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A novel modeling approach to optimize oxygen-steam ratios in coal gasification process



Milad Arabloo ^{a,1}, Alireza Bahadori ^{b,*}, Mohammad M. Ghiasi ^c, Moonyong Lee ^d, Ali Abbas ^e, Sohrab Zendehboudi ^f

- ^a Young Researchers and Elites Club, North Tehran Branch, Islamic Azad University, Tehran, Iran
- ^b Southern Cross University, School of Environment, Science and Engineering, Lismore, NSW, Australia
- ^c National Iranian Gas Company (NIGC), South Pars Gas Complex (SPGC), Asaluyeh, Iran
- ^d School of Chemical Engineering, Yeungnam University, Gyeungsan, Republic of Korea
- ^e School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, NSW, Australia
- f Department of Chemical Engineering, Massachusetts Institute of Technology (MIT), Cambridge, MA, USA

HIGHLIGHTS

- Support Vector Machine Algorithm is used to estimate oxygen-steam ratios in coal gasification process.
- The coupled simulated annealing optimization tool obtains the optimal model parameters.
- The model has been developed and tested using 100 series of the data.
- Excellent agreement between the results of model and reported data is observed.

ARTICLE INFO

Article history: Received 24 November 2013 Received in revised form 11 November 2014 Accepted 19 February 2015 Available online 4 March 2015

Keywords: Coal gasification Oxygen-steam ratio Low carbon emission Support vector machine

ABSTRACT

Coal gasification operation appears to be an essential element in the advanced energy systems, where the reaction between oxygen, steam and coal results in production of syngas (e.g., a mixture of carbon monoxide and hydrogen) under elevated pressure and temperature conditions. An efficient design for gasification process is expected if proper oxygen/steam rations are selected such that a thermal balance is established between the exothermic and endothermic reactions, leading to yield maximization of desired products in most cases. In this article, a rigorous modeling approach using support vector machine (SVM) algorithm is developed to estimate optimum oxygen-steam ratios required to balance the released heat and heat requirement in coal gasification process. An acceptable match between modeling outputs and real data is noticed so that the average absolute error is lower than 1.0%.

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1. Introduction

In coal industry, coal gasification is considered as an important technology to produce a variety of sustainable energy products and electricity with low emissions. The technique has been recognized to generate gas which has many applications in different industrial sectors including chemicals, fuels and chemical intermediates [1–5]. The coal gasification is largely utilized in fuel gas production in partial oxidation and pyrolytic processes in which methane,

The below reactions with contribution of steam, oxygen and carbon clearly describe the chemistry of coal gasification process [8,9]. Ref. No. [10] lists the standard enthalpy change of the reactions at the temperature of 298 K:

Gasification:

$$C + O_2 \rightarrow CO_2 - 393.5 \, kJ$$
 (1)

$$C + H_2O \rightarrow CO + H_2 + 131.3 \, kJ$$
 (2)

$$C + 2H_2O \rightarrow CO_2 + H_2 + 90.2 \,kJ$$
 (3)
 $C + CO_2 \rightarrow 2CO + 172.4 \,kJ$ (4)

Partial oxidation:

$$C + 0.5O_2 \rightarrow CO - 110.5 \,\mathrm{kJ}$$
 (5)

carbon monoxide and hydrogen are the main fuel elements in the product gas [6,7].

^{*} Corresponding author. Tel.: +61 2 6626 9412.

E-mail addresses: milad.arabloo@gmail.com (M. Arabloo), Alireza.bahadori@scu.edu.au (A. Bahadori).

¹ Tel.: +98 9171405706.

Water gas shift:

$$CO + H_2O \rightarrow CO_2 + H_2 - 41.1 \, kJ$$
 (6)

Methanation:

$$2CO + 2H_2 \rightarrow CH_4 + CO_2 - 247.3 \, k$$
 (7)

$$CO + 3H_2 \rightarrow CH_4 + H_2O - 206.1 \, kJ$$
 (8)

$$CO_2 + 4H_2 \rightarrow CH_4 + H_2O - 165\,kJ \eqno(9)$$

$$C + 2H_2 \rightarrow CH_4 - 74.8 \, \text{kJ}$$
 (10)

