

# Estimation of the Silica Solubility in the Superheated Steam Using LSSVM Modeling Approach

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*The presence of silica (SiO<sub>2</sub>) in boiler water causes precipitation and creates hard silicate scale on steam turbine blades. This study assessed the ability of least squares support vector machines (LSSVM) modeling approaches to estimate the solubility of SiO<sub>2</sub> in the steam of boilers. A genetic algorithm (GA) and population-based stochastic search algorithms were employed to identify the optimal LSSVM method variables. Results indicate that the GA-LSSVM can be used to model the complicated nonlinear relationship between the input and output variables. To predict the solubility of SiO<sub>2</sub> in the steam of boilers, the GA-LSSVM model generated the mean absolute error (MAE) and the coefficient of determination (R<sup>2</sup>) values of 1.8831 and 0.9997, respectively, for the entire data set. The proposed model provides a distinctly promising approach to estimating the solubility of SiO<sub>2</sub> in the steam of boilers. © 2015 American Institute of Chemical Engineers Environ Prog, 35: 596–602, 2016*

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## INTRODUCTION

Depending upon amounts of mill scale and iron oxide to be removed in conjunction with the operating pressure, boilers commonly undergo an alkaline boil-out, followed by acid cleaning if required. Carryover is often caused by a faulty boiler water condition. The purity of steam, as outlined in the design specification (with consideration of total solids in the boiler water), should be taken into consideration when designing and operating boilers [1–5].

The maximum total dissolved solids in boiler water at which the required steam purity can be obtained, should be declared by the boiler manufacturer [5–10]. The silica (SiO<sub>2</sub>) concentration of boiler water is a very important parameter for both steam turbine boilers. Several SiO<sub>2</sub> compounds have been found in various studies of turbine blade deposition. Among them, amorphous SiO<sub>2</sub> is the most common [11–15]. SiO<sub>2</sub> deposition increases the thermal resistance, which can lead to tube failure in the boilers [11–24].

Recently, Ahmadi and colleagues made many attempts to apply different intelligent based methods to solve various upstream challenging problems [25–36]. For example, Ahmadi *et al.*, employed a machine learning based approach to predict the permeability of oil reservoir [35].

In this article, a machine learning method using a new type of network modelling named least squares support vector machine (LSSVM) was developed to prepare a robust and rapid predictive model for monitoring the SiO<sub>2</sub> solubility in the steam of boilers. The proposed LSSVM model was developed implementing the actual SiO<sub>2</sub> solubility in the steam of boilers.

To demonstrate the efficiency, generalization and reliability of the LSSVM method suggested in this paper, the LSSVM results were compared with the relevant, actual SiO<sub>2</sub> solubility in the steam of boilers. The outcomes from this study showed that the LSSVM model can predict the SiO<sub>2</sub> solubility in the steam of boilers with high accuracy. When lacking suitable experimental and/or actual data, the predictive model introduced is an efficient way to estimate the SiO<sub>2</sub> solubility in the steam of boilers, especially in the initial design or development stages.

## THEORY

### LSSVM and GA

Vapnik and co-workers developed an effective method called the support vector machine (SVM) at AT&T Bell Laboratories in 1995 [30,35–37]. This approach merged the benefits of ANNs (treatment of large amounts of extremely nonlinear data) and nonlinear regression, leading to the sparseness of the outcome and high generalization aptitude [25,26,30,38]. Furthermore, this particular type of machine learning method is superior to conventional intelligent methods (like ANN) because of: avoidance of determining the number of hidden neurons, containing fewer optimizing parameters, and less Over-fitting complications than ANN methods. The SVM is mainly appropriate for regression and classification issues [25,26,30,37]. The SVM method may be

computationally challenging, as it requires the answer of quadratic programming (QP) [25,26,30,39].

