SIMULATION-BASED PREDICTIVE EMISSION MONITORING SYSTEM

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ABSTRACT

A development and investigation of mathematical models for Predictive Emission Monitoring Systems (PEMS) in order to reconstruct the missing data on the base of low frequent direct measurements are discussed. A comparative analysis is provided among variety of individual and hybrid models using real experimental data. Practical recommendations are derived for design of PEMS oriented to thermal power plants.

INTRODUCTION

The main functions of the emission monitoring systems in thermal power stations are the measurements and the registration of the harmful emissions and the preparation of the reports for the inspections for environmental protection.

The Regulating agencies in USA and in the countries of the EC have regulated two ways of reporting data (readings) formation in the emission monitoring systems (Eberhard 1995; Joseph and Macak 1996; Ekhus and Black; Gimonez et al.; EPA Handbook 1997; US Environmental Protection Agency 2000):

- By using direct measurements in the Continuous Emission Monitoring Systems (CEMS), which is the traditional approach;
- By using mathematical models based on the indirect measurements for realization of the ecological goals, known as Predictive Emission Monitoring Systems (PEMS).

In both of the reporting data sources the requirements of the national legislations (Bulgarian Ministry of Environmental Protection) and the statutory procedures and the standards in USA and EC should be satisfied (EPA Handbook 1997; Alberta Environmental Protection 1998; US Environmental Protection Agency 2000; Code of Federal Regulations, Part 60; Code of Federal Regulations, Part 75).

The Predictive Emission Monitoring has strengthened its position in USA and it's provided for with the respective normative documents (Eberhard 1995; Ekhus and Black; Topical Report №17 2001; Ghien et al. 2003). PEMS have been introduced in power stations in USA and Europe with total capacity of 10000 MW. The emission monitoring on the base of indirect measurements is considered as an alternative of the traditional approach (CEMS). Besides the carrying out of the basic functions, the predictive monitoring systems enable realization of optimal control of the combustion processes under the ecological restrictions, realization of some diagnostic functions as well as usage for generation of recommendations for operational and control activities, which will improve the total effectiveness of the equipment works on lower investment expenses.

The main goals of the current study are construction and investigation of mathematical models for PEMS applied to thermal power plant and development of procedures for missing data reconstruction on the base of low frequent direct measurements when CEMS and PEMS work together.

The criteria for discrimination of the particular solutions are: accuracy, validity for all the technological regimes, operational reliability and maintenance expenses.

RECONSTRUCTION OF THE MISSING DATA IN THE EMISSION MONITORING SYSTEMS

The aim of this study is development of Predictive Emission Monitoring Systems (PEMS) in thermal power station on the base of expert knowledge and by using simulation approach. The system for ecological monitoring of the considered project is realized as multiplex system for consecutive analysis of the pollutants for each gas outlet. The used scheme allows multifunctional carrying out of the Continuous Emission Monitoring Systems (CEMS) for realization of optimal control of the combustion processes except for performance of its main purpose. The time period of multiplexing of each gas outlet is To = 150 s (2.5 min). In this way the analysis data of oxygen (O_2), nitrogen oxides (NO_x) and sulphur dioxide (SO_2) for each gas outlet enter every 5 min, 10 min, or 15 min depending on the number of the working steam generators (respectively 1, 2 or 3).

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The determination of the substituted values of gas emissions of O_2, NO_x and SO_2 for each gas outlet (every 2.5 min) is accomplished according to the principals of the predictive emission monitoring. The high accuracy of the predictive emission monitoring makes it equivalent and in some cases better than the continuous emission monitoring or sometimes it's the only possible method.

The necessary information for reconstruction of the missing data of the components of the flue gases is delivered from two sources:

- From the continuous emission monitoring system, which analyses the concentrations of O_2, NO_x and SO_2 of the waste flue gases in each gas outlet at the above mentioned time intervals.
- The basic technological variables enter from the decentralized control system of the unit.

The using of simple interpolation methods is feasible only under certain regimes. In other cases the obtained substituted data contains considerable errors. That imposed development of methods for reconstruction of the missing data, which are valid in all the technological conditions. These methods could be classified as follows:

- without using of indirect sources of information – interpolation and/or filtration;
- by using indirect sources of information – regression relations and/or neural networks;
- combined approach – with interpolation and by using of indirect sources of information.

MATHEMATICAL MODELS FOR PEMS

Detailed analysis of the predictive abilities of eight types of mathematical models is provided. They describe the relationships between the O_2, NO_x and SO_2 concentration in one side flue gases duct as a function of the direct measurements in the same duct (but with a bigger sample time), the direct measurements of gases concentration in the neighbor duct and all available additional measurements received from SCADA or DCS.

The investigated mathematical models are given in Table 1.

