

MATHEMATICAL MODEL OF NO_x PRODUCTION AND EFFECT OF UNDERPRESSURE ON THEIR PRODUCTION

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ABSTRACT

A large number of the studies have indicated that chemical indoor air pollution has become an important environmental factor which influences the population's health. Nitrogen monoxide and nitrogen dioxide are mainly produced by combustion at high temperatures and are formed by reactions between nitrogen and oxygen. Both nitrogen in the fuel and nitrogen in the air participate in reaction, NO is further oxidized and transferred into NO₂ in the atmosphere. Nitrogen dioxide is the most toxic of the nitrogen oxides and is the most important from view-point of health.

In Slovakia it is possible to assess that about 40% of the emissions of nitrogen oxides originate from road traffic, about 50% from combustion and about 10% come from industrial processes. During several last years the emissions of nitrogen oxides have increased. There are great differences between annual average value of nitrogen in the countryside and in the big cities. Outdoor average concentration level of nitrogen oxides are presented.

People are mainly exposed to indoor nitrogen oxides. Indoor air can be contaminated from the use of gas for heating and cooking appliances. The most important indoor source of nitrogen oxides is gas burning in the kitchen. Finally concerning the indoor environment, indoor air can be contaminated by using gas for heating and cooking and this probably involves a certain health hazard. Indoor average concentrations level of nitrogen oxides are also presented. In order to improve the chemical indoor air quality we need to estimate the indoor sources NO_x production. The aims of this paper are to survey the occurrence of nitrogen oxides exposure in the building environment and to estimate the indoor NO_x production on the base of the mathematical model using the dimensional analysis. The own model of NO_x production in steam boilers based on supporting characteristic variables, which are connected with the combustion process is presented by authors. As well the comparison of results obtained from direct measurements with the results obtained from the created mathematical model has been accomplished.

KEYWORDS

Nitrogen oxides, mathematical model, indoor environment.

INTRODUCTION

It is well-known that the oxide of nitrogen production in the combustion products is the process that has not been exactly described so far on all variables which are connected with its production. According to as the crucial are considered the main factors:

excess of combustion air, recirculation of combustion products, multistage supply of the combustion air, multistage combustion and construction of burners.

It is very difficult to influence the NO_x production through some of the above mentioned factors. Regulation of combustion process by means of change in the amount of combustion air would provide a possibility and after essential boiler reconstruction comes into consideration the oxides of nitrogen production regulation in combustion process by means of combustion products recirculation.

A rare approach to the NO_x production determination brings Prof. Karták. Mathematical models presented by him intervene into the field of chemical composition of coal, determination of the solid coal weight shares in combustible matter, weight content of nitrogen in combustible matter, weight volatile share in combustible matter etc. which the common runner of the combustion device cannot find out through simple methods accessible to his technical equipment possibilities.

At heating up of the coal particle before ignition in the furnace the gaseous combustible matter and nitrogenous substances liberate. With regard to the high concentration of oxygen the burning of gaseous components is realized kinetically with intensive NO formation. Through burning up of the gaseous components the content of nitrogenous substances in the mixture decreases and in further increase of nitrogenous substances the formation of NO is less intensive regarding to the lower oxygen content and diffusive rundown of the process. The share of NO formed by kinetic or diffusive way is but approximately the same considering the different period of duration in the individual stages. The concept on the course of burning of nitrogenous substances in two stages justifies also the effect of the outgassing speed on the CO content.

The difficulty in prediction of the NO_x emissions amount during combustion of fossil fuels is caused mostly by the complexity of the mechanism in oxide of nitrogen origin which depends on many factors. Some partial mechanisms are not quite clarified so far and it is not possible to describe them exactly. Also the empirical correlations among the fuel properties, combustion regime and NO_x emissions are not sufficiently known. For informative calculations are used the mathematical models of NO_x production. These are usually assembled from the results obtained from bigger amount of laboratory measurements and measurements on real objects.

PARAMETERS FOR MATHEMATICAL NO_x PRODUCTION MODEL

As it is not always possible to influence the NO_x production on the existing devices by means of the above presented factors, new ways of intervention into the combustion process are searched with the aim to reduce the oxide of nitrogen production to the possibly minimum limit. The research task of oxide of nitrogen production in combustion process was to find out the measure of NO_x influencing by means of regulation in such parameters which the combustion process directly characterize, i.e. fuel efficiency Q [J/s], amount of the combustion air Q [m/s], underpressure in boiler p [Pa] and parameters which characterize the combustion device, i.e., e.g., rated boiler capacity P [kg/s].

All the given variables are presented in basic dimensions, what is at the same time a condition to utilize the dimensional analysis for creation the NO_x production mathematical model.

