

Innovative prediction model of carbon monoxide emission from deep mined coal oxidation

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Due to great impacts to air pollution caused by residual coal oxidation in underground mine gob, monitoring and forecasting of hazardous gases emissions have become important topics in mining engineering and environmental research today. This paper presents a robot monitoring system for carbon monoxide emission from coal oxidation in spontaneous combustion condition. According to the terahertz-wave absorption spectrum, the CO concentrations are measured by using terahertz time-domain spectroscopy (THz-TDS) technique. Based on the measured values, an innovative method of CO concentration prediction has been developed by using least square support vector machine (LSSVM) with a novel hyper-parameter selection. The hourly CO concentrations have been predicted using the SVM and the hybrid LSSVM models respectively. Results show that the hybrid LSSVM has better accuracy. Statistic estimators have been employed to compare performances of the models. It has been concluded that the errors decrease and coefficients of determination increase for hybrid LSSVM model, hence it has definite practice significance and application value.

Key words: Coal oxidation, hazardous gas, terahertz spectroscopy technique, support vector machine

INTRODUCTION

Coal is the prime energy resource in most countries, 60% of them located in three countries: the United States, Russia, and China. Uncontrolled coal fires are a serious problem in many coal-producing countries and become an environmental and economic problem of international magnitude [1].

Although written accounts of coal fires date back to at least the time of Alexander the Great, the worldwide spread of coal fires has increased dramatically since the industrial revolution. Currently, thousands of coal fires are burning—some for centuries and many uncontrollably, with flames up to 20 m and temperatures exceeding

1000°C—from eastern Asia and northern China into the coal basins of Russia, Europe, Africa, north and south America, and Australia [2,3].

Coal fire is a global catastrophe, some of its prime impacts are [4,5]: (a) Emission of many toxic gases, such as carbon monoxide (CO), carbon dioxide (CO₂), sulfur oxides (SO_x), methane (CH₄), and nitrogen oxides (NO_x). Among these noxious gases, CO₂ and CH₄ contribute to global warming. (b) Geomorphic effects include land subsidence, surface cracks, faults, and other geologic structures. This paper also presents an innovative method of CO concentration prediction using a novel hyper parameter selection for Least Square Support Vector Machine (LSSVM) [19] regression combined with particle swarm optimal algorithm (PSO) [20]. The CO concentrations of

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hazardous gas monitoring station in coal mine gob have been used to test the effectiveness of this method. Statistic estimators including mean absolute percentage error (MAPE), mean absolute error (MAE) and root mean square error (RMSE) and coefficient of determination (R2) have been employed to compare performances of the models.

EXPERIMENTAL

Hazardous gas samples were collected from the gob in an actual coal mine and analyzed by terahertz measurement to obtain the carbon monoxide concentration.

The monitoring system for CO concentration detection is shown in Fig. 1. To collect these samples, multiple sample collection tubes were placed in the gob behind the scraper conveyor. The gas from the gob was collected through these tubes using a pump, and pumped into a ball sample vessel. This full sample vessel was transferred to the laboratory for analysis. The pump system to remove gas from the gob using suction was an electric rotary vane vacuum pump with an explosion-proof motor.

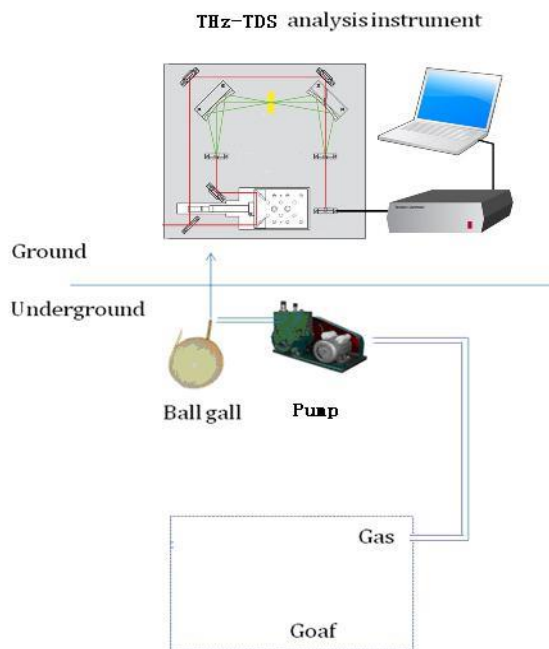


Fig. 1. Monitoring system for CO concentration detection.

