to be examined with more physicochemical data of geothermal water and more experimental data of kinetic behavior of polymerization and adsorption of silicic acid. Finally, we will construct an AI system predicting the deposition rate of silica scales from physicochemical data of geothermal waters (geochemical result, polymerization of silicic acid and adsorption of silicic acid) as input data.

1. INTRODUCTION

There are various challenges in the utilization and development of geothermal energy including social and technical issues. The most common technical issues in the utilization of geothermal energy are corrosion and scaling inside the pipeline and geothermal well. Corrosion may occur when dealing with acidic geothermal fluid or when acidic solution is injected to prevent scaling. On the other hand, scaling may happen particularly from a water-dominated geothermal system. Several types of scale have been reported such as carbonate, silica/silicate, sulfate, and sulfide, which precipitate at production well, surface facilities, reinjection well, and/or even reservoir rock around the reinjection well. All of them can significantly hinder electricity production from geothermal energy. Of those locations, silica/silicate scale can form in all of them. The current understanding suggests that silica scale formation is generally controlled by the interaction between dissolved silicic and the metal surface (initiation), and the interaction between silicic acid and the surface of silica scale (growth). However, despite the vast studies on silica scaling, there has not been a universally applicable mitigation method for the problem. This is likely due to the unique characteristics of geothermal water in each field and the complexity of scale formation mechanism.

Recently, artificial intelligence (AI) has been applied in many fields of scientific research such as to reconstruct and simulate event at Large Hadron Collider facility, synthesis of new materials, and fast diagnosis of various disease and disorder (Deiana et al., 2022). In particular, geothermal energy sector has seen a sharp increase in the utilization of AI since 2018 (Okoroafor et al., 2022). AI is being used in the optimization of geothermal energy exploration such as reservoir temperature estimation, determination of production drilling, and development of enhance geothermal system (e.g., Al Shibli and Mathew, 2019; Shahdi, et al., 2021; Moraga et al., 2022; Wang et al., 2023). In this study, we attempt to use AI to better understand and quantify silica scaling. This study aims to construct an AI model which able to quickly determine parameters that control the polymerization of silicic acid and its adsorption on the surface of silica gel (model surface material of silica scale). Furthermore, the AI model is also expected to accurately predict the behavior of polymerization and adsorption of silicic acid based on some input parameters. The model is built on the basis of empirical data from lots of onsite experiments in several geothermal power plants. Physicochemical properties of geothermal water were used as input parameter along with the saturation index of silica, silicate, and oxide minerals. Finally, the kinetic model from this study will be integrated with the empirical data of formation rate of silica scale from metal plate immersion experiments. The integrated models are used to construct an AI system for the prediction of the deposition rate of silica scale and determine the most appropriate mitigation method. The system is expected to greatly contribute to the effective utilization of geothermal energy through the mitigation of scaling problem.

2. METHODOLOGY

2.1 Physicochemical Data and Calculation of Mineral Saturation Index

The physicochemical properties of the geothermal water such as pH and concentrations of major anions and cations were obtained from the operating geothermal power plants. This includes Na, K, Ca, Mg, Cl, and SO_4. In addition, minor metals such as Fe and Al, and total concentration of silica (Si-T) were analyzed using inductively coupled plasma atomic emission spectroscopy (ICP-AES). The data were used as input parameters in the AI training data. Furthermore, the data were also used to calculate the saturation index of minerals. The calculation was done by Geochemist's Workbench® software on the basis of Thermo.tdat (version 2022) thermodynamic database from Lawrence Livermore National Library (LLNL). In this study, silicate and oxide minerals were selected as minerals of interest referring to Juhri et al., 2023. In total, 23 minerals were included (see Figure 1). The saturation index was defined as log(Q/K), where Q is the ion product in geothermal water and K is the solubility product of the corresponding mineral. This data was also used as input parameter of the AI training data.

