Approximate Modelling of Nitrogen Oxide Production from Solid Fuel Combustion

Mária Čarnogurská[1*], Miroslav Příhoda[2]

[1]Department of Power Engineering, Faculty of Mechanical Engineering, Technical University of Košice, 042 00 Košice, Slovak Republic.

[2]Department of Thermal Engineering, Faculty of Materials Science and Technology, VSB – Technical University of Ostrava, 708 33 Ostrava-Poruba, Czech Republic.

*Corresponding Author

Received: 08 February 2023/ Revised: 15 February 2023/ Accepted: 20 February 2023/ Published: 28-02-2023

***Abstract*—** *The mathematical model of nitrogen oxides production described in the paper is developed on the basis of dimensional analysis. The theory of dimensional analysis is used when a mathematical description of a phenomenon is lacking. The aim of using this method was to find out what is the relationship between the parameters of an operating hard coal combustion plant (boiler output, fuel calorific value, quantity and temperature of combustion air, negative pressure in the boiler and flue gas temperature) and the nitrogen oxides produced. The results obtained from the developed model are compared with the values measured on a real device.*

***Keywords*— modelling, dimensional analysis, nitrogen oxides.**

I. INTRODUCTION

The production of nitrogen oxides during the combustion of fossil fuels in large boilers is influenced by a number of operating parameters. The dependence between the amount of nitrogen oxides produced and the individual parameters can also be expressed by means of dimensional analysis. The NO_x generation model described in the paper was developed based on the results of measurements on a specific boiler. The information obtained from a given boiler can then be transferred to any other boiler that is physically similar to the analysed model.

II. DESCRIPTION OF THE MODEL

Currently, several mathematical models of nitrogen oxide production are known [1-3], which are based on the analysis of fuel composition and combustion reaction rates. Knowledge of the fuel composition and reaction rates is not sufficient to describe the actual combustion process in detail. Therefore, the derived models are not always relevant. Other research works [4-5] investigate e.g. the residence time of powdered fuel in the reduction zone or simulate the combustion process using CFD methods.

Dimensional analysis, based on the principle of dimensional homogeneity of equations, was used to derive the presented mathematical model. In the general case, it is always a complete physical equation that expresses the dependence of a total of n selected relevant physical quantities V_1, V_2, ..., V_n of different dimensions [6-9]. The equation has the form:

$$\varphi\left(V_1, V_2, ..., V_n\right) = 0 \tag{1}$$

Of the relevant quantities affecting NO_x emissions, those that characterise the operation of the boiler were included in the mathematical model. These quantities were selected based on the experience of the boiler operator. The values of all quantities were measured continuously. These are:

- ✓ lower calorific value of coal Q_c $(\mathrm{J \cdot kg^{-1}})$
- ✓ mass flow rate of steam $Q_{m,s}$ $(\mathrm{kg \cdot s^{-1}})$

- ✓ volume flow rate of combustion air $Q_{V,\mathrm{air}}$ ($m^3 \cdot s^{-1}$)
- ✓ negative pressure in the boiler p_v (Pa)
- ✓ flue gas temperature at boiler outlet T_{fg} (K)
- ✓ combustion air temperature T_{air} (K)

Relation (1) for selected relevant quantities, including nitrogen oxides, takes the form

$$f(Q_c, Q_{m,s}\; Q_{V,\mathrm{air}}, p_v, NO_x, T_{fg}, T_{air}) = 0 \tag{2}$$

Temperature occurs twice in the selected quantities in relation (2). Measurements on the boiler analysed showed that the T_{fg}/T_{air} ratio was practically unchanged. Its value was 0.852. In the next solution, according to the rules of dimensional analysis, the temperature can occur only once. In the following model it is the flue gas temperature at the boiler outlet T_{fg}.

The constructed dimensional matrix is made of all dimensions of the selected quantities. The condition for the use of dimensional analysis is that the units of the respective physical quantities in the dimensional matrix are transformed into SI units. E.g. Q_c ($J \cdot kg^{-1} \approx N \cdot m \cdot kg^{-1} \approx kg \cdot m \cdot s^{-2} \cdot m \cdot kg^{-1} = m^2 \cdot s^{-2}$).