Suykens and Vandewalle [25,26,30,40] recommended an improved form of SVM called LSSVM, leading to the discovery of a group of linear calculations that are more user-friendly than QP problems. However, most of the key advantages of SVM are reserved [25,26,30,38]. The structure of LSSVM is explained concisely as follows:

We assume training group with  $N$  data points  $\{x_k, y_k\}_{k=1}^N$ , where  $x_k \in \mathcal{R}^n$  stands for the input vector at the training point,  $k$ , and  $y_k \in \mathcal{R}$  is the relevant magnitude of the target. Based on the concept of LSSVM, introduced by Suykens [25,26,30,40], the unknown nonlinear function can be approximated by

$$y(x) = \sum_{k=1}^N \alpha_k K(x, x_k) + b \quad (1)$$

$K(x, x_k)$  represents the kernel function meeting the Mercer condition [25,26,30,40], and parameters  $\alpha_k \in \mathcal{R}$  ( $k=1, 2, \dots, N$ ) and  $b$  can be acquired using the following equation [25,26,30,40]:

$$\begin{bmatrix} 0 & 1_v^T \\ 1_v & \Omega + \gamma^{-1}I \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ y \end{bmatrix} \quad (2)$$

where  $y = [y_1 \dots y_N]^T$ ,  $1_v = [1 \dots 1]^T$ ,  $\alpha = [\alpha_1 \dots \alpha_N]^T$ ,  $I$  stands for an identity matrix and  $\Omega$  is a  $N \times N$  kernel matrix;  $\Omega_{kl} = \varphi(x_k)^T \cdot \varphi(x_l) = K(x_k, x_l) \forall k, l = 1, \dots, N$ . The conventional types of the kernel function are as follow [25,26,30,40]:

$$K(x, x_k) = x_k^T x \quad (\text{Linear kernel}) \quad (3)$$

$$K(x, x_k) = (\tau + x_k^T x)^d \quad (\text{Polynomial kernel of degree } d) \quad (4)$$

$$K(x, x_k) = \exp(-x - x_k^2 / \sigma^2) \quad (\text{Radial basis function RBF kernel}) \quad (5)$$

When considering a RBF kernel function, the generalization efficiency and performance of the LSSVM is affected by two regulating variables comprising the regularization variable ( $\gamma$ ) and the RBF kernel variable ( $\sigma^2$ ). As explained by Ahmadi and colleagues [25,26,30,41], the implementation of nonpopulation-based optimization methods are not suitable choices in such conditions because of the high nonlinearity of the SVM approach. Consequently, a genetic algorithm (GA) as a robust and well-known optimization method was employed to optimize these two parameters.

GA is a population-based stochastic general search tool based on the mechanism of natural selection and natural genetics [25,26,30,42,43]. This method performs in an iterative way by creating new populations of chromosomes from the previous ones.

At every stage, the GA chooses chromosomes chaotically from the existing population to be parents and uses them to generate the offspring for the further peers. Upon consecutive generations, the offspring "develops" in the direction of an optimal answer. The GA employs three key forms of operators at every stage to produce the further offspring from the existing offspring comprising selection, crossover and mutation [25,26,30,44].

The descriptions of the GA method are explicated in the literature [25,26,30,36,45,46]. In addition, the concept of LSSVM is explained in Refs. 25,26,30,47–49.

