Journal of Southeast University (English Edition) Vol. 24, No. 1, pp. 55 – 58 Mar. 2008 ISSN 1003—7985

Neural network approach to predicting mercury emission from utility boiler

Yang Hongmin[1,2] Zhou Bo[1]

([1]School of Power Engineering, Nanjing Normal University, Nanjing 210042, China)

([2]Institute for Combustion Science and Environmental Technology, Western Kentucky University, Bowling Green, KY 42101, USA)

Abstract: The feasibility of using an ANN method to predict the mercury emission and speciation in the flue gas of a power station under un-tested combustion/operational conditions is evaluated. Based on existing field testing datasets for the emissions of three utility boilers, a 3-layer back-propagation network is applied to predict the mercury speciation at the stack. The whole prediction procedure includes: collection of data, structuring an artificial neural network (ANN) model, training process and error evaluation. A total of 59 parameters of coal and ash analyses and power plant operating conditions are treated as input variables, and the actual mercury emissions and their speciation data are used to supervise the training process and verify the performance of prediction modeling. The precision of model prediction (root-mean-square error is 0.8 $\mu g/Nm^3$ for elemental mercury and 0.9 $\mu g/Nm^3$ for total mercury) is acceptable since the spikes of semi-mercury continuous emission monitor (SCEM) with wet conversion modules are taken into consideration.

Key words: mercury speciations; electric utility boiler; prediction; artificial neural network

A recent report by the Environmental Protection Agency (EPA) on emissions of hazardous air pollutants by electric utilities predicts that emissions of air toxics from coal-fired utilities will increase by 10% to 30% by the year 2010[1]. Mercury from coal-fired utilities is identified as the most hazardous air pollutant of the greatest potential public health concern. The U. S. announced the clear skies initiative in 2002, which targeted the reduction of NO_x, SO_2 and mercury by 70% by 2018[2].

Mercury in the flue gas usually exists in three forms[3]: oxidized (Hg[2+]), elemental (Hg[0]) and particle-bound (Hg[P]). Total mercury concentration in flue gas is indicated as Hg[T]. Due to its high volatility, mercury usually exists in a vapour form. Oxidized mercury is soluble in water and can be removed in wet scrubbers[4]. On the other hand, elemental mercury usually escapes emission control equipment and is emitted into the atmosphere.

Artificial neural network (ANN) modeling is a technique that may offer advantages in the modeling process that follows nonlinear relationships[5]. ANN modeling uses historical data to "learn" the patterns that occur between given inputs and outputs of the model, and then simulates the outputs under non-tested conditions. The use of neural networks applied to air pollution is a trend of increasing interest[6-7]. The method tends to be a "blackbox" method, where the equations describing complex situations are not known. Therefore, an ANN may be suitable for predicting mercury emissions and for the power generation where the fundamental transformation mechanism is not fully understood and the irregular effects on the results are too complex to deal with by using traditional data mining theory.

In this paper, the feasibility of using an ANN to predict the mercury emissions in the flue gas of a power station under un-tested combustion/operational conditions is evaluated using a 3-layer back-propagation network based on the existing field data at the stack. Although EERC developed a method based on ANN to estimate mercury speciation in flue gas for individual power plants[8], the interest of this paper is focused on the prediction of mercury in a time series according to the changes in complex multifactors.

1 Mercury Measurement for Utility Boiler

There are three primary forms of mercury emission from coal-fired boilers of power station: gaseous elemental mercury (Hg[0]), gaseous oxidized mercury, and particle bound mercury (Hg[P]). Most oxidized mercury in flue gas is in the divalent state (Hg[2+]). Oxidized mercury is soluble and has a tendency to be adsorbed by a particulate matter. The instrumentation used in this study is a semi-mercury continuous emission monitor (SCEM). The SCEM used is the Sir Galahad from PS Analytical. It uses a gold trap to extract the mercury from the flue gas and measures the mercury concentration by an atomic fluorescence detector. The ontario hydro method (OHM), an ASTM standard method for measuring and speciating mercury in utilities flue gas, is used to verify the SCEM reading. The mercury content in coal and ash samples is analyzed by the leco advanced mercury analyzer 254 following the ASTM direct combustion method. The AMA 254 has a detection limit of 0.01 ng and a detection range of 0.05 to 600 ng.