2.2 Onsite Experimental Procedures

A number of onsite experiments have been conducted in many geothermal power plants in Indonesia and Japan. Polymerization experiment of silicic acid was conducted for 90 minutes where adequate amount of geothermal water was sampled every 5 – 15 minutes. From these samples, concentration of monosilicic acid (Si-M) was determined on-site by a spectrophotometric analysis while total concentrations of silicic acid (Si-T), aluminum (Al-T), and iron (Fe-T) were determined in laboratory by ICP-AES. Furthermore, adsorption experiment on silica gel (D-50-1000AW) was conducted to observe the interaction between various dissolved species with the surface of silica gel which represent the surface of pre-formed silica scale. The specific surface area of the silica gel was known to be 28 m^2/g. Both polymerization and adsorption experiments were conducted at temperature range of 90 – 95 °C.

The data obtained from the polymerization and adsorption experiments were compiled as polymerization rate and adsorption rate which then used as output parameters of AI training data. Note that polymerization and adsorption data were presented as change of concentration of monosilicic acid and total silicic acid, respectively. Therefore, the value ranges from 0 to negative where 0 means constant concentration and negative value means the concentration decreased. More negative value indicates higher polymerization rate and higher adsorption rate.

2.3 Machine Learning Setup

2.3.1 Training data

The training data were from the onsite experiment results at 5 geothermal power plants. In total, 20 experiment results were used for the AI training. The input parameters of the training data consist of major characteristics and saturation index of minerals. The pH ranged from 3.95 to 9.32, the total concentration of major anions-cations ranged from 1,527 to 38,072 mg/l, and the total concentration of silicic acid ranged from 388 to 1,276 mg/l. These data accommodate wide ranges of pH, salinity, and silicic acid content. Furthermore, the total concentrations of Al and Fe were generally low where they range from 0.01 to 1.77 mg/l and 0.006 to 2.1 mg/l, respectively. Furthermore, the output parameters of the training data consist of polymerization rate and adsorption rate. Each were represented by the change of Si-M and Si-T concentrations respectively, at 10, 30, 45, 60, and 90 minutes.

2.3.2 Preprocessing

The training data (input and output parameters) were preprocessed before used for AI training. All input parameters (major characteristic and saturation index of minerals) were normalized using minimum-maximum method, except for the ratio of Si-M/Si-T. The ratio of Si-M/Si-T was normalized using absolute maximum method where 1 is the maximum value. Furthermore, the output parameters (adsorption and polymerization behavior) were also normalized using absolute maximum method where 0 is the maximum value. This assumes Si-M or Si-T concentration will not increase over reaction time.

2.3.3 AI Prediction and Model Evaluation

The AI models were built based on the neural network analysis using Keras, an open-source neural network library developed by Google, which runs on top of TensorFlow platform. The produced models were then evaluated using 3 geothermal water data from 3 different power plants. The input parameters for the prediction represent acidic to weakly alkaline pH conditions, low to high salinity, Si-T, Al-T, and Fe-T concentrations (Table 1). Results from the AI prediction were then compared to the polymerization and adsorption experiment result from each respective geothermal power plant. The accuracy of the prediction was quantified based on the value of root mean square error in percent scale (Despotovic et al., 2016). The value of RMSE was calculated using the equation 1 below, where $H_{i,m}$ is measured data from onsite experiments and $H_{i,c}$ is calculated data by AI model. From this RMSE value, the models are categorized into excellent (<10%), good (10-20%), fair (20-30%), and poor (>30%) (Jamieson et al., 1991; Heinemann and Schmidhalter, 2012; Li et al., 2013).

$$\%RMSE = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(H_{i,m}-H_{i,c}\right)^2}}{\frac{1}{n}\sum_{i=1}^{n} H_{i,m}} \times 100 \qquad \ldots\ldots\ldots.\ (1)$$

Table 1: Characteristics of geothermal water used for the prediction and evaluation.

	pH	Na	K	Ca	Mg	Cl	SO_4	Si-T	Si-M / Si-T	Al-T	Fe-T
Geothermal water 1	5.61	1,180	200	7.9	0.43	1,800	646	889	0.902	0.48	0.04
Geothermal water 2	7.20	1,130	190	7.8	0.44	1,700	618	784	0.496	0.47	0.04
Geothermal water 3	6.30 or 5.02[*)]	10,249	2,817	708.8	0.50	21,200	74	1,276	0.720	0.01	1.40

[*)] pH was 6.30 for polymerization experiment and 5.02 for the adsorption experiment. all values are in ppm except for pH.

