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# Modelling of nitrogen oxides distribution in the hearth of gas-fired industrial furnace

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**Abstract:** A model is proposed for calculating the formation and transportation of nitrogen oxides in the combustion chamber of an industrial furnace heated by gaseous fuels burning. The calculations use a three-dimensional stationary description of turbulent flow and mixing of fuel and oxidizer flows in the presence of heat transfer, mass transfer, and momentum between them transfer. Simulation of the spatial pattern of nitrogen oxides formation in the working space of the furnace is performed in the programming and computing suite SCAN. It is shown that the temperature non-uniformity over the hearth surface is not too pronounced due to the organization of the inclined flow inlet in the direction of the hearth, which is a desirable feature of the furnace operation. The highest concentration of combustion products is observed in the zone of maximum temperatures. In addition, the existence of two zones of the highest generation of oxides has been determined. The first zone is located approximately in the center of the hearth, and the second is located on the far external surface of the furnace. The possibility of using the developed model in the SCAN complex for carrying out parametric studies and engineering calculations, as well as for modification in the direction of adjusting and adapting the model to the regime-constructive features of specific energy technological devices, is noted.

## 1. Introduction

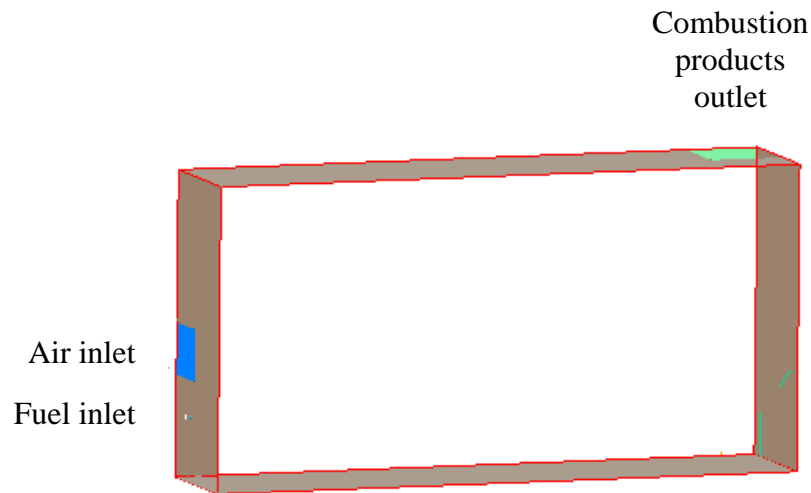
When organizing the process of thermochemical regeneration in industrial furnaces, not only fuel saving is achieved, but also a reduction in emissions of harmful substances into the atmosphere. In the partitioned example of the developed programming and computing suite SCAN [1], a model is presented for calculating the formation and transportation of nitrogen oxides in the working space of the burner of a gas-fired industrial furnace. The calculations use a three-dimensional stationary description of the turbulent flow and mixing of fuel and oxidizer flows in the presence of heat transfer, mass transfer and momentum transfer between them. The purpose of the illustrative example is to describe the features of the model and the user settings of the complex for its adaptation to the calculations of the spatial distributions of velocities, temperatures and composition of the flue gases, with particular attention to the calculation of the distribution of such a dangerous environmental pollutant, as nitrogen oxides. It is assumed that the reader has been familiarized with the features and technology of carrying out thermomechanical calculations in a standard software-computing



environment PHOENICS and similar computation systems within the corresponding courses of technical universities.

## 2. Description of the problem statement and the models used

The model is designed and activated in a universal manner, but it is used for thermo-gas-mechanical calculation of a specific furnace of a real industrial design. The construction of the concerned furnace is shown in Figure 1.



**Figure 1.** Configuration of a gas-fired furnace.

It contains such basic features that are inherent in many similar devices widely used in high-temperature energy technologies, namely:

- separate inlets to inject fuel (natural gas) and oxidant (air), ensuring the angular inclination of incoming flows towards each other to improve mixing conditions;
- thermally insulated external walls;
- fixed temperature of the combustion chamber bottom; and
- removal of combustion products, together with the resulting gas contamination, through an outlet located in the corner of the furnace arch.

In the process of mixing fuel and oxidizer entering the furnace of rectangular shape through holes of the given configuration and dimensions, the mixture is ignited, which (under the stable conditions) leads to steady burning, in which the gaseous fuel is consumed to form combustion products with the release of a large amount of heat.

In the given model, gaseous fuel is represented as a generalized hydrocarbon compound,  $C_xH_y$ , where the subscripts "x" and "y" are calculated by the composition of natural gas. Their values should, in general, ensure the correct ratio of "C" to "H" in a particular natural gas. In a numerical example, natural gas is treated as pure methane, i.e.  $x = 1$ , and  $y = 4$ .