2 Determination of ANN Topology Architecture and Selection of Impact Parameters

The ANN technique uniquely uses input and output data sets and directly "learns" the patterns inherent in the data. The key fact of an ANN model which makes it desirable is the ability to learn patterns from a data set. The ability of an ANN model is derived from the power of various interconnected processing units, "neuron-type" units, known as perceptrons, to function through pattern recognition in a data set. Once the perceptrons are interconnected with each other, a powerful processing technique with the ability to learn and self-organize from an extensive data set is established. The topology approach is used to construct the studied ANN

Received 2007-01-05.

Biography: Yang Hongmin (1972—), male, doctor, professor, yanghongmin@njnu.edu.cn.

Foundation items: The National Basic Research Program of China (973 Program) (No. 2006CB200302), the Natural Science Foundation of Jiangsu Province (No. BK2007224).

Citation: Yang Hongmin, Zhou Bo. Neural network approach to predicting mercury emission from utility boiler[J]. Journal of Southeast University (English Edition), 2008, 24(1): 55 – 58.

model, with input layer, output layer and hidden layer design. The topology design requires a number of model factors, including the type of learning, the number of hidden layers, the number of neurons in the hidden layers, and the number of neurons in the input and output layers. The architecture of topology used in this study is shown in Fig. 1. It consists of multilayer perceptrons with 59 input neurons which correspond to 59 impact parameters, one hidden layer with 200 neurons, and two output neurons for predicting results. The functions that govern weighting and activation of the perceptrons are the activation functions, which are logistic $[1/(1+e^{x})]$ in all the cases.

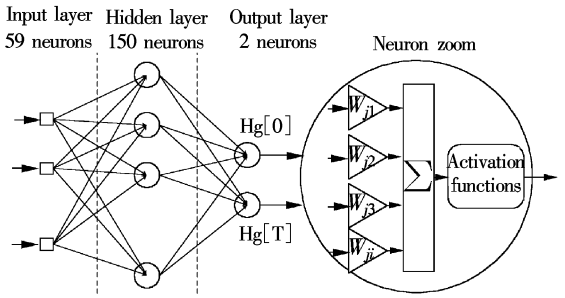

Fig. 1 Architecture of ANN topology structure used in mercury prediction

Two different datasets are used in ANN modeling. One is used to train the neural network (training dataset, 50% of the cases) and the other one is used to validate the prediction model and calculate the root-mean-square (RMS) value (testing dataset, 50% of the cases) after the training is finished. A comparison between the RMS values for two datasets obtained for the three full boilers has been made. An excellent match is achieved for all the cases. The selected impact parameters for the ANN model to predict mercury at the stack are listed in Tab. 1. The total input vector datasets are divided into three groups: ① Coal-fired boiler configuration, ② Coal and ash properties and ③ Plant operation information from power plants. Three units with different configurations of the boiler and the air pollution control devices, as listed in Tab. 2, are chosen to perform the training and testing procedures. The SCEM system is located at the stack and it monitors the mercury emissions and their speciation for two weeks continuously. The sampling frequency is 5 min/point. The hourly-averaged mercury data are treated as the satisfactory output values and are used to supervise the training process.

Tab. 1 Impact parameters selected in ANN modeling

Coal and ash properties	Coal-fired boiler configuration	Plant operation information
Data from the approximate, ultimate and XRF analysis of coal and ash	Type and configuration of FGD, ESP, SCR and combustor in power plants	Operation data such as power load, coal consumption, SCR, APH temperature, and concentrations of SO_2 and NO_x

Tab. 2 Configuration of tested units

Unit configuration	Unit 1	Unit 2	Unit 3
Combustor type	Tangential fire	Opposed wall fire	Opposed wall fire
Particulate control	Cold ESP	Cold ESP	Cold ESP
NO_x control	SCR	SCR	No
SO_x control	No	FGD	FGD

3 ANN Training Process and Results

The learning process is divided into three phases, including training, testing and prediction. Data consisting of input vectors coupled with matched output values are fed into the neural network in the first two phases, in this study, totals of 100, 180, 145 input sample vectors and hourly-averaged mercury data are involved in the training computation for these three units, respectively. A subsequent prediction phase is then used to assess the forecasting ability of the model. Data sets which are used in the prediction phase are collected in another 5 to 8 day's field testing. It also consists of 100, 180, 145 impact vectors and hourly averaged mercury data which are isolated from the data sets in the training phase. This ensures that each phase will be performed using data it has never seen before.

The general back-propagation (GBP) technique is deployed for the training and testing processes. The network learns by comparing the model output with actual outputs, and then makes adjustments to the hidden layers in a "backward propagation" to allow the ANN model to learn how to predict the output more effectively.