3. RESULTS AND DISCUSSION

3.1 Correlation Matrix

Correlation matrix (Figures 1 and 2) shows correlation coefficient between input parameters and output parameters. This is done to identify which variables are strongly correlated to the polymerization rate and adsorption rate of silicic acid. Therefore, they will be selected to seek for a better AI model. Figure 1a shows that K, Si-T, and Fe-T are strongly correlated to the polymerization rate of silicic acid. Note that polymerization is expressed as the decrease in Si-M concentration (negative value), hence the negative correlation coefficients of K, Si-T, and Fe-T mean they positively affect the rate of polymerization. On the contrary, Si-M/Si-T (degree of polymerization at initial condition) is slightly correlated to polymerization rate of silicic acid. Among input parameters, Na, K, Ca, Mg, and Cl are strongly correlated to each other. Figure 1b also shows that K, Si-T, and Fe-T are also correlated to the adsorption rate of silicic acid on the surface of silicic acid.

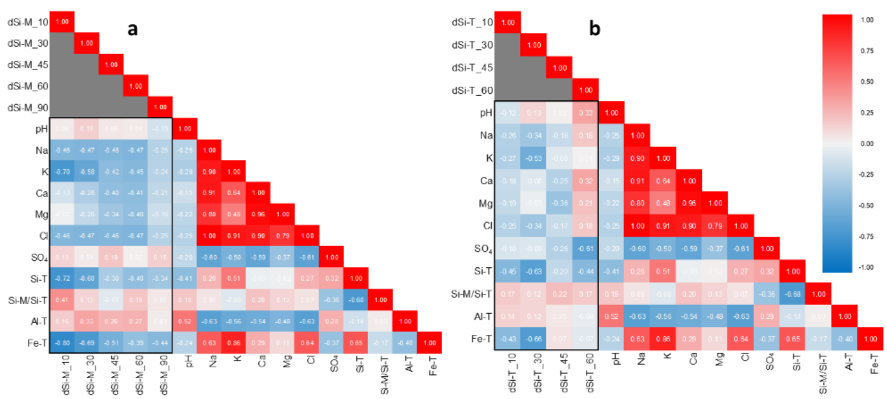

Figure 1: Correlation matrix of major characteristics of geothermal water with polymerization behavior of silicic acid (a) and its adsorption on the surface of silica gel (b).