Gas samples were collected at different points in the mine. Collection tubes were placed in the gob near the air return roadway. Boundaries for the model were based on a workface in a coalmine in

northern China, which has a U-type ventilation mode. The intake airflow and return airflow are on the top and bottom, respectively, of the front of this model.

The gas samples were analyzed using a THz-TDS system which is used to measure THz absorption of carbon monoxide following the pioneering works [21].

According to the principle of radiation transfer [22-24], the radiation emitted from the source and traveling through the gas cell can be absorbed by the CO gas. The spectra of absorption coefficient for CO gas are presented in Fig. 2 at three different concentration levels, i.e., 0.5%, 1%, and 2%. CO gas is known to have a number of equispaced signature spectral lines that are at very precise frequency locations.

It can be seen that the frequency positions of the spectral lines did not change for the different concentration conditions; however, there was a significant change in the intensity of the lines from one concentration level to another. As concentration increases, so does the intensity of the rotational transition lines. There is evidently a near linear relationship between the pressure and the change in intensity of the absorption peaks. This is also true for all rotational lines in CO gas.

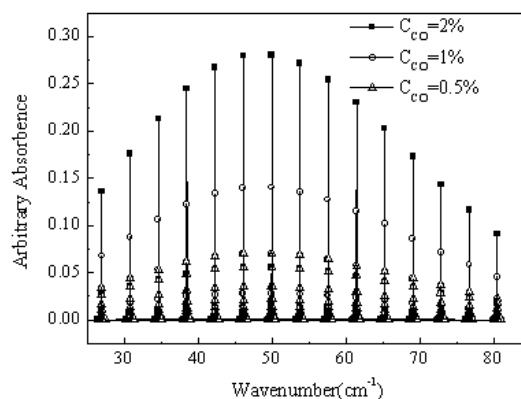


Fig. 2. Absorption spectrum of CO at different concentrations.

The measurements in this study demonstrate that varying the concentration of the gas affects only the amplitude of the absorption lines and not their exact position. This is critical in air pollution studies when trying to single out a specific gas (such as CO) from a field sample with unknown constituents.

PREDICTION MODEL

Support vector machine (SVM) has been used in many applications, for example, the pattern recognition problem and fault diagnose with high dimension and nonlinearity [25, 26]. The hybrid Least square support vector machine (LSSVM) [27] as a novel approach for CO concentration prediction has been applied to data from the hazardous gas monitoring system. LSSVM is reformulations to the standard support vector machines which result in a set of linear equations instead of a quadratic programming problem of SVM.

LSSVM is a learning algorithm. It uses a hypothesis space of linear function in a high dimensional feature space by using the kernel theory. In this paper, this algorithm is trained by optimization theory. Consider a given training set $(x_i, y_i), i = 1, 2, \dots, n$, where x_i and y_i are the input and the output of the i th example, n denotes the number of samples. The support vector method approach aims at constructing a regression function of the following form:

$$y = \omega^T \varphi(x_i) + b \tag{1}$$

where $\varphi(x_i)$ is a nonlinear function which maps the feature space of input into a higher dimension feature space and can be reached by the kernel strategy, $\omega \in R^n$ is coefficient vector and $b \in R$ is bias term. These unknown coefficients ω and b can be obtained through solving the following optimization problem:

$$\begin{aligned} \min J(\omega, \mathbf{e}) &= \frac{1}{2} \omega^T \omega + \frac{\gamma}{2} \sum_{i=1}^N e_i^2 \\ \text{s.t.} \quad & y_i [\omega^T \varphi(x_i) + b] = 1 - e_i \quad i = 1, \dots, N \end{aligned} \tag{2}$$

where $J(\omega, \mathbf{e})$ is structure risk, In equation (2), the first term, measures the inverse of the margin distance. In order to obtain the minimum structural risk, the first term should be minimized. γ is the regularization parameter, determining the trade-off between the fitting error minimization and smoothness. \mathbf{e} is a slack variable, which ensures classification validity under linear non-separable