The standard back-propagation method is based on the following popular gradient descent learning[9]:

$$\Delta w_{ij}(n) = \eta \delta_i(n) x_j(n) \tag{1}$$

where $\Delta w_{ij}(n)$ is the correction applied to the weight w_{ij}; η is the learning rate parameter; $\delta_i(n)$ is the local gradient which points to the required changes in network weights; and $x_j(n)$ is the output of neuron j at iteration n. A slower learning rate is needed for this complex input situation. Here we set it as 0.01. The momentum learning method is an improvement on the gradient descent search technique. In the momentum learning method, the equation to update the weights becomes

$$\Delta w_{ij}(n) = \eta \delta_i(n) x_j(n) + \alpha[w_{ij}(n) - w_{ij}(n-1)] \tag{2}$$

where α is the momentum constant, and here we choose it as 0.005. The momentum rate is analogous to the momentum in physics. A high momentum rate is used to give the network a higher inertia or tendency to proceed in a straight direction.

Using the maximum and minimum values found within each data channel of the network, all the input and output data are normalized. Using a reverse process, the output results produced by the network are then denormalized to provide the actual output values. The train continues until the number of learning stages reaches a specified value or the error of the model output compared with the actual output reaches a desirable minimum value.

The control statistical parameters used are the coefficient of multiple determination (R_2) and the root mean square error (RMSE). R_2 indicates the proportion of the variation of dependent variables (outputs) over the variation of the independent variables (inputs). The R_2 value of 1.0 indicates a perfect model fit. The RMSE provides useable statistical information to verify model forecasts because the smaller the RMSE, the higher the precision of model prediction. The error is expressed by the RMS value, which can be calculated by

$$E = \frac{1}{2}\left[\sum\sum |t_{ip} - o_{ip}|^2\right]^{1/2} \quad (3)$$

where E is the RMS error; t is the network output (target) and o represents the desirable output vectors over all patterns (p).

In this study, the training dataset including 100, 180, 145 input vectors and hourly-averaged mercury speciation data for units 1, 2 and 3, respectively, are used to train the ANN model. With the completion of the training and testing phases of the ANN model, the comparison between the model prediction and real measurement values in a time series is shown in Fig. 2 for individual testing units. In these figures, some unexpected spikes are found in the time series of measurement of mercury speciation which are normally suspected to relate to the SCEM with the wet conversion module. Fortunately, the prediction results show that the ANN model can tolerate the systematic error in the training process and correct these spike data. The R_2 (model fit) for gaseous elemental mercury is 0.856, and for gaseous total mercury it is 0.93. The RMS error is 0.8 μg/Nm^3 for gaseous elemental mercury and 0.9 μg/Nm^3 for gaseous total mercury, respectively. The normalized prediction and measurement values are summarized in the same plotting as shown in Fig. 3, most of the data are close to the line with a slope of 1.0 ($y = x$). This is much more clear to compare the difference between prediction and measurement. For some values with high actual measurement, the deviation results from the spike of the wet SCEM system.

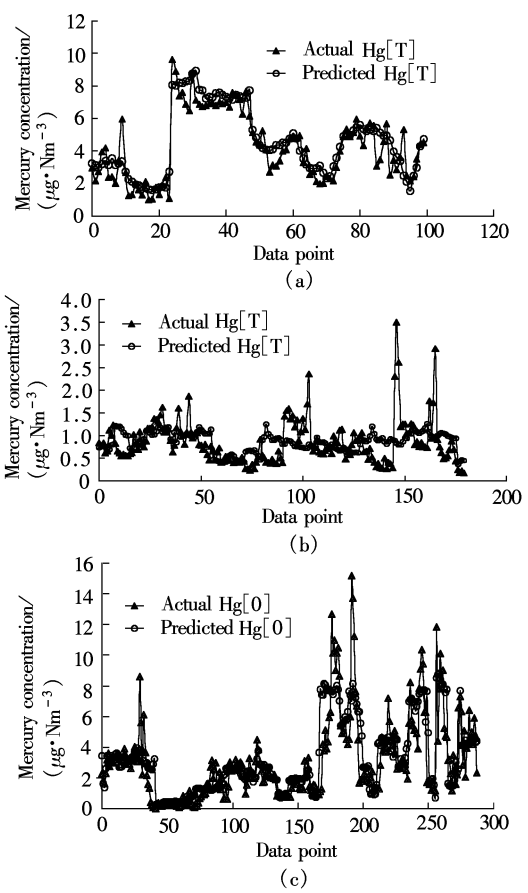

Fig. 2 Comparison of the mercury concentration between actual value and prediction. (a) Unit 1; (b) Unit 2; (c) Unit 3