For the six selected quantities, the matrix will have n = 6 columns and m = 4 rows. Its shape is

$$\begin{array}{c} \\ \mathrm{m} \\ \mathrm{s} \\ \mathrm{kg} \\ \mathrm{K} \end{array} \begin{array}{cccccc} Q_c & Q_{m,s} & Q_{V,\mathrm{air}} & p_v & NO_x & T_{fg} \\ 2 & 0 & 3 & -1 & -3 & 0 \\ -2 & -1 & -1 & -2 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{array} \tag{3}$$

Finding dimensionless arguments (similarity criteria) that indicate the interdependence of the selected variables is done by the following procedure. The matrix (3) is split into two parts. One part represents the square matrix and the other part the complementary matrix (4). The unknown quantities x_1 to x_6 are added to both matrices so that their indices reflect the order of the selected quantity in the respective matrix - see equation (6)

$$\left\| \begin{array}{cccc} 2 & 0 & 3 & 0 \\ -2 & -1 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{array} \right\| \cdot \left\| \begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_6 \end{array} \right\| = (-1) \cdot \left\| \begin{array}{cc} -3 & -1 \\ 0 & -2 \\ 1 & 1 \\ 0 & 0 \end{array} \right\| \cdot \left\| \begin{array}{c} x_5 \\ x_4 \end{array} \right\| \tag{4}$$

From equation (4), the unknown quantities x_1 to x_6 are found. These unknowns then characterize the dimensionless arguments π for which

$$\pi = \prod_{i=1}^{n} V_i^{x_i} \tag{5}$$

Then one can write

$$\pi = Q_c^{x_1} \cdot Q_{m,s}^{x_2} \cdot Q_{V,\mathrm{air}}^{x_3} \cdot p_v^{x_4} \cdot NO_x^{x_5} \cdot T_{fg}^{x_6} \tag{6}$$

The choice of the redundant unknowns x_5 and x_4 from the right-hand side of equation (4) is made twice according to procedure (7)

$$\begin{array}{r} \\ \text{1. st sel.} \\ \text{2. nd sel.} \end{array} \begin{array}{cc} x_5 & x_4 \\ 1 & 0 \\ 0 & 1 \end{array} \tag{7}$$

The solution of equation (4) leads to a system of linear equations of the form

$$\begin{array}{rcl} 2\cdot x_1 \quad +3\cdot x_3 & = & 3\cdot x_5 \quad +x_4 \\ -2\cdot x_1 \quad - \; x_2 \quad - \; x_3 & = & 2\cdot x_4 \\ x_2 & = & -x_5 \quad -x_4 \\ x_6 & = & 0 \end{array} \tag{8}$$

The solution of system (8) results in two independent vectors (dimensionless arguments) π .

$$\begin{array}{c|cccccc|} & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \\ \pi_1 & 0 & -1 & 1 & 0 & 1 & 0 \\ \pi_2 & -1 & -1 & 1 & 1 & 0 & 0 \end{array} \tag{9}$$

The "minus" sign for a given unknown x_i, in the solution (9) indicates that the physical quantity in relation (6), amplified to the corresponding unknown x_i, will be in the denominator of the resulting argument, and the "plus" sign informs that the corresponding quantity will be in the numerator. Based on the above, two dimensionless arguments π of the form (10) can be established

$$\pi_1 = \frac{Q_{V,\text{air}} \cdot NO_{\text{x}}}{Q_{m,\text{s}}} \quad (1) \quad \text{and} \quad \pi_2 = \frac{Q_{V,\text{air}} \cdot p_{\text{v}}}{Q_{\text{c}} \cdot Q_{m,\text{s}}} \quad (1) \tag{10}$$

Dividing criterion π_1 by criterion π_2 yields a new criterion π_3 of the form (11)

$$\pi_3 = \frac{Q_{\text{c}} \cdot NO_{\text{x}}}{p_{\text{v}}} \quad (1) \tag{11}$$

Since the dimensionless argument π_3 contains the quantity NO_{x}, the dependence of which on other quantities in the black coal combustion process we want to determine, this argument can be expressed as a function of the argument π_2

$$\pi_3 = \varphi(\pi_2) \tag{12}$$

The argument π_3 can be displayed as a function of the dependent variable of the function π_2 in power form (13)

$$\pi_3 = A \cdot \pi_2^B \quad (1) \tag{13}$$

Logarithming equation (13) yields a line equation of the form

$$\log \pi_3 = \log A + \log B \cdot \log \pi_2 \tag{14}$$

The constant *A* and the regression coefficient *B* can be determined e.g. using an Excel spreadsheet (Fig. 1 and Fig. 2). Their values are $A = 0.0117$, $B = -0.7584$.