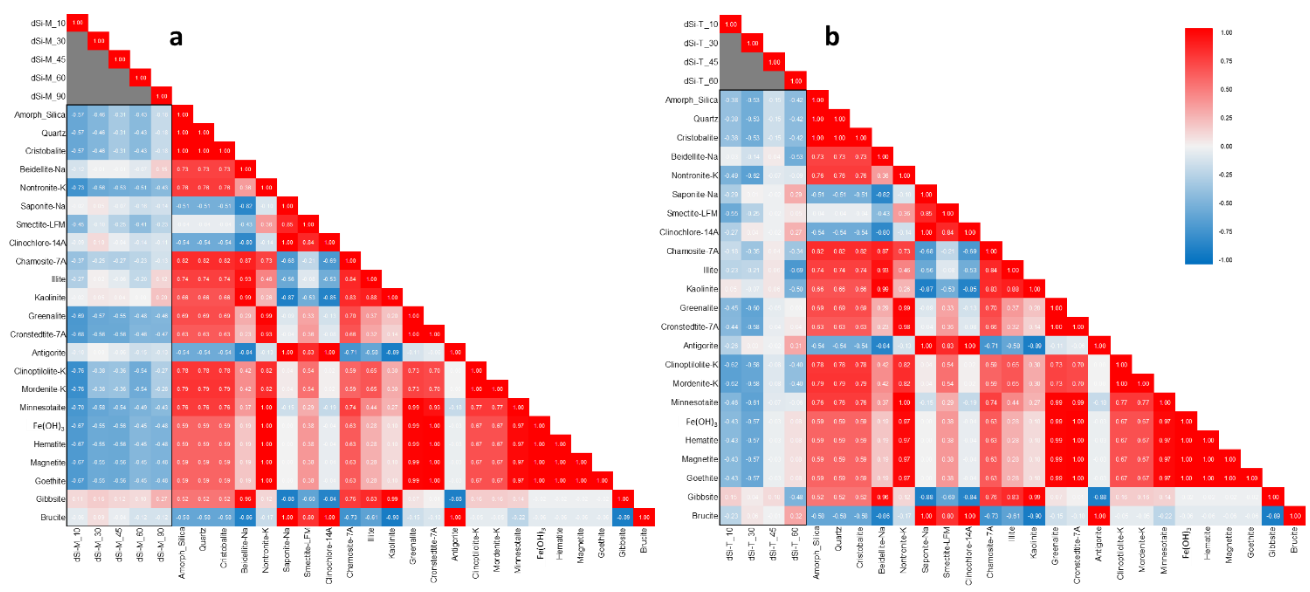

Figure 2: Correlation matrix of saturation index of minerals with polymerization behavior of silicic acid (a) and its adsorption on the surface of silica gel (b).

Figure 2a and 2b show that the saturation index of many minerals is correlated to the polymerization and adsorption rate of silicic acid, respectively. This includes silica minerals (amorphous silica, quartz, and cristobalite), iron-silicates (nontronite, greenalite, cronstedtite, and minnesotaite), alumino-silicates (clinoptilolite and mordenite), and iron oxides ($Fe(OH)_3$, hematite, magnetite, and goethite).

3.2 Factor Analysis

Factor analysis was carried out to examine the degree of influence or impact that each input parameter has on the polymerization rate and adsorption rate of silicic acid (output parameters). In this study, a Partial Derivative (PaD) method was used to calculate the contribution of each input parameter (Gevrey et al., 2003). Result of the factor analysis can be seen in Figure 3.

Total concentration of silicic acid and iron affect the rate of polymerization more strongly than other input parameters. Si-T concentration at initial condition contributes -7.72% and Fe-T concentration contributes -7.56% (Figure 3a). This implies that higher concentrations of Si-T and Fe-T at initial stage causes faster decrease in the Si-M concentration, i.e., faster polymerization rate. This is in accordance with the previous studies that demonstrates the importance of Fe in the polymerization of silicic acid and formation of silica scale (Manceau et al., 1995; Pokrovski et al., 2003; Juhri et al., 2022). Furthermore, concentrations of Ca, Mg, and SO_4 at initial condition also significantly contribute to the polymerization of silicic acid (-3.70%, -2.75%, and -2.61%, respectively). Among the minerals considered in this study, goethite (FeOOH) shows the highest contribution (-2.56%) followed by cronstedtite ($Fe^{2+}{}_2Fe^{3+}{}_2SiO_5(OH)_4$) (-2.10%), quartz ($SiO_2$) (-2.09%), and brucite ($Mg(OH)_2$) (-2.00%). On the contrary, K concentration at initial stage gives the most adverse effect on the polymerization of silicic acid as it has 6.42% contribution, significantly higher than the rest of input parameters. Saturation index of beidellite and illite also strongly prohibit the polymerization of silicic acid with high positive contribution of 2.28% and 2.17%, respectively. Other input parameters such as Al-T, pH, and amorphous silica show mild negative and positive contributions at the same time.