All these variables are simply measurable directly in operation, what allows us subsequently to compare the NO_x production during particular working conditions on the chosen combustion device on the basis of direct measurements and by means of the created mathematical model described in the following chapter.

APPLICATION OF DIMENSIONAL ANALYSIS

Mathematical model describing NO_x formation is based on formation of dimensionless arguments π_i from the stated variables influencing the oxide of nitrogen formation. Their valuable property is, that in all existing systems of units they have the same numerical size and they have no dimension.

Formation of a mathematical model rests in derivation of functional dependence from the expressed dimensionless variables which in general has always exponential character. Transformation of this function into logarithmic coordinates corresponds to linear character, that makes the work with model easier and enables simply to determine the parameters of linear function. The model presented in the article has a universal validity for all combustion devices, that are noted for at least approximate geometric characteristics. For every combustion device the parameters of linear function i.e. the location constant and regression coefficient has to be determined separately. Construction of the model starts from the assumption that in the combustion device there is no sucking of the wrong air through leakages ($Q_n = \text{const.}$) and the existing type of the flame is respected.

The general relation among the selected variables which effect the combustion process and the NO_x production can be put down in the form

$$\Psi (Q_u, P_k, Q_{vz}, p_p, \text{NO}_x) = 0 \quad (1)$$

The created dimensional matrix-relation (2) has the rank of matrix $r = 3$ and its lines are dimensionally independent on themselves. From $n = 5$ independent variables at rank of the matrix r , can be set up $n-r$ of dimensionless arguments.

	Q_u	P_k	Q_{vz}	P_p	NO_x
m	2	0	3	-1	-3
s	-2	-1	-1	-2	0
kg	0	1	0	1	1

For the general form of the argument π is valid

$$\pi = Q_u^{x_1} \cdot P_k^{x_2} \cdot Q_{vz}^{x_3} \cdot p_p^{x_4} \cdot \text{NO}_x^{x_5} \quad (3)$$

From the condition that the left side identically equals to one (ordinary number Π), the resulting exponent of every basic dimension equals to zero. By applying this condition for every from r basic dimensions we obtain a system of three linear equations with five unknowns. To solve it we have to select two unknowns (and this always twice) and to calculate the rest.

For the selected $x_4 = 0$ and $x_5 = 1$ the exponents will be calculated from the linear equations system $x_1 = 0, x_2 = -1, x_3 = 1$

For the selected $x_4 = 1$ and $x_5 = 0$ the exponents will be calculated from the linear equations system $x_1 = -1, x_2 = -1, x_3 = 1$.

For dimensional arguments is then valid:

	x_1	x_2	x_3	x_4	x_5
π_1	0	-1	1	0	1
π_2	-1	-1	1	1	0

The searched dimensional homogeneous function in dimensionless form is

$$\Psi (\pi_1, \pi_2) = 0, \quad (4)$$

or after adjustment and backward transformation of dimensions for the particular variables, the function will have the form

$$\Psi \left(\frac{Q_{vz} \cdot NO_x}{P_k}, \frac{Q_{vz} \cdot P_p}{Q_u \cdot P_k} \right) = 0 \quad (5)$$

The real course of the dependence of dimensionless arguments π_1 to π_2 calculated according to the relation (5) from the measured values.

The transformation of the relation (5) in logarithmic coordinates represents the equation of the straight line the course of which is shown on figure 1

$$\pi_1 = A \cdot \pi_2^B \quad (6)$$

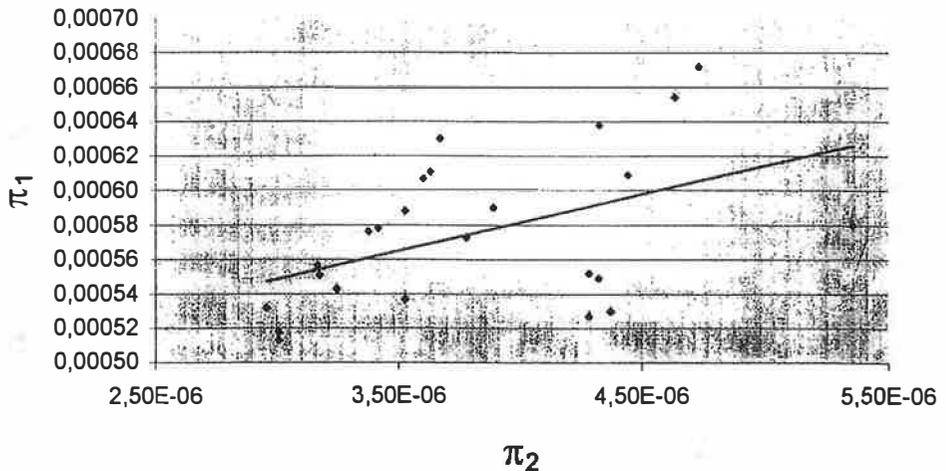


Figure 1 The logarithmic π_1 and π_2 dependence

After completing of relation (6) by relation (5) and its modification we obtain the relation characterizing the NO_x production in the form

$$NO_x = A \cdot P_k^{1-B} \cdot Q_{vz}^{B-1} \cdot Q_u^{-B} \cdot p_p^B \quad (7)$$