Theoretically, it is possible to make a thermal balance between endothermic and exothermic reactions for the purpose of design of gasification processes. To attain this goal, the feed rate is an important parameter to be changed [10]. For instance, the amounts of steam and oxygen required for Reactions (2) and (5) are 0.45 and 0.27 mol/mole of carbon, respectively; while the ratio of oxygen to steam is equal to 0.6. Other influential reactions in the process are given as below:

$$C + H_2O \to CO + H_2 + 131.3 \, kJ \tag{11} \label{eq:11}$$

$$1.2C + 0.6O_2 \rightarrow 1.2CO - 131.3 \, k \text{]} \tag{12}$$

Net:
$$2.2C + H_2O + 0.6O_2 \rightarrow 2.2CO + H_2$$
 (13)

It has been proved that a number of reactions take place throughout the coal gasification operation, simultaneously. Hence the process control in terms of operating conditions is not an easy task. However, the maximum amount of desirable products is achievable if the key process variables such as pressure, temperature, oxygen/steam ratio, reaction time, and feed, recycle and product flow rates are carefully selected [11,12]. For example, the process under low temperature, elevated pressure and recycled hydrogen can lead to synthesis of high-energy fuel gas (e.g., methane) in practical cases. [10]. It is worth noting that the oxygen-steam ratio is taken into account as an importation input variable if the target is to optimize a coal gasification process [10].

Based on the importance of input parameters for the coal gasification process, it seems necessary to determine the combined influence of pressure and temperature on oxygen/steam ratio through developing a proper predictive tool. Therefore, an extensive effort was made to find out the relationship between the process conditions and performance and then present an efficient strategy which is useful to properly design coal gasification processes. The high capable technique employed in this study is on the basis of support vector machine (SVM) algorithm that offers accurate and reliable predictions. More discussion on the topic along with systematic statistical analysis are provided in the subsequent sections.

2. Methodology for the development of SVM-based predictive tool

2.1. LSSVM modeling

Based on the machine learning theory, a strong predictive model which is called SVM was developed [13–15]. This strategy has been widely utilized in two important categories; namely, regression analysis and classification [16–20]. It has been proved that artificial neural network (ANN) systems have serious drawbacks, though they can be safely used for a number of cases in science and engineering subjects. Describing one of disadvantages, several parameters such as type of activation function and number of hidden layers and nodes should be carefully chosen to properly model the behavior of a certain process. On the other hand, determination of these network variables is generally obtained through a trial and error procedure which is time-consuming and costly [21–25]. The gradient descent search process to optimize the model's weights and biases may converge to a local minimum solution.

Therefore, global solution is not guaranteed, since there is always the chance of getting stuck in a bad local solution [24–28]. Although it offers satisfactory results in some cases but often tends to over-fit the training data [24,29]. The over-fitting problem is a critical issue that usually leads to poor generalization performance. There are several criteria which may demonstrate the superiority of SVM-based models over the ANN-based methods including: more guaranteed to converge toward the global optimum; no need to identify the network topology in advance; less likely to be over-fitted to the training data; fewer adjustable parameters and acceptable generalization performance [17].

The SVM is a supervised learning technique from the field of machine learning applicable to both regression and classification analysis [14,16,18,20,30–33]. On the other hand, one of the major drawbacks of the SVM is the necessity to solve a large-scale quadratic programming problem [34]. This disadvantage has been overcome by modifying the traditional SVM to the least-squares SVM (LS-SVM), which solves linear equations (linear programming), instead of quadratic programming problems to reduce the complexity of optimization process [13,33,35]. Considering the problem of approximating a given dataset $\{(x_1, y_2), (x_2, y_2), \ldots, (x_N, y_N)\}$ with a nonlinear function:

$$f(x) = \langle w, \Phi(x) \rangle + b \tag{14}$$

where $\langle .,. \rangle$ represents a dot product; $\Phi(x)$ represents the nonlinear function that performs regression; b and w are bias terms and weight vector, respectively. In the LS-SVM, the optimization problem for function estimation is formulated as [34,36]:

$$\min_{w,b,e} J(w,e) = \frac{1}{2} \|w\|^2 + \frac{1}{2} \gamma \sum_{k=1}^{N} e_k^2$$
 (15)