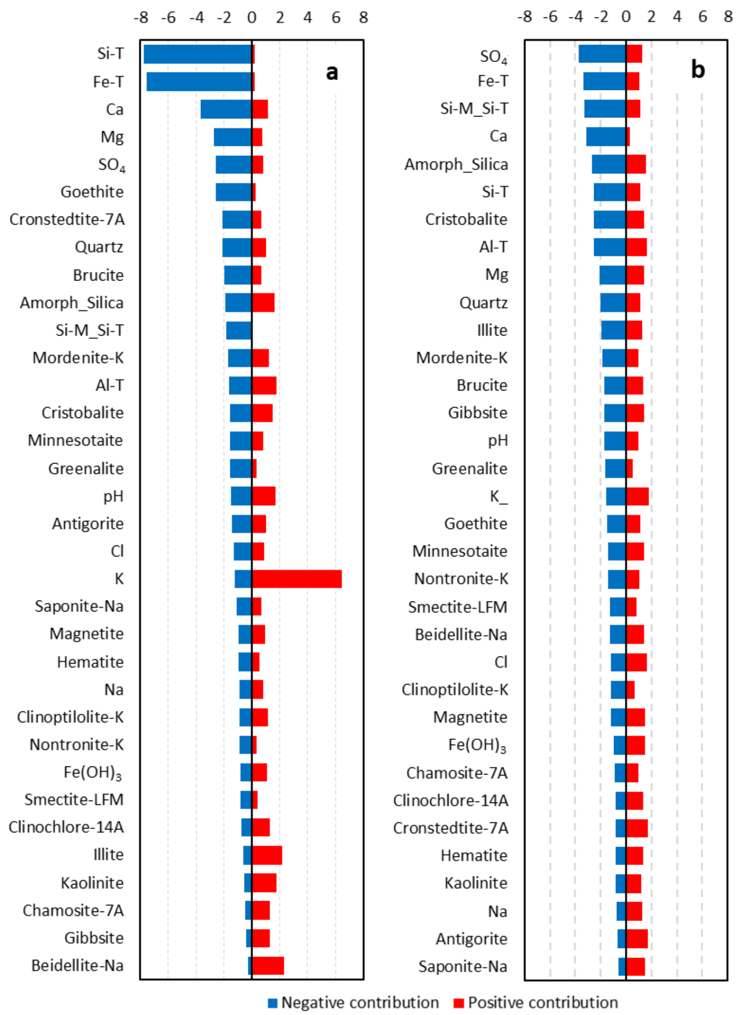

Figure 3: Contribution factor of input parameters (major characteristics of geothermal water and saturation index of minerals) to the polymerization of silicic acid (a) and its adsorption on the surface of silica gel (b).

As seen in Figure 3b, concentration of SO_4 at initial condition contribute the most to the adsorption of silicic acid (-3.72%). Furthermore, Fe-T concentration, ratio of Si-M/Si-T, and Ca concentration also give fair contribution of -3.37%, -3.31%, and -3.11% respectively. However, factor analysis result suggests that many input parameters have similar negative contribution value. In general, saturation index of silica minerals (amorphous silica, cristobalite, and quartz) contributed the most to the adsorption of silicic acid. Similarly, many input parameters also give fair positive contribution. Concentrations of K (1.79%), Al-T (1.64%), and Cl (1.61%); and saturation index of antigorite (1.72%), cronstedtite (1.69%), and amorphous silica (1.59%), are among the most positively contributing input parameters, implying that they adversely affect the adsorption rate of silicic acid on the surface of silica gel.

3.3 Prediction

3.3.1 Polymerization rate of silicic acid

Figure 4 shows the result of prediction of polymerization behavior based on 3 geothermal waters using 3 different approaches (Table 2). The first model (Model A) was built using all the input parameters which consists of 34 variables (11 major characteristics and 23 saturation index of minerals). In general, Model A is categorized as a good model as the overall RMSE(%) value is 10.5. Specifically, the model predicted the polymerization behavior of geothermal water 1 (low pH, intermediate salinity and Si content) more accurately than geothermal water 2 and 3. The second model (Model B) was built based on the variables that are strongly correlated to the polymerization rate (16 variables). The overall accuracy was worse than Model A, with RMSE(%) value of 15.7. Model B actually predicted the polymerization behavior of geothermal water 1 and 2 (neutral pH pH, intermediate salinity and Si content) better than Model A, but much worse in predicting the polymerization behavior of geothermal water 3 (neutral pH, high salinity and Si content). Finally, Model C was built based on selected variables whose contribution value are higher than the average. Overall, the RMSE(%) value of this model is only slightly higher than that of Model A. This model accurately predicted the polymerization behavior of geothermal water 1 and 2 but overestimated the polymerization rate of geothermal water 3.