case. This optimization problem including the constraints can be solved by using the Lagrange function as following:

$$\begin{aligned} L(\omega, e_i, b, \alpha_i) &= \frac{1}{2} \omega^T \omega + \frac{\gamma}{2} \sum_{i=1}^N e_i^2 \\ &- \sum_{i=1}^N \alpha_i \{ y_i [\omega^T \varphi(x_i) + b] + e_i - 1 \} \end{aligned} \tag{3}$$

where α_i is the Lagrange multipliers. Considering the optimization conditions by Karush-Kuhn-Tucker (KKT), the optimal condition about (2) can be obtained as following:

$$\begin{cases} \frac{\partial L}{\partial \omega} = 0 \Rightarrow \omega = \sum_{i=1}^N \alpha_i y_i \varphi(x_i) \\ \frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{i=1}^N \alpha_i y_i = 0 \\ \frac{\partial L}{\partial \alpha_i} = 0 \Rightarrow y_i [\omega^T \varphi(x_i) + b] + e_i - 1 = 0 \\ \frac{\partial L}{\partial e_i} = 0 \Rightarrow \gamma e_i = \alpha_i \end{cases} \tag{4}$$

where $i = 1, 2, \dots, N$.

Eliminating the parameter ω and b in equation (4), these equality constraints can be transformed as following:

$$\begin{bmatrix} 0 & \mathbf{y}^T \\ \mathbf{y} & \mathbf{\Omega} + \frac{\mathbf{I}}{\gamma} \end{bmatrix} \begin{bmatrix} b \\ \mathbf{a} \end{bmatrix} = \begin{bmatrix} 0 \\ \mathbf{Q} \end{bmatrix} \tag{5}$$

where \mathbf{I} is the identity matrix,

$$\Omega_{ij} = y_i y_j \varphi(x_i)^T \varphi(x_j).$$

The solution of \mathbf{a} and b can be obtained by solving (5) and substitute to (1). (1) is presented as:

$$f(x) = \sum_n \alpha_i \varphi(x_i)^T \varphi(x_j) + b \tag{6}$$

According to the Mercer rule, the kernel function $K(x_i, x_j)$ is introduced, thus the kernel function is expressed as:

$$K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j) \tag{7}$$

In LSSVM, quadratic programming problem is changed as the problem of solving linear equation groups, which simplifies the calculation quantity.

Combining equation (6) with equation (7), equation (6) is expressed as:

$$f(x) = \sum_n \alpha_i K(x_i, x_j) + b \quad (8)$$

There are various kernels used in the LSSVM. Different kernel function presents the different mapping from the input space to the feature space. As a result, LSSVM model changes with the different kernel function selections. The radial basis function (RBF) is used as the kernel function of the LSSVM because RBF kernel tends to give good performances under general smoothness assumptions. RBF-kernel function is presented as following:

$$K(x, y) = \exp\left(-\frac{\|x - y\|^2}{2\sigma^2}\right) \quad (9)$$

where σ is the kernel parameter and controls the LSSVM's regression or classification ability. In equation (2), γ is the regularization parameter determining the fitting error minimization and smoothness. They are important parameters in the LSSVM algorithm.

In LSSVM model, the parameter γ and parameter σ of the RBF function are chosen according to experience. In this way, for different sample sets, the optimal parameter values are difficult to be found, which affects the fault diagnosis efficiency and accuracy. However, it needs an exhaustive search over the space of hyper-parameters, which must be time consuming. This procedure needs to locate the interval of feasible solution and a suitable sampling step. In order to acquire the better classification accuracy, the particle swarm optimization algorithm (PSO) is used to find the optimal solution of these parameters in LSSVM.

The basic idea of particle swarm optimization can be described in an explicit way: each individual in particle swarm, referred to as a 'particle', represents a potential solution; each particle moves its position in search domain and updates its velocity according to its own flying experience and

neighbors' flying experience, aiming at a better position for itself.