s.t.
$$y_k = e_k + \langle w, \Phi(x_k) \rangle + b$$
 $k = 1, \dots, N$ (16)

where $e_k \in R$ are error variables; and $\gamma \geqslant 0$ is a regularization constant. To solve this optimization problem, Lagrange function is developed as [34,36]:

$$L_{\text{LS-SVM}} = \frac{1}{2} \|w\|^2 + \frac{1}{2} \gamma \sum_{k=1}^{N} e_k^2 - \sum_{k=1}^{N} \alpha_k \{e_k + \langle w, \Phi(x_k) \rangle + b - y_k\}$$
 (17)

where $\alpha_k \in R$ are Lagrange multipliers. The solution of Eq. (17) can be determined by partially differentiating the Lagrange function with respect to w, b, e_k and α_k [34,36]:

$$\begin{cases} \frac{\partial L_{\text{LS-SVM}}}{\partial w} = 0 \to w = \sum_{k=1}^{N} \alpha_k \Phi(x_k) \\ \frac{\partial L_{\text{LS-SVM}}}{\partial b} = 0 \to \sum_{k=1}^{N} \alpha_k = 0 \\ \frac{\partial L_{\text{LS-SVM}}}{\partial e_k} = 0 \to \alpha_k = \gamma e_k \\ \frac{\partial L_{\text{LS-SVM}}}{\partial \alpha_k} = 0 \to \langle w, \Phi(x_k) \rangle + b + e_k - y_k = 0 \end{cases}$$

$$(18)$$

By defining $1_v = [1; \ldots; 1], Y = [y_1; \ldots; y_N], \alpha = [\alpha_1; \ldots; \alpha_N]$ and eliminating w and e, the following linear equations are obtained [34]:

$$\begin{bmatrix} 0 & 1_N^T \\ 1_N & \Omega + \gamma^{-1} I_N \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ Y \end{bmatrix}$$
 (19)

where I_N refers to the $N \times N$ identity matrix and Ω is the kernel matrix that is defined as [34]:

$$\Omega_{lk} = \Phi(x_l)\Phi(x_k) = K(x_l, x_k), \quad l, k = 1, ...N$$
 (20)

There are several kernel functions that can be used here including linear, polynomial, spline, and radial basis functions [37,38]. On

the other hand, radial basis, and polynomial functions are most widely used functions.

$$K(x_k, x_l) = \exp(-\|x_k - x_l\|^2 / \sigma^2)$$
 (21)

$$K(x_k, x_l) = \left(1 + x_k^T x_l/c\right)^d \tag{22}$$

where σ denotes the width of the RBF which controls the regression ability and d is the polynomial degree.

2.2. Data gathering and preprocessing

Experimental data used in this study were collected from literature [10] and reported in Table 1. For modeling purpose, independent variables including temperature and pressure have been selected as input parameters and the value of oxygen-steam ratio was assigned as the target (output) variable. Fig. 1 shows a graphical illustration of variation of the applied oxygen-steam ratio data with temperature and pressure as predicted by the tool.

In the next step the data set was divided into three sub-data sets including the "training set", the "validation set", and the "test set". Generally, the training data are used to develop the network. The second part namely validation set is used for selecting optimal parameters of the LS-SVM model and also to avoid the over-fitting problems. The task of remaining data, i.e., test set, is to evaluate the capability of the trained model [17,39]. This division is commonly performed randomly. For this purpose, 70%, 15%, and 15% of the main data sets are randomly selected for the training, validation, and test sets, respectively.

During the computation, the widely used kernel function, i.e., radial basis function (RBF), has been implemented. It has the following general form [39,40]:

$$K(x_k, x_l) = \exp(-\|x_k - x_l\|^2 / \sigma^2)$$
 (23)

In Eq. (23), σ stands for a decision variable which is obtained throughout the optimization computations [39].

Table 1Statistical description of the applied data [10] for developing predictive models.

Parameter	Min	Max	Average
Temperature (K)	900	1500	1239
Pressure (kPa)	101	4053	2465
Oxygen-steam ratio (m3(n)/kg)	0.7	12.1	7.4

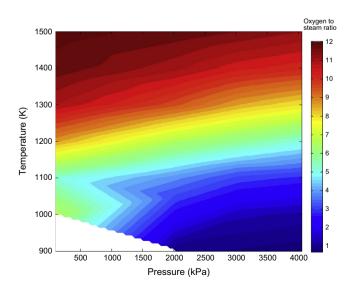


Fig. 1. Graphical illustration of domain of applied data [10] for oxygen-steam ratio modeling.