Regression straight line for the calculation of location constant A and of the regression coefficient B by the method of the smallest squares from the relation (6) has the form:

$$\log \pi_1 = \log A + B \cdot \log \pi_2 \quad (8)$$

or in general

$$y = a + b \cdot x$$

On the basis of the calculated coefficients a and b, the coefficients A and B for the straight line in logarithmic coordinates are determined. The location constant A, i.e. the

distance on the axis π_1 , from the starting point of the coordinates system and the regression coefficient B i.e. the line slope is evaluated for the given type of the combustion device on the basis of measurements of individual relevant variables according to the following relations:

$$a = \frac{\sum x_i^2 \cdot \sum y_i - \sum x_i \sum x_i \cdot y_i}{n \cdot \sum x_i^2 - (\sum x_i)^2}$$

$$b = \frac{n \cdot \sum x_i \cdot y_i - \sum x_i \cdot \sum y_i}{n \cdot \sum x_i^2 - (\sum x_i)^2}$$

where $\sum x_i = \sum \log \pi_2$ (1..... 24 measurements)
 $\sum y_i = \sum \log \pi_1$ (1..... 24 measurements)

For the boiler at its rated boiler capacity from 180 t/hour to 210 t/hour were during combustion of bituminous coal at fuel efficiency from 24.35 MJ/kg to 25.15MJ/kg calculated the coefficient $a = -2,0095$ and the coefficient $b = 0,227088$.

Because $a = \log A \Rightarrow A = 10^a = 10^{-2,0095}$, then $A = 0,009784$
 $b = B \Rightarrow B = 0,227088$.

For the given combustion device the NO_x production will be regulated by the adjusted relation (7) in the form

$$\text{NO}_x = 0,009784 \cdot P_k^{0,77291} \cdot Q_{vz}^{-0,77291} \cdot Q_u^{-0,227088} \cdot p_p^{0,227088} \quad (9)$$

Under the assumption, that the heating power of the fuel will be during the combustion process taken as constant, it is possible to regulate the production of NO_x emissions during the constant rated boiler capacity by means of the amount of the combustion air and underpressure of the combustion products.

$$\text{NO}_x = K_1 \cdot Q_{vz}^{b-1} \cdot p_p^b \quad (10)$$

where $K_1 = 0,009784 \cdot P_k^{0,772912} \cdot p_p^{-0,227088}$

The amount of the combustion air Q_{vz} for the required rated boiler capacity is calculated by the control automatic machine. It modifies then this amount automatically according to the relation (10) to the constant

$$K_2 = Q_{vz}^{b-1}, \quad t.j. \quad K_2 = Q_{vz}^{-0,77291}$$

The working regime of the boiler will be then characterized by creation of oxides of nitrogen which will be controlled by the functional dependence of the form

$$NO_x = K \cdot p_p^{0,227088} \quad (11)$$

where $K = K_1 \cdot K_2$

From the view of the possible regulation of combustion process in the next step the maximum allowed value of the produced NO_x is selected and from the relation (11) the required underpressure to achieve this selected value is subsequently determined and this must fully respect also the stability of burning. Regulation of underpressure will be realized by regulation of blower fans load.

RESULTS OBTAINED FROM DIRECT MEASUREMENTS AND FROM THE MATHEMATICAL MODEL

Examination of the possibility in NO_x creation regulation by regulation of combustion products underpressure according to the relation (11) has been accomplished for the underpressure range from 2 to 100 Pa. Respecting the stability of burning the information on NO_x formation obtained from direct measurements and from the mathematical model in the field of combustion products underpressure between 50 and 110 Pa will be decisive.

Figure 2 represents the dependence of NO_x formation at the rated boiler capacity of $P_k = 50$ kg/s, of the fuel efficiency $Q_n = 25150000$ J/kg and the amount of combustion air $Q_{vz} = 61,11111$ m³/s. At underpressure $P_p = 110$ Pa through direct measurement the searched value of combustion products was $NO_x = 475$ mg/m³ and by means of calculation from the model the oxide of nitrogen production is 508 mg/m³. The relative mistake in NO_x determination in this case is rather big and it represents 7.01561 % in comparison with the measured value. By underpressure regulation in the field of the burning stability the decrease of the oxide of nitrogen production can be achieved from the maximum value 508 mg/m³ of combustion products to 425 mg/m³, which represents a 17 % decrease of nitrogen during the boiler performance at underpressure of 50 Pa in comparison with its performance at the underpressure of 110 Pa.