The evaluation of the investigated mathematical models accuracy is accomplished by calculation the relative mean square error (MSE) (δ) between predicted and directly measured values for the same discrete time. The following formulas are used:

$$\delta = \frac{\sigma_C}{m_C} 100, \%, \quad (1)$$

where $\sigma_C = \frac{1}{N-1} \sum_{i=1}^{N} \left(\hat{C}_i - C_i^e \right)^2$,

$$m_C = \frac{1}{N} \sum_{i=1}^{N} C_i^e ,$$

where N is the size of the test data set; $\hat{C}_i$ are the predicted values of the gas concentrations obtained from the mathematical models and C_i^e are the corresponding measured values.

Table 1: Investigated mathematical models

№	Description of the used sources of information and the type of mathematical relationships	Notation
1	Equal concentrations in the output ducts A and B	MA1
2	Definition of the concentration using direct measurements and interpolation	MA2
3	Correction using the ratio between "wet" oxygen concentrations in the output ducts A and B	MA3
4	Mathematical models derived on the base of direct measurements	MA4
5	Hybrid mathematical models (direct measurements)	MA2+MA3
		MA2+MA4
		MA2+MA3+MA4
6	Model based on the ratio "front"/"back" oxygen concentration	MB1
7	Mathematical models on the base of control actions and states	MB2
	- Regressive models	MB21
	- Neural Network models	MB22
8	Combined mathematical model	MA2+MB2

The most appropriate mathematical models for development of predictive monitoring systems are presented and discussed in the following sections.

MATHEMATICAL MODELS USING DIRECT MEASUREMENTS

Concentration determination by interpolation of direct measurements (Model MA2)

Direct measurements only from CEMS during the corresponding sample time are used depending on the load of the power station. When one, two or three units work simultaneously direct measurements in each one of the gas outlets "left" (A) and "right" (B) are carried

out respectively every 5 min, 10 min or 15 min. The opportunity to reconstruct the missing measurements in order to provide a set with 2.5 min sample interval by interpolation is investigated.

The reconstruction of the missing data for the gas concentrations is accomplished using Lagrange interpolation polynomial. The interpolation approach defines a function f(x), which pass through given number of experimental measurements A_i (Fig. 1). Using this function the missing values B_1, B_2, B_3, B_4 and B_5 of the relevant component $y(x_i)$ are calculated.

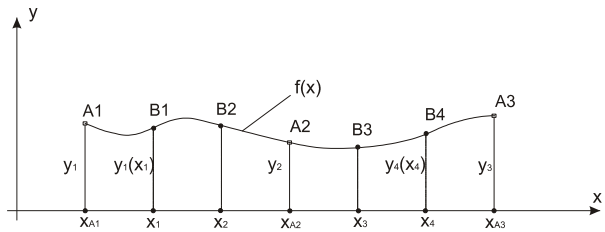

Figure 1: Interpolation procedure

The interpolation could be realized in the following way:

- depending on the number of the points used for interpolation (2, 3, 4,...);
- with averaging or not the interpolated values, using or not moving horizon of interpolation.

During the reconstruction of the missing values of NO_x the relative mean square error (δ) increases linearly depending on the sampling time. The results for δ are presented in Table 2.

Table 2: Summarized interpolation results

Number of the working units	One unit $T_0 = 5$ min	Two units $T_0 = 10$ min	Three units $T_0 = 15$ min
δ, %	3.48	5.45	6.79

Using of «wet» oxygen (Model MA3)

The information sources are:

- specially installed sensors on the base of zirconium oxide (ZrO_2) in each of the gas outlet ducts A and B, measuring continuously the concentrations of the "wet" oxygen O_2^{WAe} and O_2^{WBe};
- the Continuous Emission Monitoring Systems (CEMS).

The missing concentrations of the gas components O_2, NO_x and SO_2 in the gas outlet duct, where there is no current measurement when in the other gas outlet duct of the same unit there is measurement by the Continuous Emission Monitoring Systems (CEMS), are using linear relation. For example the missing concentration of NO_x^B in the outlet duct B is estimated using the following expression:

$$\hat{NO}_x^B = \frac{O_2^{WAe}}{O_2^{WBe}} NO_x^{Ae} \qquad (2)$$

In Table 3 the average values of the relative mean square error δ for the predicted estimations of NO_x and SO_2 obtained from the multitude simulations are presented.

Table 3: Average values of δ

Gas	NO_x	SO_2
δ, %	5.77	1.68

Mathematical models using the direct measurements in the gas outlet ducts A and B (Model MA4)

This mathematical model is created on the base of the data from the Decentralized Control System (DCS) and the Continuous Emission Monitoring Systems (CEMS).