In this study, Coupled Simulated Annealing (CSA) technique [41] was applied to obtain the optimum values of the σ^2 and γ . Indeed, the CSA enhances the optimization process quality. A group of simulated annealing processes coupled by their acceptance probabilities characterizes the CSA [41]. The simulated annealing processes are parallel to each other. In the CSA technique, each single simulated annealing process has information on the status of all others' costs. The information between single SA processes is shared via an acceptance probability function and coupling term [41]. In the classical SA, a metropolis rule [42] is frequently utilized to determine the acceptance probability of an uphill move; the CSA, in contrast, considers other current solutions along with the solutions' costs through a coupling term ψ in the state set $\eta \in S$, in which S denotes the set of all possible solutions [41,43]. The following expression represents the acceptance probability function, A^{η} [41.43]:

$$A^{\eta}(\psi, x_i \to y_i) = \frac{\exp[(E(x_i) - \max_{x_i \in \eta} E(x_i))/T_k^a]}{\psi}$$
 (24)

where T_k^a stands for the acceptance temperature; x_i and y_i denote the individual solutions and their corresponding probing solution, respectively. The coupling term is defined as follows [41,43]:

$$\psi = \sum_{\forall \int \eta} \exp[(E(\mathbf{x}_i) - \max_{\mathbf{x}_i \in \eta} E(\mathbf{x}_i))/T_k^a]$$
 (25)

The average mean square error (MSE) between the desired and predicted output values, as defined by Eq. (26), was considered as an objective function

$$MSE = \frac{1}{n} \sum_{i} (d_i - p_i)^2$$
 (26)

where d and p are the target value and predicted output, respectively.

Table 2Optimized parameters of the developed LSSVM model by CSA [41] optimization technique.

Parameter	Optimized value		
$\frac{\gamma}{\sigma^2}$	1.209042E+04 1.99122		

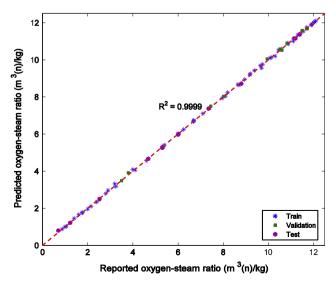


Fig. 2. Comparison between the applied data [10] and results of developed LS-SVM model.

3. Results and discussion

3.1. Evaluation of developed models

In this study, we employed an efficient optimization method, known as coupled simulated annealing, to determine the optimal magnitudes of LS-SVM parameters (e.g., σ^2 and γ) as reported in Table 2.

Cross plots of the proposed model's predictions versus the database values from [10], is demonstrated in Fig. 2. As it is clear in Fig. 2, almost all points lie on the bisector of the first quadrant (45° line), which suggests validity of the developed model. In addition, relative deviations between the outputs of developed models and corresponding utilized data are depicted in Fig. 3. Fig. 4 shows the performance of proposed tool for the prediction of oxygen–steam ratio as a function of pressure for various operating temperatures with literature reported data [10]. Table 3 shows the proposed method yields accurate results with average absolute deviation percentage of less than 0.5% in comparison with

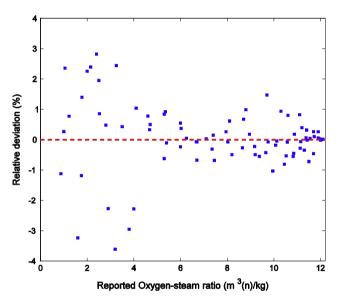


Fig. 3. Relative deviation of the predicted values from applied database [10].

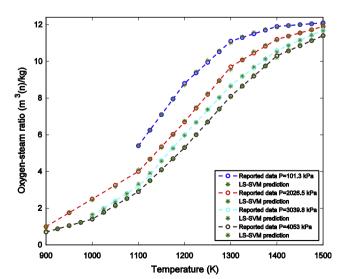


Fig. 4. Performance of proposed method for prediction of oxygen–steam ratio in comparison with database [10].

literature reported data [10]. To make a judgment based on results and plots, it can be concluded that the developed methods are sufficiently accurate for estimating oxygen–steam ratio in coal gasification process.