According to the simple PSO model, the velocity V_i for each dimension of the i th particle can be updated as follow:

$$V_{i+1} = wV_i + c_1r_1(P_i - X_i) + c_2r_2(P_g - X_i) \quad (10)$$

where w is the inertia weight coefficient; c_1 and c_2 are two positive constants called acceleration coefficients; P_1 and P_2 P_i and P_g are the local individual best location and the global best location; r_1 and r_2 are random numbers in the range of [0,1]. The new position X_i for i th particle can be expressed as:

$$X_{i+1} = X_i + V_{i+1} \quad (11)$$

In the standard PSO, if $0 < w < 1$ and $V_{i+1} < V_i$, there exists a certain number that when the generation number is more than it, the current global best position P_g of the swarm does not vary, and consequently, all components of V_i , will be smaller than a given error, and the particle will stop evolution. Even if a better solution exists in this direction, the particle swarm may stop evolution before finding this position and fall into premature convergence. This is the reason why the standard PSO may fall into local optimum solution.

To solve the problem of premature convergence, we use the stochastic particle swarm optimization (SPSO) algorithm [28, 29]. Here set the inertia weight $w = 0$, substituting equation (10) into equation (11), the following equation can be obtained:

$$X_{i+1} = X_i + c_1r_1(P_i - X_i) + c_2r_2(P_g - X_i) \quad (12)$$

In order to improve the global searching ability, P_g is maintained to be the historic best position, and an extra particle j with the position X_j is generated randomly in the searching domain. In this way, the following updating procedure is obtained:

$$\begin{cases} P_j = X_j \\ P_g = \arg \min(P_i, P_j) \end{cases} \quad (13)$$

This means that if $P_g = P_j$, the random particle j locates at the best position and the new random particle will be searched repeatedly, therefore at least one particle is generated in the searching domain randomly to improve the global searching ability.

In the SPSO-LSSVM model, the appropriate parameters are selected by the SPSO algorithm, which can find the optimal parameter value quickly. As what has been mentioned above, γ and σ^2 become the swarms, then the dimension of the swarms is two. These swarms can be expressed as following:

$$\begin{aligned} \gamma_i &= [\gamma_{i1}, \gamma_{i2}, \dots, \gamma_{id}] \\ \sigma^2_i &= [\sigma^2_{i1}, \sigma^2_{i2}, \dots, \sigma^2_{id}] \end{aligned} \quad (14)$$

The key factor to determine the optimized hyper-parameters using SPSO is how to define the fitness function which evaluates the goodness of individual. The fitness function can evaluate the objective values of all particles. The choice of the fitness function is very important because it is on this basis that the SPSO evaluates the goodness of each particle solution for the LSSVM regression system. In function regression, the fitness function is the sum square error between the real output data of the system and the output data of the LSSVM model in the same input. In this study, the fitness function used is expressed as follows:

$$F(\gamma, \sigma^2) = \sum_{i=1}^N \left\{ \left[\frac{y_{ireg} - y_i}{y} \right]^2 \right\} \quad (15)$$

where y_i is real output data and y_{ireg} is the output data of the LSSVM model in the same input.

RESULTS AND DISCUSSION

Having constructed both the SVM and hybrid LSSVM models, the parameters would have had to be calibrated and evaluated. CO levels have been predicted by both SVM and LSSVM models for the field measurements.

The data taking part in the learning and testing steps of the models have been those collected from a period of 40 days in 2010 and 2011 respectively. In

those days, the CO concentration was measured every 1 h so the CO level was predicted on hourly basis for each day. In both SVM and LSSVM models, 80 percent of the data were used for training the models and the rest were used for testing the models.

Optimization of these parameters has been done by a systematic grid search of the parameters using leave-one-out cross validation on the training set. First, a broad range of parameters settings are investigated with large steps. Second, after identifying a promising region, this region is searched in more details. The test set is used as an independent set to calculate the final prediction error. Furthermore, the test error is not used to select the optimal model but its size is compared to test set errors with other settings to identify possible overtraining.