## METHODOLOGY

### GA-LSSVM Model

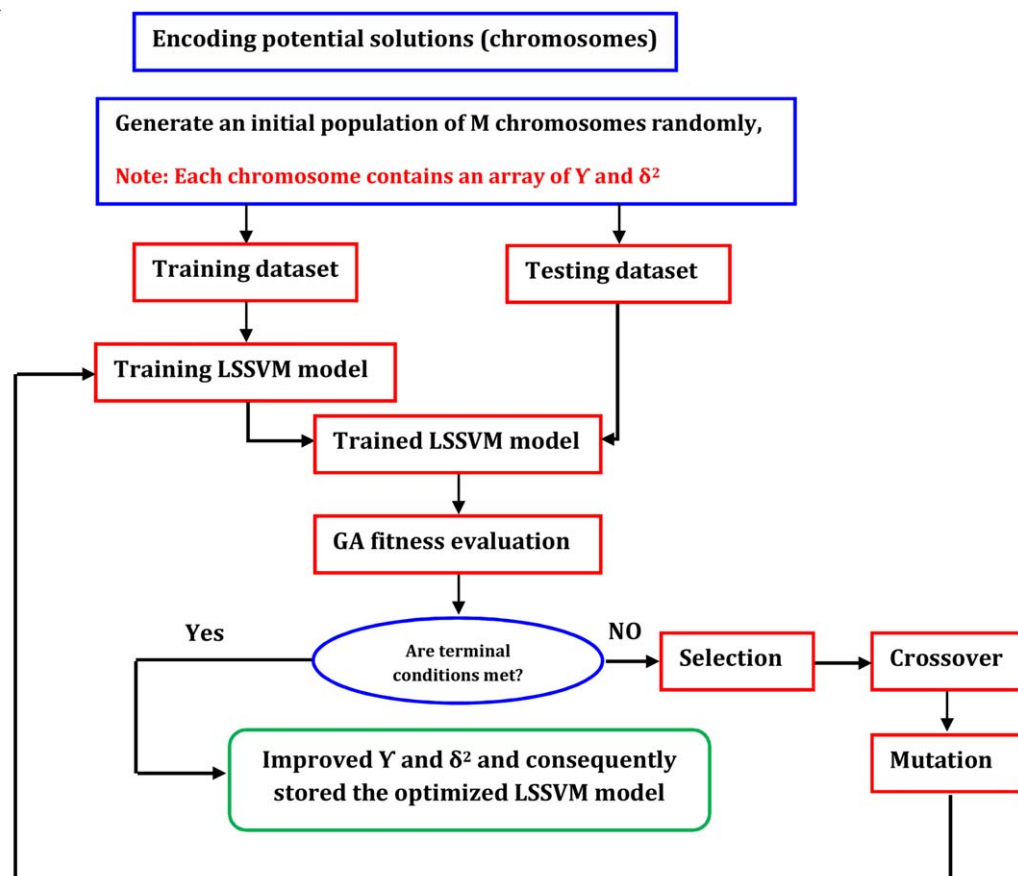
An efficient GA-LSSVM tool was employed to estimate the solubility of SiO<sub>2</sub> in steam of boilers as a function of the water SiO<sub>2</sub> content and pressure. To gain the generalized LSSVM tool, two adjustable variables need to be optimized, comprising the regularization variable  $\gamma$  and the kernel variable conforming to the kernel type.

Specifying a suitable regularization parameter  $\gamma$ , the kernel function and the subsequent kernel variable is essential, and is generally calculated by the comprehended usage type [50]. The RBF kernel is often used in nonlinear function prediction and nonlinear modeling issues [47]. The RBF kernel is an applicable option for kernel function because of the outstanding overall efficiency and fewer variables of the RBF kernel compared to the other kernel functions [51,52].

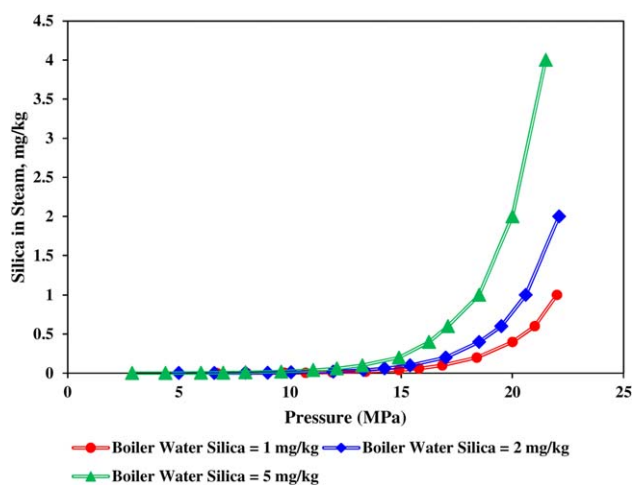
GA was employed as an efficient search strategy to make a suitable choice for the regularization and RBF kernel variables ( $\gamma$  and  $\sigma^2$ ). Figure 1 presents a box-chart of GA-LSSVM for optimizing  $\gamma$  and  $\sigma^2$ .

The following items present a thorough explanation of the LSSVM modeling process.