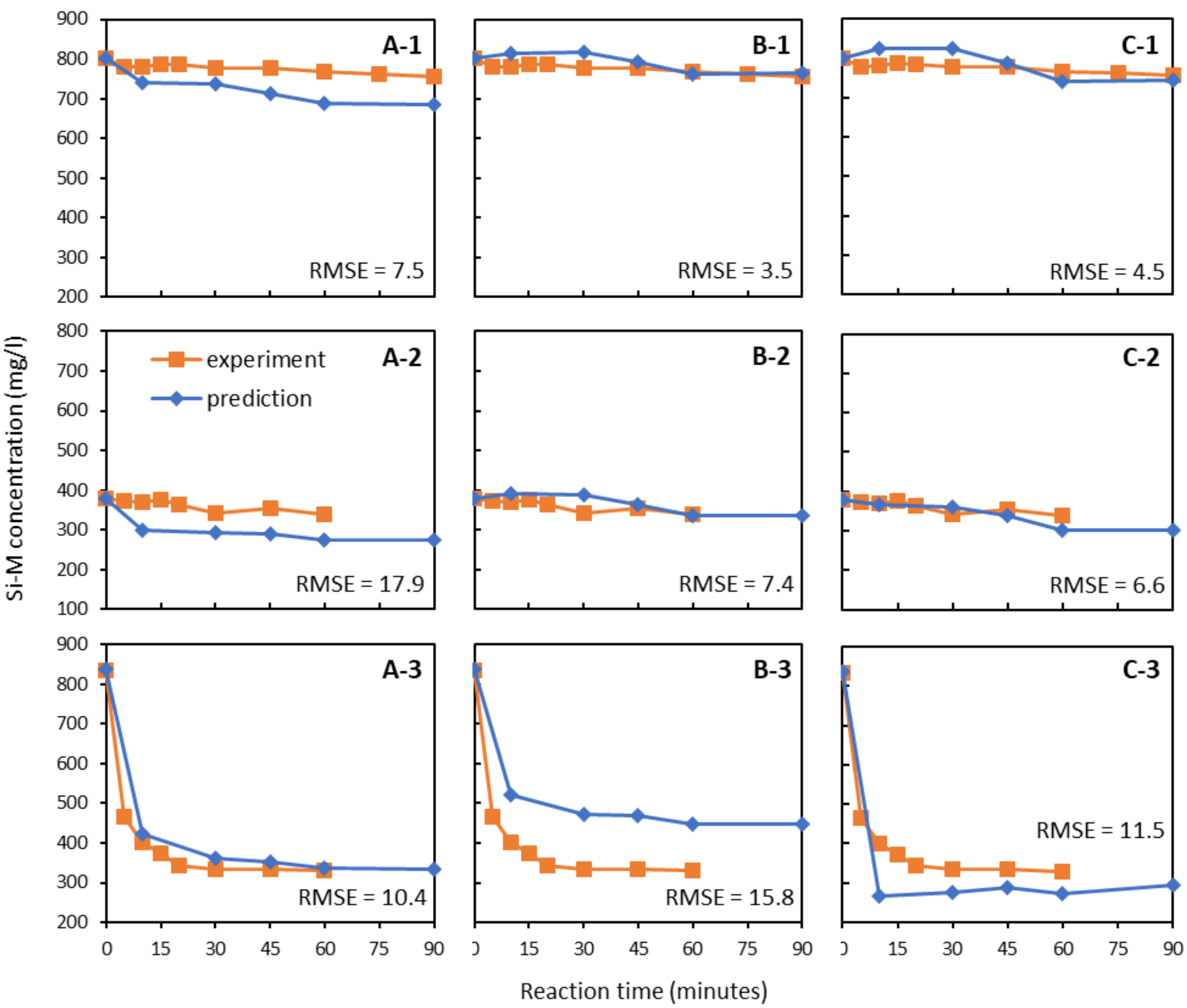

Figure 4: Change in the concentration of monosilicic acid (Si-M) during on-site polymerization experiments and its prediction by AI models with all major characteristics and saturation index of minerals as input (A), selected input based on correlation matrix (B), and selected input based on contribution factor (C).

Table 2: Detail of models used for the prediction of polymerization rate of silicic acid.

	Model A	Model B	Model C
Input parameters	All major characteristics (34 variables) of geothermal water and saturation index of minerals	Only parameters (16 variables) that have correlation value of >|0.50|.	Only parameters (23 variables) that have contribution value higher than the average
RMSE(%)	10.5	15.7	10.8

3.3.1 Adsorption rate of silicic acid on the surface of silica gel

Figure 5 shows the result of prediction of adsorption behavior of silicic acid in 3 geothermal waters on the surface of silica gel using 3 different approaches (Table 3). The first model (Model A) was built using all the input parameters. In general, Model A gave an excellent accuracy in predicting the adsorption behavior of geothermal water 1 and 3 with RMSE(%) value of 2.9 and 2.5, respectively. Prediction for geothermal water 2 was the least accurate with RMSE value of 4.8%. Model B was built with fewer input parameters (16 variables) selected based on the correlation of the input parameters to the output (Figure 1 and 2). Model B generally gave a more accurate prediction (RMSE = 3.2%), specifically for geothermal water 1 and 3. However, it gave a less accurate for geothermal water 2. Model C was also built from fewer input parameters (27 variables) selected based on AI's contribution factor analysis (Figure 3). Model C generally gave the most accurate prediction of the adsorption behavior of silicic acid in 3 geothermal waters. Model C gave a more accurate prediction for geothermal water 2 and 3 than Model A and B, but slightly less accurate prediction than Model B for geothermal water 1.