The results are further analyzed using statistical indices. The statistical indices used in the analysis are mean absolute percentage error (MAPE), mean absolute error (MAE) and root mean square error (RMSE) and coefficient of determination (R^2). These parameters have been defined as below:

$$MAPE = \frac{1}{N} \sum_{i=1}^N \left[\frac{|y'_i - y_i|}{y_i} \right] \times 100\% \quad (16)$$

$$MAE = \frac{1}{N} \sum_{i=1}^N |y'_i - y_i| \quad (17)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^N [y'_i - y_i]^2}{N}} \quad (18)$$

$$R^2 = 1 - \frac{\sum_{i=1}^N [y'_i - y_i]^2}{\sum_{i=1}^N [\bar{y}_i - y_i]^2} \quad (19)$$

Where y_i is the observation value, \bar{y}_i is the average value and y' is the predicted value. The MAE and the MAPE correct the 'canceling out' effects; moreover, MAPE takes into account the different scales at which this measure can be computed. RMSE gives a relatively high weight to large errors. This means the RMSE is most useful when large errors are particularly undesirable. The MAE and the RMSE can be used together to diagnose the variation in the errors in a set of

forecasts. The RMSE will always be larger or equal to the MAE; the greater difference between them, the greater the variance in the individual errors in the sample. All errors are negatively oriented scores, so lower values are better. The computations were made with the Windows XP operating system and MATLAB.

Hourly CO concentrations predicted by SVM model have been shown in Fig. 3.

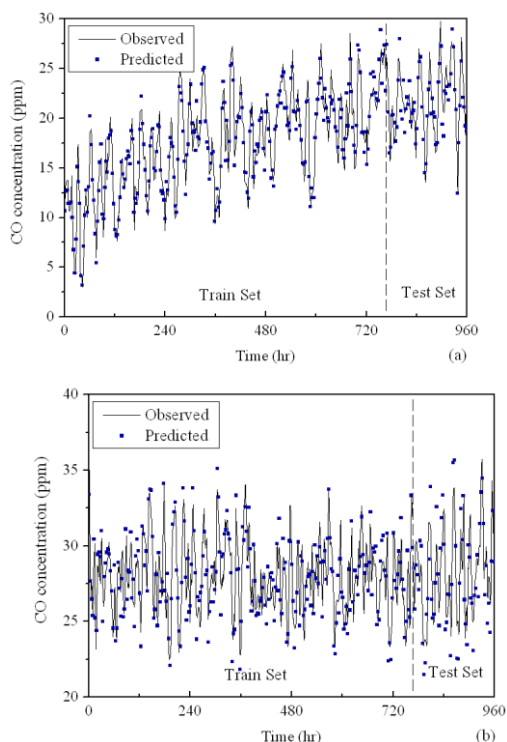


Fig. 3. Hourly CO concentrations predicted by SVM model in (a) 2010 and (b) 2011.

Correlations between prediction and measured values in the test stage have been determined using R^2 as shown in Fig. 4. Coefficients of determination for each period were 0.767 and 0.683 respectively. This means that the SVM model can predict CO concentration fluctuations within an acceptable limit. However, grid search and modeling was found to be very much time consuming. Also, there as been a significant amount of multicollinearity among the CO concentration predictors. Multicollinearity can make it difficult to correctly identify the most important contributors to a physical process. Also the large number of the predictors, reduce the earning rate of the prediction

process, hence, size reduction methods like LSSVM, can be useful solution for this predicament.

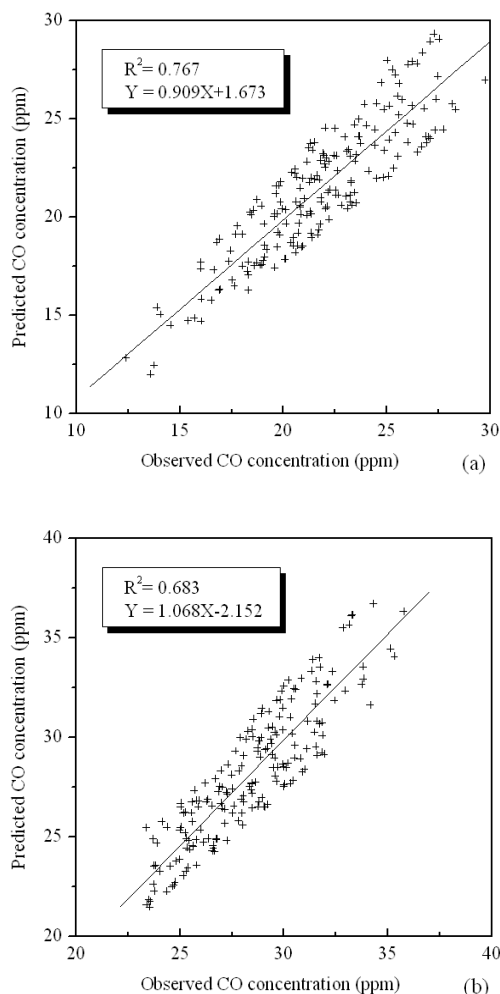


Fig. 4. Correlation between measured CO concentrations and SVM predictions predicted by SVM model during testing stages in (a) 2010 and (b) 2011.