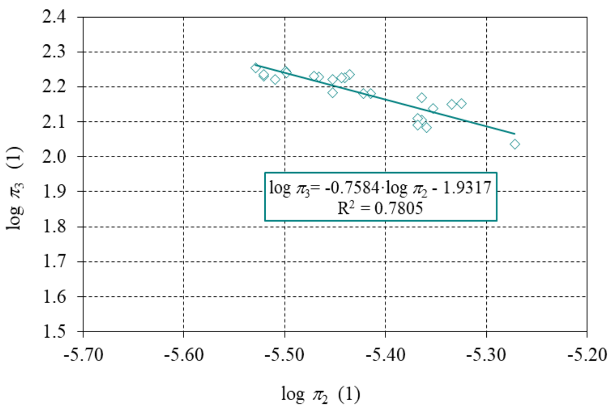

FIGURE 1: Dependence of dimensionless arguments in the sense of equation (14)

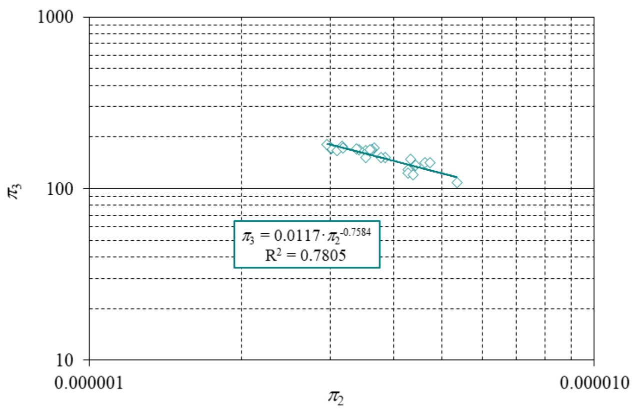

FIGURE 2: Dependence of dimensionless arguments in the sense of equation (13)

With the help of dimensional analysis, the NO_x production formation model will have the following form of dependence of the relevant dimensional quantities during the burning of black coal according to (13)

$$\frac{Q_c \cdot NO_x}{p_v} = A \cdot \left(\frac{Q_{V,air} \cdot p_v}{Q_c \cdot Q_{m,s}} \right)^B \tag{15}$$

The functional dependence of the formation of nitrogen oxides on other operating parameters will be in the form

$$NO_x = A \cdot Q_{V,air}^B \cdot Q_{m,s}^{-B} \cdot p_v^{1+B} \cdot Q_c^{-1-B} \tag{16}$$

After adding the calculated values of the constant A and the regression coefficient B to the expression (16), the relation for the production of nitrogen oxide has the form

$$NO_x = 0.0117 \cdot \left(\frac{Q_{V,air}}{Q_{m,s}} \right)^{-0.7584} \cdot \left(\frac{p_v}{Q_c} \right)^{1-0.7584} \quad (\text{kg·m}^{-3}) \tag{17}$$

The general shape of the dependence of NO_x on selected relevant quantities is represented by the expression (18)

$$NO_x = C \cdot \left(\frac{Q_{V,air}}{Q_{m,s}} \right)^m \cdot \left(\frac{p_v}{Q_c} \right)^n \quad (\text{kg·m}^{-3}) \tag{18}$$

where individual constants represent values: C = 0.0117, m = -0.7584, n = 0.2416.

Relationship (18) represents a mathematical model of NO_x production during the burning of black coal. Based on it, the calculated values of produced NO_x at specific measured values of the relevant variables are shown in Fig. 3. The deviation in NO_x expression ranges from +9.92 to -12.23%. The mean deviation is -0.21%.