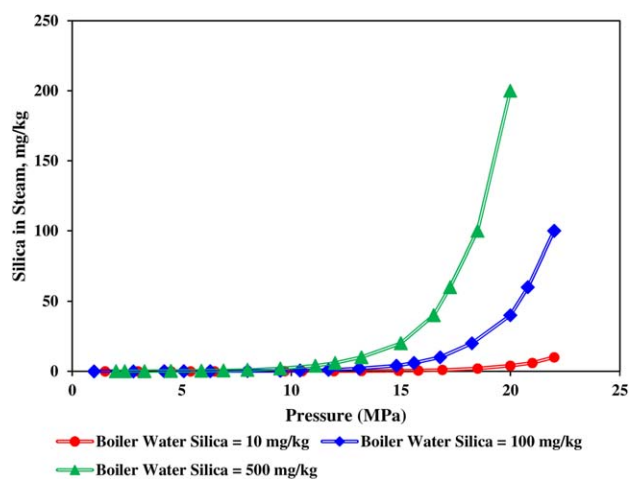
1. Splitting all data samples into training (80%) and testing (20%) groups. The training group is used to evolve the LSSVM method, and the testing group is used to validate the LSSVM approach. It should be noted that the testing data bank was not previously used in optimization of LSSVM approach. In other words, testing data bank was completely different from training data bank employed for optimizing adjustable LSSVM parameters.
2. Training the LSSVM approach with the training data points and the initial variable combination ( $\gamma$  and  $\sigma^2$ ). The optimal variable combination ( $\gamma$  and  $\sigma^2$ ) is examined using the GA method. The stages of a GA for modifying the variables of the suggested LSSVM are described as follows:
  - i. GA begins with a set of random candidate solutions (represented by chromosomes) called a population. Each chromosome contains an array of these two parameters ( $\gamma$  and  $\sigma^2$ ). Therefore, every parameter that needs to be optimized is denoted as a gene.
  - ii. Assess the fitness of each chromosome in the population using a fitness function.
  - iii. According to their appointed fitness magnitudes, some chromosomes in the existing offspring are chosen to be a portion of the population assessed throughout the subsequent creation. The chosen chromosomes are used to create fresh offspring via GA operators (mutation and crossover) to assemble the population for further creation.
  - iv. Crossover stands for the progression of taking two parent answers and generating a population from them. After the selection process, the offspring is developed with improved chromosomes.
  - v. The mutation stands for the progression of chaotically altering the magnitudes of genes throughout an offspring. The chief aim of a mutation is to present fresh genetic matter into the offspring, which would enhance the genetic variety. The mutation avoids the GA from being stuck in a local optimum.
  - vi. Employ a freshly created offspring (new parameter combination) for the next run of the approach.
  - vii. This process is repeated until some stopping criteria (e.g. when an acceptable answer is specified or the



**Figure 1.** Flow chart of the LSSVM parameters selection based on GA. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]



**Figure 2.**  $\text{SiO}_2$  solubility in the steam of boilers as a function of pressure for a water  $\text{SiO}_2$  content less than 10 mg/kg [12]. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]



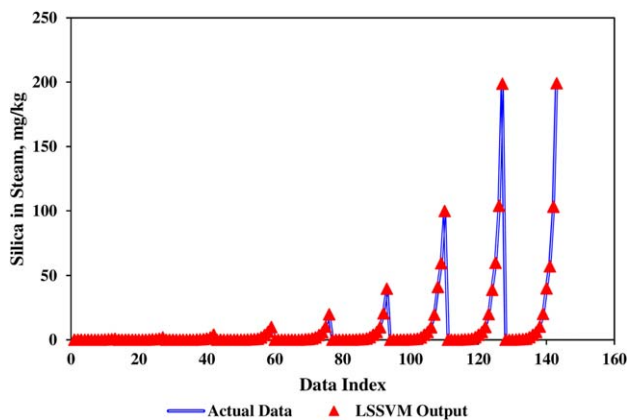
**Figure 3.**  $\text{SiO}_2$  solubility in the steam of boilers versus pressure for a water  $\text{SiO}_2$  content greater than 10 mg/kg [12]. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

number of generations that the GA is allowed to execute) are fulfilled.

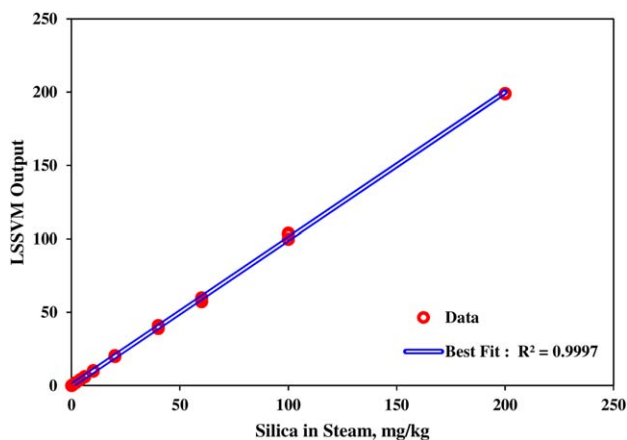
3. Implementing the optimal variable combination, i.e.  $\gamma$  and  $\sigma^2$ , to assemble the LSSVM approach. Inputting the testing data group into the LSSVM approach gaining the

prediction values. The accuracy of the LSSVM model estimated ability can be verified by the test.