The corresponding concentrations of the gas components in the ducts A and B O_2^{Ae}, NO_2^{Ae} and SO_2^{Ae} respectively O_2^{Be}, NO_2^{Be} and SO_2^{Be} are measured in accordance with the the set sequence for analysis. For calculation of the gas emission vector in the duct B $\hat{\mathbf{C}}_\mathbf{B}(k)$, when only the emissions in the duct A are measured, the next relation is used:

$$\hat{\mathbf{C}}_\mathbf{B}(k) = f(V^L, V^R, O_2^{fe}, O_2^{be}, T, O_2^{Ae}, O_2^{WBe}, NO_x^{Ae}, SO_2^{Ae}) \qquad (3)$$

The dependence for the emissions in the duct A is determined in analogous way.

The relative errors for prediction of the gas emissions from the mathematical models are given in Table 4.

Table 4: Relative errors of the gas emissions prediction

δ, %	O_2	NO_x	SO_2	$\bar{\delta}$
Exit flue A	3.46	3.22	3.74	3.47
Exit flue B	3.36	3.29	3.59	3.41

The experimental values (*) and the predictive values of the concentrations of NO_x in the duct B, where δ=3.29%, are illustrated at Figure 2.

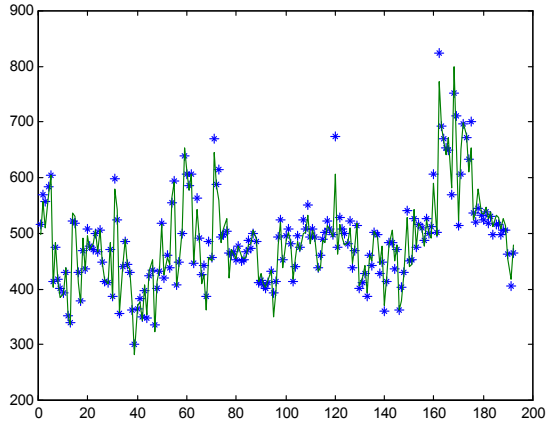

Figure 2: Experimental and predicted values of the NO_x concentrations

MATHEMATICAL MODELS BASED ON THE UNIT STATE AND CONTOL DATA (MODEL MB2)

The development of these mathematical models is based on the data from the unit Decentralized Control System. It's not necessary ecological monitoring system to be available. The physical insightconsiderations and the preliminary investigations of the models have shown their sensibility to the total air flow rate V and to the fuel flow rate B. The mathematical models are individually derived for prediction of the gas concentrations in each one of the exit ducts A and B. For example the created model for exit duct A has the following form:

$$\hat{\mathbf{C}}_{\mathbf{A}}(k) = f(B^L, B^R, V^L, V^R, O_2^{fe}, O_2^{be}, T) \qquad (4)$$

where $\hat{\mathbf{C}}_{\mathbf{A}}$ is a vector of the predicted concentrations of gas components $\hat{O}_2^A$, $N\hat{O}_x^A$ and $S\hat{O}_2^A$.

All the variables in the right part of the equation (4) are measured continuously and are defined as follows:

B^L and B^R are the fuel flow rate correspondingly in the left and in the right combustion chamber;

V^L and V^R are respectively the flow rate of the total air in left and right air duct;

O_2^{fm} and O_2^{bm} are the measured concentrations in the front and the back part of the corresponding combustion chamber;

T is the temperature before the secondary steam superheater.

Relation approximations by regressive models (Model MB21) and neural network models (Model MB22) are studied. The average values of the unit emissions of both flue gas ducts are accepted as representative value.

Regressive models (Model MB21)

In Table 5 the relative mean square errors (δ) of the predicted values of the gas concentrations, given from the regressive model (Model MB21) in comperison to the real experimental data are shown.

Table 5: Results from the regressive model

Gas	O_2	NO_x	SO_2
δ, %	3.22	6.91	4.07

Neural network models (Model MB22)

According to the dependence (4) mathematical models based on neural networks (Model MB22) for prediction of the concentrations of O_2, NO_x and SO_2 in each of the gas outlet ducts A and B are developed. The highest prediction accuracy is achieved by using two layers neural networks of Cascade-Forward Backdrop type with sigmoid transfer function in the hidden layer and with linear one in the output layer.

The relative mean square error (δ), comparing the predicted values of the gas concentrations towards the real experimental data, are given in Table 6.