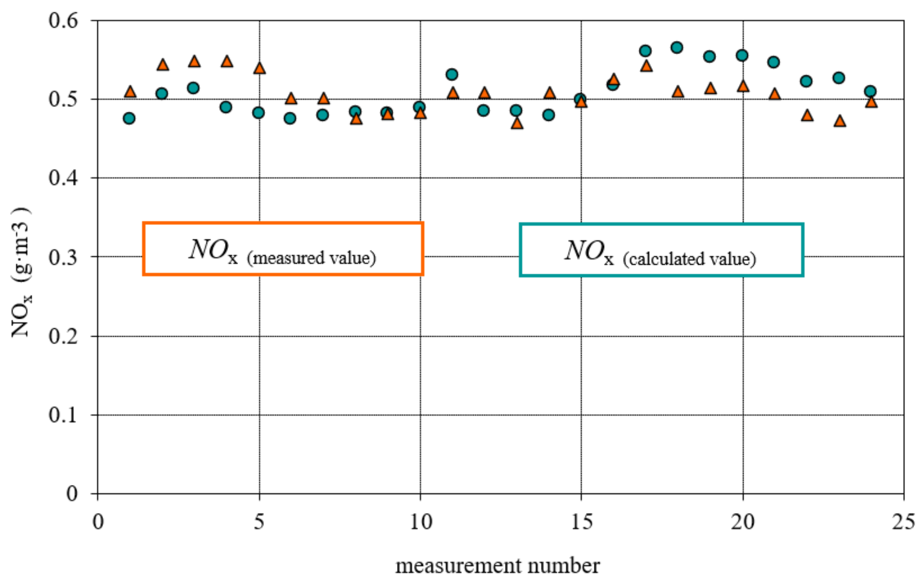

FIGURE 3: Measured and calculated NO_x values

III. CONCLUSION

The difference between the measured and calculated values according to relation (18) can be justified by the fact that, when choosing the relevant quantities, all the influences on which NO_x depends on the combustion of fossil fuels were certainly not taken into account. For a more relevant description of the combustion process it would be necessary to include flame temperature among the selected variables. Because its measurement in online operation of the boiler is a problem, it was not included in the basic model of the boiler. Another variable that could be considered is the mass flow of the coal burned. In addition, the presented results are from a relatively small sample of measurements (only 24). With a large enough sample of data (on the order of 10^2), the results would be more accurate [10].

When using a method for determining NO_x production based on dimensional analysis, it is irrelevant to know the details of the combustion device itself, regarding its construction, combustion air distribution system, location of burners, etc. It is also irrelevant to investigate what happens if it changes during combustion, e.g. fuel moisture. All these influences are reflected in the model in the measured values of the quantities that make up the model itself.

ACKNOWLEDGEMENTS

This paper was written with the financial support of the granting agency VEGA within the project solution 1/0532/22 and from FMT VŠB-TUO within the project solutions SP 2023/034.

REFERENCES

[1] J. B. Zeľdovič, G. I. Barenblatt, V. B. Librovič, G. M. Machviladze, "Mathematical theory of combustion and explosion". Nauka, Moscow, 1980, p. 31-35, (in Russian).

[2] Z. Ibler, J. Karták, "Models for calculating the emission of nitrogen oxide during the combustion of fossil fuels". Energetika, 1990, 40/9/10, p. 346-347. (in Czech).

[3] L. J. Muzio, G. C. Quartucy, "Implementing NO_x Control: Research to application. Prog. Energy Combust. Sci," 1997, 23, 233-266. PII: SO360-12&5(a7)00002-6.

[4] M. Xu, J. L. T. Azevedo, M. G. Carvalho, "Modelling of the combustion process and NO_x emission in a utility boiler". 2000. Fuel, 79, 13, 1611-1619.

[5] J. Zhu., Q. Lu, T. Niu, G. Song, N. Yongjie, "NO emission on pulverized coal combustion in high temperature air from circulating fluidized bed - An experimental study." 2009. Fuel Processing Technology, 90, 5, 664-670.

[6] M. Čarnogurská, "Dimensional analysis and the theory of similarity and modeling in practice". Košice, Elfa, s. r. o., 1998, 64 p. (in Slovak).

[7] J. Kožešník, „Physical similarity and construction of models". Jčm+f, Praha 1948. (in Czech).

[8] J. Kožešník, "Similarity theory and modeling". Academia, Praha 1983. (in Czech).

[9] M. Čarnogurská, "Fundamentals of mathematical and physical modeling in fluid mechanics and thermodynamics". Vienala, Košice, 2000, 176 s., (in Slovak).

[10] http://www.fhpv.unipo.sk/cvt/statistika/stbasic2.htm, online 27.1.2023.