The optimal LSSVM parameters of  $\gamma=130765442292.5722$  and  $\sigma^2=25.80639327532004$  for the estimated solubility of  $\text{SiO}_2$  in the steam of boilers were obtained  $\text{SiO}_2$ .



**Figure 4.** Actual versus predicted SiO<sub>2</sub> solubility in the steam of boilers based on the GA-LSSVM technique. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]



**Figure 5.** Plot of GA-LSSVM predicted against the experimental SiO<sub>2</sub> solubility in the steam of boilers. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

## RESULTS AND DISCUSSIONS

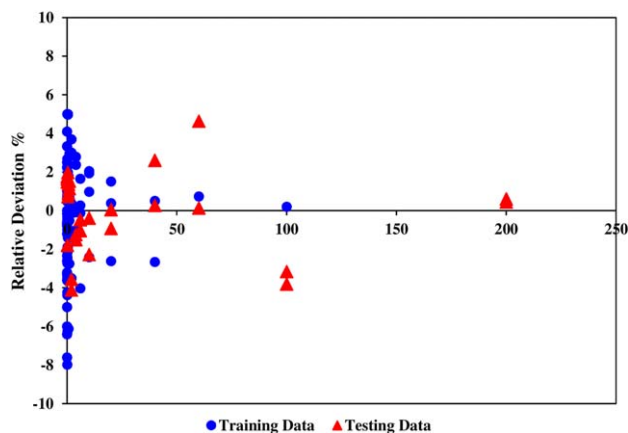
An efficient machine learning method, i.e., GA-LSSVM was employed to assemble the predictive method for estimating the SiO<sub>2</sub> solubility in the steam of boilers.

The real behavior of the SiO<sub>2</sub> solubility in the steam of boilers versus the corresponding pressure when SiO<sub>2</sub> content lower than 10 mg/kg was demonstrated in Figure 2. Furthermore, Figure 3 shows the real trend of the solubility of SiO<sub>2</sub> in the steam of boilers versus the corresponding pressure for the SiO<sub>2</sub> content greater than 10 mg/kg.

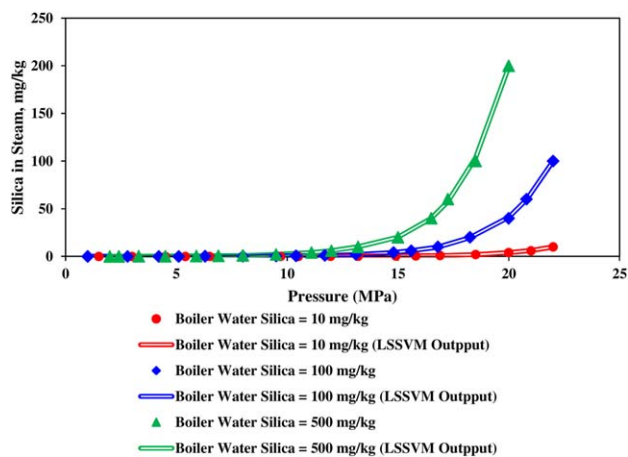
The predicted SiO<sub>2</sub> solubility in the steam of boilers and the equivalent measured data were compared to assess the estimation accuracy of the GA-LSSVM tool (Figure 4). As depicted in Figure 4, there is no considerable difference between the estimated and measured solubility of SiO<sub>2</sub> in steam of boilers.

The regression plot for the whole data samples accompanied by the coefficient of determination ( $R^2$ ) and its linear fitting correlation for the SiO<sub>2</sub> solubility in the steam of boilers (see Figure 5) are presented.

In Figure 5, the blue line characterizes the finest fit linear regression line between the model outputs and measured data. The  $R^2$  magnitude indicates the correlation between the



**Figure 6.** Relative deviations between the experimental and predicted SiO<sub>2</sub> solubility in the steam of boilers during the training and testing process based on the GA-LSSVM technique. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]



**Figure 7.** Comparison of estimated and measured SiO<sub>2</sub> solubility in the steam of boilers versus pressure for water SiO<sub>2</sub> contents greater than 10 mg/kg [12]. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