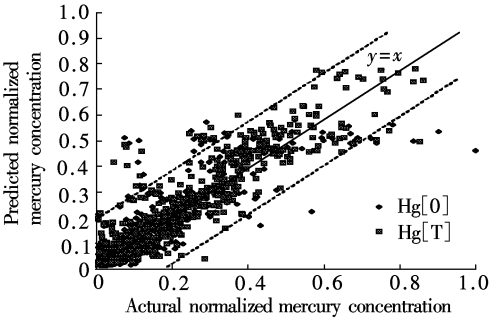

Fig. 3 Plot of normalized mercury emission obtained with ANN modeling vs. actual measurement

4 Conclusion

The feasibility of using an artificial neural network to predict mercury emissions at a stack of a utility boiler is investigated, and positive conclusions can be drawn as follows: Three layers of the back-propagation network can predict hourly-averaged mercury emissions with acceptable discrepancies. Comprehensive 59 impact parameters on mercury emissions are considered in the prediction process. The accuracy of the modeling strongly depends on the selection and collection of these impact parameters. The R_2 (model fit) of this model for gaseous elemental mercury is 0.856, and for gaseous total mercury is 0.93. The precision of model prediction (RMS error is 0.8 μg/Nm^3 for gaseous elemental mercury and 0.9 μg/Nm^3 for gaseous total mercury) suggests that ANN does hold promise for predicting mercury emissions and their speciation if the spikes of mercury SCEM with the wet conversion module are taken into consideration.

References

[1] US Environmental Protection Agency. Mercury study report to Congress, volume Ⅰ: executive summary, EPA-452/R-97-003 [R]. Washington DC: Office of Air Quality Planning and Standards and Office of Research and Development, 1997.

[2] US Environmental Protection Agency. *Clear skies legislation introduced in Congress proposal will improve air quality, prevent premature deaths, illnesses* [M]. Washington, DC: EPA Press, 2002.

[3] Galbreath K C, Zygarlicke C J. Mercury transformations in coal combustion flue gas [J]. *Fuel Processing Technology*, 2000, **65**(1): 289 − 310.

[4] Livengood C D, Huang H S, Mendelsohn M H, et al. Development of mercury control technology for coal-fired systems [C]//*Proceeding of the* 210*th ACS National Meeting*. Chicago, IL, 1995: 325 − 331.

[5] Müller B, Reinhardt J. *Neural networks*: *an introduction*[M]. New York: Springer-Verlag, 1990.

[6] Gardner M W, Dorling S R. Artificial neural networks (the multiplayer perceptron)—a review of applications in the atmospheric sciences [J]. *Atmos Environ*, 1998, **32**(14/15): 2627 − 2636.

[7] Luis E O, Beatriz M T. A method to estimate emission rates from industrial stacks based on neural networks [J]. *Chemosphere*, 2004, **57**(7): 691 − 696.

[8] Jensen R R, Karki S, Salehfar H. Artificial neural network-based estimation of mercury speciation in combustion flue gases[J]. *Fuel Processing Technology*, 2004, **85**(6/7): 451 − 462.

[9] Aleksander I, Morton H. *An introduction to neural computing* [M]. 2nd ed. London: Chapman and Hall, 1995.

利用人工神经网络理论预测电站锅炉汞组分的释放

杨宏旻[1,2] 周 波[1]

([1] 南京师范大学动力工程学院,南京 210042)
([2] 西肯塔基大学燃烧科学与环境技术研究所, 美国鲍灵格林 42101)

摘要:对利用人工神经网络方法来预测电站锅炉在未知的燃烧或运行工况下烟气中汞组分进行了可行性评估. 基于已掌握的三个电站锅炉现场测试的汞排放数据库,建立了一个三层误差反向传播神经网络模型用以对烟囱处汞排放的组分进行预测. 全部预测过程包括:数据的采集整理、构建人工神经网络模型、训练过程和误差评估4部分. 总共选取了59个煤样、灰样以及电站运行工况参数作为输入变量,利用部分实际汞排放测试数据来指导训练过程,其余的实测数据用来校验网络预测模型的准确性. 结果表明,模型获得的预测精度对单质汞元素的均方根误差为0.8 μg/Nm^3,对全汞的均方根误差为0.9 μg/Nm^3. 这样的误差在当考虑到现场采用半连续释放测量(SCEM)方法,由湿法测试模块所产生的峰值误差时是完全可以接受的.

关键词:汞组分;电力锅炉;预测;人工神经网络
中图分类号:X51