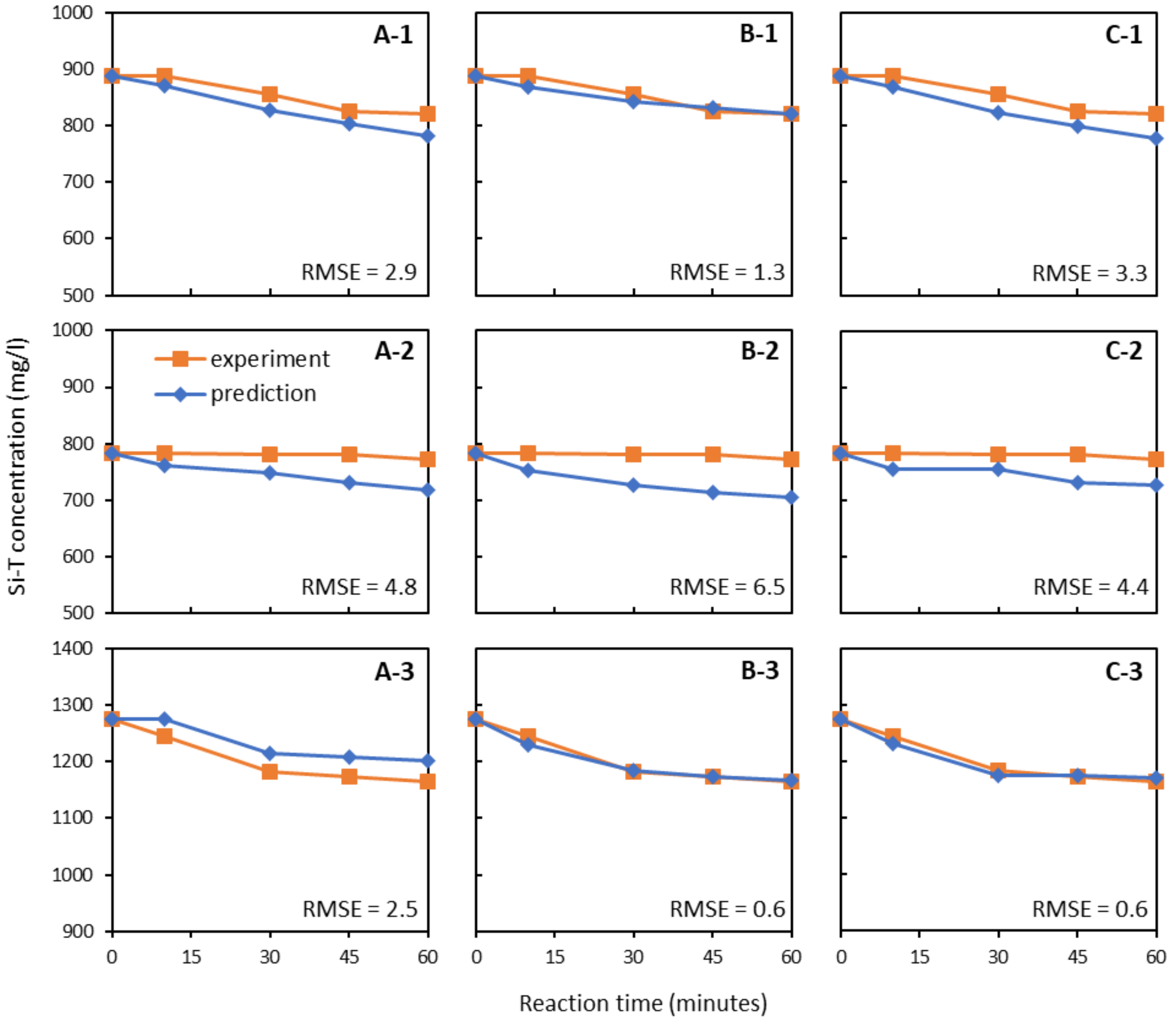

Figure 5: Change in the total concentration of silicic acid (Si-M) during on-site adsorption experiments and its prediction by AI models with all major characteristics and saturation index of minerals as input (A), selected input based on correlation matrix (B), and selected input based on contribution factor (C).

Table 3: Detail of models used for the prediction of adsorption rate of silicic acid.

	Model A	Model B	Model C
Input parameters	All major characteristics (34 variables) of geothermal water and saturation index of minerals	Only parameters (16 variables) that have correlation value of >|0.50|.	Only parameters (27 variables) that have contribution value higher than the average
RMSE(%)	3.3	3.2	2.7

4. CONCLUSIONS AND IMPLICATIONS

This study provides a preliminary result of AI modelling for polymerization and adsorption behavior of silicic acid, as well as proposes its AI modelling procedure. Polymerization rate of silicic acid and its adsorption on the surface of silica gel were strongly correlated to the Fe-T despite its low concentration. Contribution factor analysis also showed that Fe-T was among the most contributing variables to the polymerization and adsorption rate of silicic acid, along with Si-T and SO_4 concentrations. The AI models for the prediction of the polymerization of silicic acid were considered good models based on their RMSE(%) values. Moreover, the AI models for the prediction of adsorption behavior of silicic acid on the surface of silica gel were considered excellent.

This study is a steppingstone towards the prediction of silica scale formation rate and prevention of its initiation. Further, the established AI models should be examined with more physicochemical data of geothermal water and more experimental data of kinetic behavior of polymerization and adsorption of silicic acid. Finally, the kinetic model will be integrated with the empirical data of formation rate of silica scale through metal plate immersion experiments to construct an AI system for the prediction of the deposition rate of silica scale. The system is expected to greatly contribute to the effective utilization of geothermal energy through the mitigation of scaling problem.

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