The LSSVM method has been used in this research to reduce the size of the input data. Hourly prediction results of hybrid LSSVM model are shown in Fig. 5. Similar to the SVM model, correlations between prediction and measured values in the test stage have been determined for LSSVM model as shown in Fig. 6. Coefficients of determination for each period were found to be 0.838 and 0.78 respectively.

Results of the two SVM and hybrid LSSVM models have been compared and discussed statistically and their respective computation times are illustrated in Table 1. It can be seen that the hybrid LSSVM model has higher coefficient of determination and fewer errors than the SVM

model. Thus, the hybrid LSSVM model produced more accurate results and size reduction had positive effect on the model performance. Moreover, the hybrid LSSVM model achieves faster training speed and grid search. As it was observed, the total calculation time obviously is saved. The reduction of the input vector dimensions is resulted in the reduction of the SVM calculations and shortening the SVM training periods. Due to the effects of many factors on air pollution concentrations, a small error has remained. However in this case, the hybrid LSSVM has been found a better and faster predictive model.

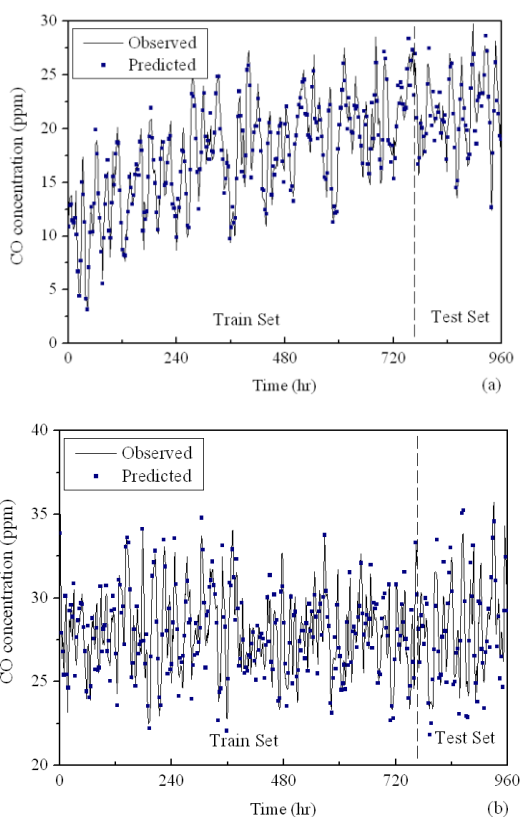


Fig. 5. Hourly CO concentrations predicted by LSSVM model in (a) 2010 and (b) 2011.

As seen in Table 1, the RMSE and MAR have decreased by using LSSVM method. This means that LSSVM is able to remove unqualified variables and noises, hence, the positive effect of the LSSVM is more sensible. Also, the MAPE has decreased in both the tasting and training processes by using hybrid LSSVM. In other words, LSSVM method can increase model prediction efficiency.