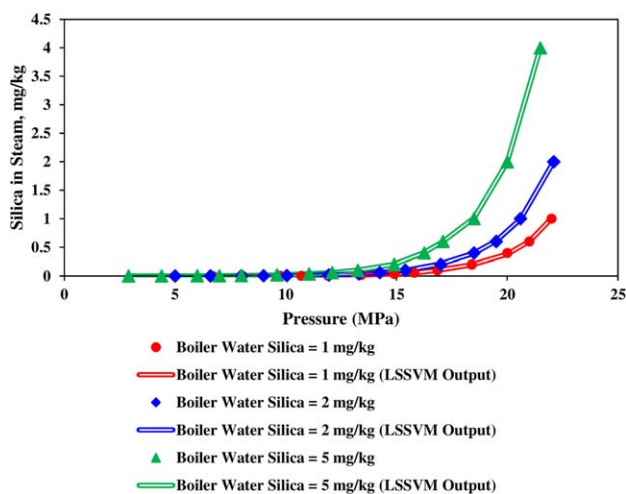
GA-LSSVM outcomes and measured data.  $R^2 \approx 1$  reveals a perfect linear correlation between the GA-LSSVM results and actual values. On the other hand,  $R^2 \approx 0$  reveals that no linear correlation between the GA-LSSVM results and measured data.  $R^2$  is calculated via the below formula:

$$R^2 = 1 - \frac{\sum_{i=1}^N (y_i^{\text{exp}} - y_i^{\text{pre}})^2}{\sum_{i=1}^N (y_i^{\text{exp}} - \bar{y}^{\text{exp}})^2} \quad (6)$$

where  $N$  is the whole number of data samples included,  $y_i^{\text{exp}}$  is the measured data at the sampling point  $i$ ,  $y_i^{\text{pre}}$  is the  $i$ th target of the correlation, and  $\bar{y}^{\text{exp}}$  and  $\bar{y}^{\text{pre}}$  are the average of the measured and estimated data.

As illustrated in Figure 5, the outputs of GA-LSSVM matched the measured values quite fine, and the  $R^2$  values were greater than 0.99 in all stages including testing and





**Figure 8.** Comparison of the estimated and measured SiO<sub>2</sub> solubility in the steam of boilers versus pressure water silica content lower than 10 mg/kg [12]. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

**Table 1.** Performance of the GA-LSSVM model in terms of the statistical criteria for predicting the SiO<sub>2</sub> solubility in the steam of boilers.

	GA-LSSVM		
	Training	Testing	Overall
MSE	0.0176	1.2734	0.2635
R <sup>2</sup>	0.9999	0.9996	0.9997
MAE	1.9454	1.6270	1.8831

training. Eq. (7) represents the linear regression formula for the whole samples employed for testing and training the GA-LSSVM tool, as following as

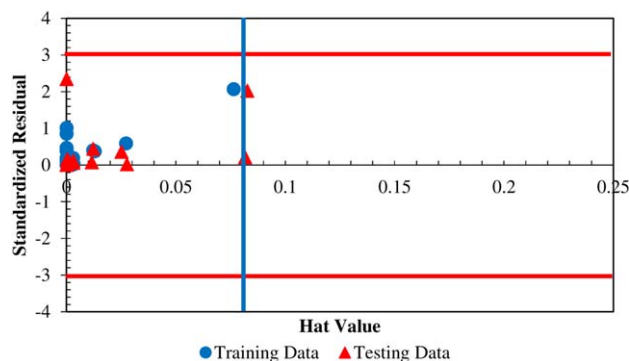
$$y = 1.0004x + 0.0087; R^2=0.9997 \quad (7)$$

The slope of the above linear equation and infinitesimal value of intercept reveals that the GA-LSSVM approach estimates the real solubility of SiO<sub>2</sub> in the steam of boilers with high accuracy.

Figure 6 depicts a scheme of the experimental data and relative error % between the measured and estimated values ( $\text{relative deviation \%} = \frac{\text{actual}-\text{predicted}}{\text{actual}} \times 100$ ) throughout the training and testing progression for the solubility of SiO<sub>2</sub> in the steam of boilers. The relative error % between the recorded and GA-LSSVM estimated values were in the range of  $\pm 6\%$  for most of the data sets (see Figure 6).