Table 6: Results from the neural models

Gas	O_2	NO_x	SO_2
δ, %	2.83	6.60	2.92

HYBRID MATHEMATICAL MODELS

Combining different types of modeling techniques the total estimation accuracy could be improved with 10-15% (Hadjiski 1999). Extensive simulation studies on the possibilities of combining the considered mathematical models and other created mathematical models in hybrid ones are carried out. The aggregation is performed by weighted summation of the models outputs. Under aggregation of two mathematical models the predicted concentration of the analyzed gas component $\hat{C}_i$ obtained from the hybrid model is calculated as follows:

$$\hat{C}_i = \alpha_i \hat{C}_{1i} + (1-\alpha_i)\hat{C}_{2i} \qquad (5)$$

By analogy at aggregation of three mathematical models the expression for $\hat{C}_i$ is:

$$\hat{C}_i = \alpha_i \hat{C}_{1i} + \beta_i \hat{C}_{2i} + (1-\alpha_i-\beta_i)\hat{C}_{3i} \qquad (6)$$

The index i in the expressions (5) and (6) is addressed to one of the gases O_2, NO_x or SO_2. The predicted concentrations of the considered gas on the individual mathematical models are denoted by $\hat{C}_{1i}, \hat{C}_{2i}$ and $\hat{C}_{3i}$. α_i and β_i represent weight coefficients, varying in the interval [0,1].

The selection of the combination of the individual mathematical models, which are investigated to be aggregated, is accomplished taking into account such criteria as accuracy, reliability of the measurement and the costs minimization for sensors and analyzers of the gas components.

A procedure for aggregation of the mathematical models, based on the methods of the nonlinear programming is proposed. In this procedure the independent variables are α_i and β_i. The objective function is equation (1) of the relative mean square error δ_i for the concentration $\hat{C}_i$, estimated by using expressions (5) or (6). The suggested procedure is developed on the base of parallel simulation computations of the individual models for test data sets completed with experimental data of the gas concentrations and subsequent aggregation of the models. On Figure 3 a graphic illustration of created hybrid mathematical model, applying the proposed aggregation procedure is presented.

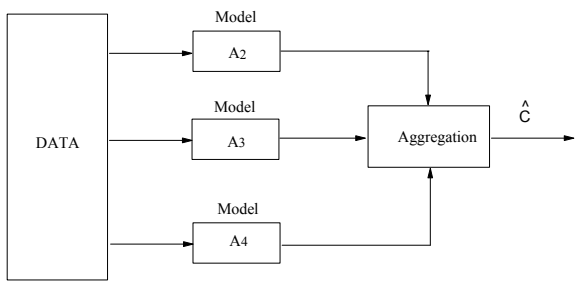

Figure 3: Hybrid mathematical model

Numerous statistical analyses have shown the dominant efficiency of the next three combinations of models used direct measurements:

1. Interpolation model (MA2) and model based on the ratio of the oxygen content in flue gas ducts A and B (MA3)

2. Interpolation model (MA2) and model based on the direct measurements (MA4)

3. Interpolation model (MA2), model using "wet" oxygen (MA3) and model based on the direct measurements (MA4).

A variety of combinations of models MA2, MA3 and MA4 with the models MB1 and MB2 are possible. The carried out analysis has shown that the hybrid models of type MA2+MB2 are more perspective for the purposes of the ecological monitoring.

The results of the accuracy evaluation of the individual models and of the hybrid models are summarized in Table 7. The investigated models are ranged according to their accuracy.

Table 7: Ranging of the models on their accuracy

Notation	Mean square error δ, %	Range position
MA1	10.7	12
MA2	6.79	10
MA3	3.72	2
MA4	3.44	1
MA2+MA3	6.43	9
MA2+MA4	6.33	8
MA2+MA3+MA4	5.4	6
MB1	9.7	11
MB21	4.73	4
MB22	4.12	3
MA2+MB21	5.91	7
MA2+MB22	5.14	5

CONCLUSIONS

The simulation results using developed algorithms for reconstruction of the missing data of the flue gases concentration could be summarized as follows:

1. The methods using direct measurements guarantee higher accuracy.

2. The ranging of the methods on the average relative mean quadratic error, presented in Table 7, shows distinguish priority of the methods based on models using direct measurements (MA4) and on measuring the "wet" oxygen (MA3).

3. The results obtained from the model based on measuring of "wet" oxygen (MA3) depend only on the direct measurement data and they are not influenced by the operational conditions. That permits these algorithms to be used in the whole range of technological regimes, namely static, quasi-static and dynamic, without applying of any adaptive procedures.

4. If during the exploatation of the "wet" oxygen sensor some difficulties of fouling and similar ones appear, which decrease the measuring precision, the interpolation model (MA2) will

remain to be efficient with the previous accuracy.

5. The hybrid mathematical model (MA2+MA3+MA4) (Figure 3) guarantee high accuracy. The eventual automatic elimination consequently of the models MA3 and MA4 will maintain the efficiency of the emission monitoring system. Thus the hybrid model (MA2+MA3+MA4) possesses robust properties with respect to the measuring conditions.

6. The models using data from the Decentralized Control System are more important in solving the task of optimization of the combustion process in the steam generators under the ecological restrictions for the gas emissions and when Continuous Emission Monitoring Systems (CEMS) is not available.

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