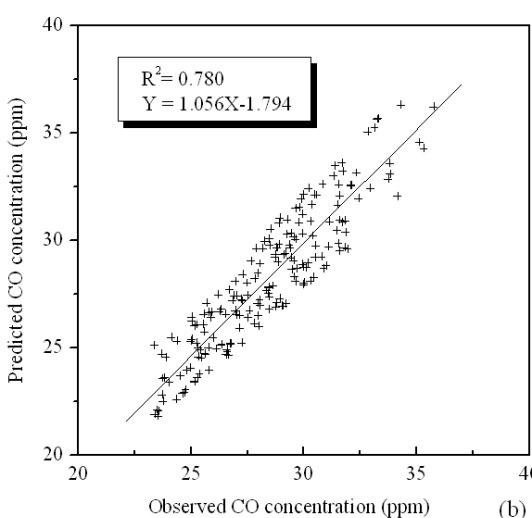
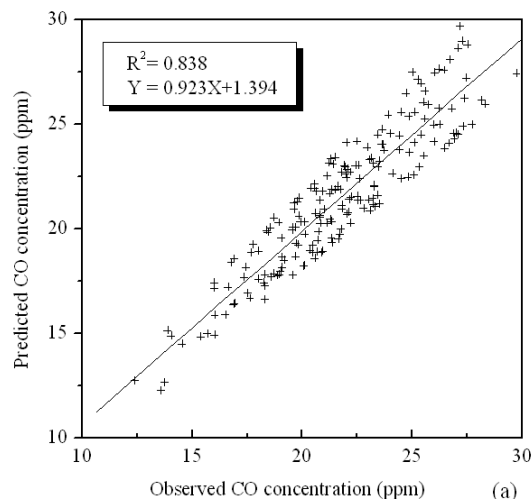


Fig. 6. Hourly CO concentrations predicted by LSSVM model in (a) 2010 and (b) 2011.

Table 1. Comparison of SVM and LSSVM models by statistics estimators.

			MAE	RMSE	MAPE	R ²	Time (s)
P ₁	LSSV	Train	0.683	0.811	0.039	0.972	68
		Test	1.173	1.358	0.054	0.838	
	SVM	Train	0.856	1.028	0.049	0.956	
		Test	1.408	1.630	0.064	0.767	
P ₂	LSSV	Train	0.725	0.832	0.026	0.877	63
		Test	1.143	1.305	0.040	0.780	
	SVM	Train	0.943	1.081	0.034	0.792	
		Test	1.371	1.566	0.048	0.683	

CONCLUSIONS

In this paper, a robot monitoring system for carbon monoxide emission from underground coal fires has been presented. The CO concentrations were measured by using terahertz time-domain spectroscopy (THz-TDS) technique according to the

absorption characteristics of CO. This paper has also presented the prediction method of hourly hazardous gas emission from coal mine gob by applying the Support Vector Machine (SVM) and Least Square Support Vector Machine (LSSVM).

It can be concluded that such models provide a more promising alternative to time series forecasting. However, the important point of this approach is the data size reduction by LSSVM. The proposed hybrid LSSVM model provides a considerable improvement in the forecasting of CO concentrations over the SVM model based on the same set of input variables. Besides, the LSSVM implementation for size reduction obviously saved time of the SVM training and grid search method.

Statistical error estimators have been used to compare performance of the SVM and the hybrid LSSVM models. Errors estimated by the MRE, MSRE and MAPE decreased as R2 decreased by implementing the LSSVM. Generally, the hybrid LSSVM models have good ability to predict air pollution in different time intervals.

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ИНОВАТИВЕН МОДЕЛ ЗА ПРЕДСКАЗВАНЕ НА ЕМИСИИ ОТ ВЪГЛЕРОДЕН МОНОКСИД ПОЛУЧЕНИ ПРИ ОКИСЛЕНИЕ НА ВЪГЛИЩА НА ГОЛЕМИ ДЪЛБОЧИНИ

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(Резюме)

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Мониторингът и прогнозирането на емисиите на опасни газове вече е важна тема в минното инженерство и изследването на околната среда. Това се дължи на замърсяването на въздуха поради остатъчното окисление в подземните минни хоризонти. В настоящата работа се представя роботизирана мониторингова система за емисиите от въглероден моноксид от спонтанното горене на въглища в мини. Концентрациите на въглеродния моноксид се измерват чрез терахерц-вълнова спектроскопия (THz-TDS). На основата на измерените стойности е разработен иновативен метод, използващ „least square support vector machine“ (LSSVM) с хипер-параметричен подбор. Часовите концентрации са предсказвани чрез моделите SVM и хибридният LSSVM. Резултатите показват, че хибридният LSSVM- модел дава по-висока точност. Направен е изводът, че грешките намаляват, а корелационните коефициенти нарастват при хибридният LSSVM-модел, поради което той определено има практическа стойност и приложимост.