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

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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.

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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%.

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

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:

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

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

$$C + 2H_2O \rightarrow CO_2 + H_2 + 90.2\,kJ \quad (3)$$

$$C + CO_2 \rightarrow 2CO + 172.4\,kJ \quad (4)$$

Partial oxidation:

$$C + 0.5O_2 \rightarrow CO - 110.5\,kJ \quad (5)$$

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Water gas shift:

$$CO + H_2O \rightarrow CO_2 + H_2 - 41.1\,\text{kJ} \tag{6}$$

Methanation:

$$2CO + 2H_2 \rightarrow CH_4 + CO_2 - 247.3\,\text{kJ} \tag{7}$$

$$CO + 3H_2 \rightarrow CH_4 + H_2O - 206.1\,\text{kJ} \tag{8}$$

$$CO_2 + 4H_2 \rightarrow CH_4 + H_2O - 165\,\text{kJ} \tag{9}$$

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

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:

$$C + H_2O \rightarrow CO + H_2 + 131.3\,\text{kJ} \tag{11}$$

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

$$\text{Net}: 2.2C + H_2O + 0.6O_2 \rightarrow 2.2CO + H_2 \tag{13}$$

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]:

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

$$\text{s.t. } y_k = e_k + \langle w, \Phi(x_k) \rangle + b \quad k = 1, \ldots, N \tag{16}$$

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]:

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

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]:

$$\begin{cases} \dfrac{\partial L_{\text{LS-SVM}}}{\partial w} = 0 \rightarrow w = \sum_{k=1}^{N}\alpha_k \Phi(x_k) \\ \dfrac{\partial L_{\text{LS-SVM}}}{\partial b} = 0 \rightarrow \sum_{k=1}^{N}\alpha_k = 0 \\ \dfrac{\partial L_{\text{LS-SVM}}}{\partial e_k} = 0 \rightarrow \alpha_k = \gamma e_k \\ \dfrac{\partial L_{\text{LS-SVM}}}{\partial \alpha_k} = 0 \rightarrow \langle w, \Phi(x_k) \rangle + b + e_k - y_k = 0 \end{cases} \tag{18}$$

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]:

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

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

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

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

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