Figure 3 presents the NO_x dependence on the amount of the combustion air at constant underpressure in the field of burning stability. The underpressure reduction to the lower limit of the burning stability brings also the reduced oxides of nitrogen production. Maximum reduction of oxide of nitrogen production during performance of the boiler on the lower limit of burning stability brings in the followed field of the combustion air amount change a decrease of NO_x by cca 80 mg/m³ of combustion products

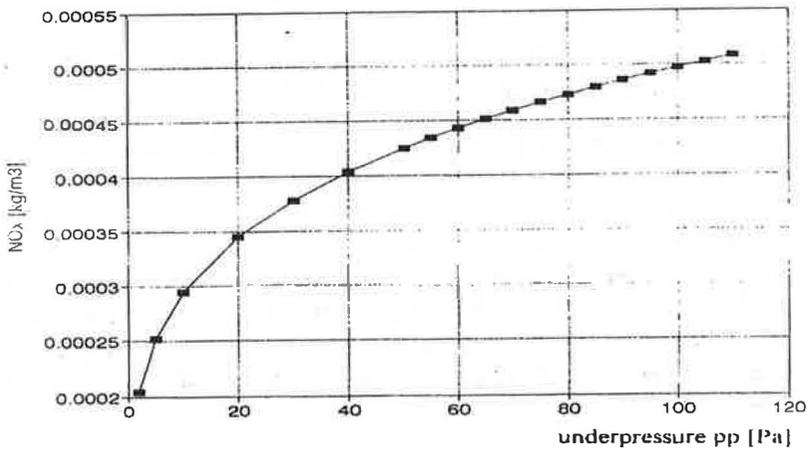


Figure 2 The NO_x production dependence on underpressure

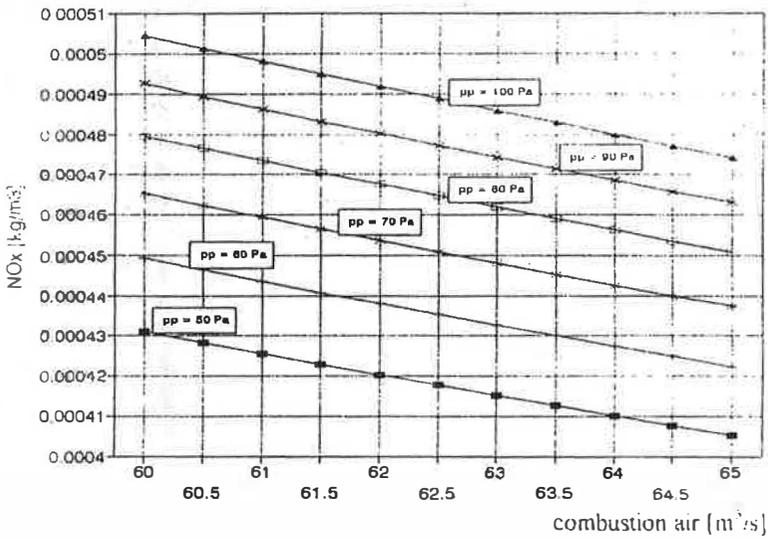


Figure 3 The NO_x production dependence on combustion air

CONCLUSION

The selected relevant variables for construction of the mathematical model presented in the article do not give a true picture of the combustion process considering the NO_x production wholly and exactly. But these are the variables which the runner of combustion devices can regulate by simply procedures and so partly effect the NO_x production.

The model has been tested and the mistake in the nitrogen oxide determination from measurements and by means of mathematical model at the number of measurements 24 moved from + 10 to -12 %. The presented mistake values occurred in the whole system of measurement only once and therefore we can consider them as irrelevant. In case of extending the model by further variables a more distinct coincidence in the measured and calculated values can be expected.

Also despite the big relative mistake in the measured and calculated NO_x values, it can be stated, that the presented mathematical model can serve for approximate determination of nitrogen oxide in the combustion process of fossil fuels and more it showed the essential trends in the possibility of NO_x production influencing in particular combustion devices.

REFERENCES

- Ibler, Z. and Kartak, J. (1990) *No_x Model Estimation during combustion of Fossil Fuels*, Energetics, 40/9/10
- Mihal'ov, P., Čarnogurska, M. and Schvarzbacherová, E. (1997) *A dimenzionális elemzés felhasználása za No_x alakulásának leírásánál*. Micro CAD '97. *Proceedings International Computer Science Conference*. Miskolc, Hungary.