All the predicted points were within the region enclosed by  $\pm 8\%$ . The relative error % between the real and GA-LSSVM estimated SiO<sub>2</sub> solubility in the steam of boilers varies between  $-8\%$  to  $+8\%$  for whole samples (see Figure 6). The relative error % of the GA-LSSVM outcomes from the real solubility of SiO<sub>2</sub> in the steam of boilers values varies between  $-7.95\%$  to  $5.00\%$ , and the absolute average relative error was 1.8831%

Figures 7 and 8 compare the outputs gained from the GA-LSSVM approach and SiO<sub>2</sub> solubility in the steam of boilers versus the relevant pressure for the different water SiO<sub>2</sub>



**Figure 9.** Detection of the probable doubtful measured SiO<sub>2</sub> solubility in steam of boilers [12] and the applicability domain of the suggested approach for the SiO<sub>2</sub> solubility in steam boilers analysis. [Color figure can be viewed in the online issue, which is available at [wileyonlinelibrary.com](http://wileyonlinelibrary.com).]

content. As shown in Figure 7, the results gained from the GA-LSSVM approach lie on the actual data samples when the water SiO<sub>2</sub> content is over 10 mg/kg with an acceptable accuracy. Moreover, Figure 8 shows the satisfactory agreement and accuracy of the predictive method for estimating the solubility of SiO<sub>2</sub> in the steam of boilers for water SiO<sub>2</sub> contents lower than 10 mg/kg.

The testing and training outputs obtained from the suggested approach for solubility of SiO<sub>2</sub> in the steam of boilers estimations were used to compute the various statistical certification indices, such as the mean absolute error (MAE), mean squared error (MSE), and correlation coefficient (*R*). The selected evaluation indexes are written as follows:

$$R = \frac{\sum_{i=1}^N (y_i^{\text{exp}} - \overline{y^{\text{exp}}})(y_i^{\text{pre}} - \overline{y^{\text{pre}}})}{\sqrt{\sum_{i=1}^N (y_i^{\text{exp}} - \overline{y^{\text{exp}}})^2 \sum_{i=1}^N (y_i^{\text{pre}} - \overline{y^{\text{pre}}})^2}} \quad (8)$$

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i^{\text{exp}} - y_i^{\text{pre}})^2 \quad (9)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |y_i^{\text{exp}} - y_i^{\text{pre}}| \quad (10)$$

Table 1 lists the statistical indices for the accuracy of the model in estimating the solubility of SiO<sub>2</sub> in the steam of boilers. The GA-LSSVM model for estimating the solubility of SiO<sub>2</sub> in the steam of boilers generated acceptable outputs in terms of the statistical evaluation indices.

The outcomes of GA-LSSVM model are reasonable and highlight the reliability of the GA-LSSVM tool for estimating the solubility of SiO<sub>2</sub> in the steam of boilers. The values of  $R^2 \approx 1$  and the low MSE and MAE by the model for both the testing and training groups highlighted the good generalization ability and estimation power of the proposed approach.

Determining the outlier of the predictive models has a significant importance in the reliability of the aforementioned tools in the given problem. Assessing the data for the SiO<sub>2</sub> solubility in steam boilers is essential, because uncertainties disturb the estimation ability of the evolved approach. The Leverage Value Statistics approach was carried out to achieve this goal [53–55]. A full description of the computational procedure and mathematical backgrounds of this method is reported in Refs. 53–55. Figure 9 presents the Williams plot for the GA-LSSVM outcomes. The existence of the majority of data samples in the ranges,  $0 \leq H \leq 0.078 - 3 \leq R \leq 3$ , shows that the GA-LSSVM approach is statistically valid and correct. In addition, it reveals

that the entire data throughout the databank are positioned within the acceptable areas of the employed approach.

#### CONCLUSION

This study examined predictive and generalization competence of the GA-LSSVM model for the solubility of SiO<sub>2</sub> in the steam of boilers at various ranges of water SiO<sub>2</sub> contents and pressures by employing an accurate data set comprising various samples gathered from previous experimental studies [22]. The water SiO<sub>2</sub> content and pressure were used as the predictor variables, whereas the solubility of SiO<sub>2</sub> in the steam of boilers was considered to be dependent variables.

All the outputs produced through the GA-LSSVM approach reveal the brilliant ability of the aforementioned method in estimating the solubility of SiO<sub>2</sub> in the steam of boilers in comparison with those demonstrated elsewhere. Furthermore, these outcomes were verified via various statistical indexes employed to evaluate the reliability of methods.

Overall, the GA-LSSVM method employed in this study displays a sound ability in estimating the solubility of SiO<sub>2</sub> in the steam of boilers under different circumstances. This can be particularly useful when designing facilities for steam boilers owing to their remarkable characteristics including user friendly environment, robustness and generalization.

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