The powerful model introduced in this paper would be a quick, accurate and simple way for engineers and researchers to effectively monitor oxygen–steam ratio at various operating conditions without implementing laboratory or/and plant trials.

Table 3Comparison of calculated values with typical data [10].

Pressure	Temperature	Reported	Predicted values	Absolute
(kPa)	(K)	oxygen-steam	using LS-SVM	relative
		ratio data [10]	model	deviation (%) ^a
4053	975	1.225	1.215	0.77
4053	1025	1.775	1.750	1.4
4053	1075	2.525	2.503	0.85
2026.5	1125	4.675	4.659	0.33
101.3	1125	6.25	6.247	0.05
4053	1150	4.1	4.057	1.04
2026.5	1150	5.35	5.300	0.92
4053	1175	4.7	4.676	0.5
2026.5	1175	6.025	6.002	0.37
101.3	1175	7.95	7.929	0.26
4053	1200	5.3	5.333	0.62
3039.8	1200	6	5.967	0.55
2026.5	1200	6.7	6.745	0.68
101.3	1200	8.8	8.713	0.99
4053	1225	6	6.014	0.24
3039.8	1225	6.675	6.679	0.07
2026.5	1225	7.45	7.501	0.69
2026.5	1250	8.2	8.240	0.49
101.3	1250	9.95	10.053	1.03
4053	1275	7.4	7.389	0.15
3039.8	1275	8.025	8.030	0.07
4053	1350	9.2	9.245	0.49
3039.8	1350	9.65	9.691	0.43
2026.5	1350	10.45	10.534	0.81
101.3	1350	11.5	11.582	0.72
4053	1450	10.85	10.898	0.45
3039.8	1450	11.15	11.157	0.07
2026.5	1450	11.55	11.545	0.04
101.3	1450	12	12.002	0.02
4053	1475	11.125	11.156	0.28
2026.5	1500	11.9	11.893	0.05
101.3	1500	12.1	12.098	0.02
Average a	absolute deviat	tion (%)		0.48

^a Absolute relative deviation (%) = $\frac{|\text{Reported value} - \text{Predicted value}|}{|\text{Reported value}|} \times 100$.

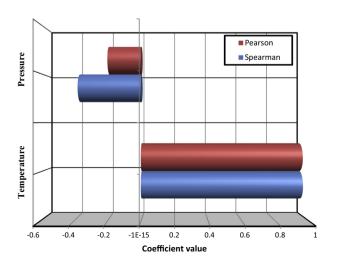


Fig. 5. Sensitivity analysis of the LS-SVM model and the dependence of oxygensteam ratio on temperature and pressure.

3.2. Sensitivity analysis

This section aims to determine the sensitivity of the LS-SVM model predictions to changes in the independent variables (i.e., temperature and pressure). As a result of the analysis, a relative variable impact value was allocated to every input variable. The analysis results provide users useful insights into the effects of all variables involved in the system. Herein, variable impact analysis was conducted using the Spearman and Pearson techniques [44]. Fig. 5 presents the degree of correlation between the input variables on the oxygen-steam ratio. These correlation coefficients have values ranging from -1 to +1. A value of +1 and -1 imply that the variables have a perfect increasing and decreasing linear relationship, respectively [35,45]. Fig. 5 reveals a low negative impact of pressure and a high positive impact of temperature on oxygen-steam ratio. These findings are in accordance with the known effects of pressure and temperature on oxygen-steam ratio in coal gasification process.

4. Conclusions

In this work, a rigorous modeling approach was presented that assists engineers for fast and accurate computation of the ratio of oxygen to steam ratio needed to sustain zero total enthalpy change in coal gasification process by means of LS-SVM modeling algorithm. The developed tool appears to considerably assist process system engineers/researchers who are working on the design and operational aspects of coal gasification plants. In addition, the comparison of real data and estimated values clearly demonstrates the precision of the predictive model that can be simply utilized for practical implications in coal processing industry. It is expected that this accurate tool will pave the way accurate predictions of oxygen–steam ratio critical in coal gasification processes which can be used by engineers for process monitoring.

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