The model assumes that the oxidizer of gas fuel is air, consisting, by volume, of 79% nitrogen and 21% oxygen. Oxygen disappears as it is consumed to oxidize the fuel hydrocarbon. It is assumed that chemical transformations occur at a terminal velocity, which is depending on the turbulent dissipation of reagent-containing vortices. The value of the dissipation is extracted, as well as the values of the effective coefficients of viscosity, thermal conductivity and diffusion, from the standard model, which operates by calculating the kinetic energy of turbulence and the rate of its dissipation according to the equations of their conservation.

Nitrogen is considered to be an inert component of the oxidizer-rich mixture, which is not subject to chemical transformations associated with combustion. In addition, memorably, the slow reactions of nitrogen oxides formation, although they depend on the local availability of fuel, nitrogen and oxygen, are carried out with such insignificant their consumption that they do not violate the general material balances. The model presents a superposition of two generally accepted mechanisms for the formation of nitrogen oxides: (1) thermal mechanism, according to the Zeldovich scheme, and (2) fuel mechanism. Oxidation of the hydrocarbon fuel, on the contrary, is assumed to be so complete and effective that carbon dioxide and water vapor are formed without intermediate compounds.

Although consideration of variability of the mixture density is carried out according to the law of ideal gas mixtures, the changes in the heat capacities of its components are not considered significant in comparison with the effective average value. Moreover, in the present example, attention is not focused on the contributions of thermal radiation effects, which are not of fundamental interest. Their account would lead to a transfer of the thermal energy of the flow to the walls and to a corresponding decrease in the overall temperature level of the gas flow. In this sense, the model is oriented to the worst scenario, somewhat higher than in reality, concerning the rate of nitrogen oxides formation.

### Geometric operations

The basic operations for creating a design of the calculation area are as follows:

- Setting the calculated area for the size of the furnace
- Placement of inlets and outlet
- Installation of external walls
- Viewing and adjusting the mesh spacing

### Solvable equations

The independent variables of the problem are the distances in three directions of the Cartesian coordinate system, X, Y, and Z,  $m$ . The conservation equations are collected by the methods used for the program-computing complex for the following dependent variables:

- Three components of the gas mixture velocity, U1, V1 and W1,  $m/s$
- Static pressure, P1,  $H/m^2$
- Kinetic energy of turbulence, KE,  $m^2/c^2$
- Rate of dissipation of kinetic energy, EP,  $m^2/c^3$
- Total enthalpy of the gas mixture flow, N1,  $J/kg$
- Mass fraction of fuel, FUEL
- Mass fraction of nitrogen oxides, YNOX
- Mixing share, MIXF

### Initial data

The following initial data are used for modeling combustion:

- Molecular weights: ( $kg/kmol$ ): W (air) = 29.0; W (fuel) = 16.0; W (products) = 28.0
- Stoichiometric ratio: 17.24
- Specific heat capacities ( $kg/kmol$ ): 1500.
- Heat of combustion ( $J/kg$ ):  $4.9e7$
- Reaction Type: Kinetically-controlled
- Reaction source: EDDY\_BREAKUP
- The fuel consumption factor:  $a = 4.0$
- Density calculation option: 3\_GASES
- Temperature calculation option: 3\_GASES-KINETIC
- Calculation option for heat capacity: 3\_GASES

- Coefficient of thermal conductivity ( $W/m \cdot K$ ): 0.0263
- System pressure ( $N/m^2$ ): 1.e5
- Temperature reference point ( $K$ ): 0.0
- Coefficient of thermal expansion: 0.00341

At the oxidant inlet:

- Temperature ( $K$ ): 312.0
- Mass fraction of fuel: 0.0
- Mass fraction of oxidizer: 1.0
- Speed in the X-direction ( $m/s$ ): 0.0
- Speed in Y direction ( $m/s$ ): - 4.0
- Speed in the Z-direction ( $m/s$ ): - 4.0
- Intensity of turbulence: 5%
- Mass fraction of nitrogen oxides: 0.0

At the fuel inlet:

- Temperature ( $K$ ): 312.0
- Mass fraction of fuel: 1.0
- Mass fraction of oxidant: 0.0
- Speed in the X-direction ( $m/s$ ): 0.0
- Speed in Y-direction ( $m/s$ ): 13.0
- Speed in the Z direction ( $m/s$ ): - 61.5
- Intensity of turbulence: 5%
- Mass fraction of nitrogen oxides: 0.0

### Used variables

The general list of variables used for modeling:

- DEN1 ( $\rho$ ) - density of the gas flow,  $kg/m^3$
- ENUT - coefficient of turbulent kinematic viscosity,  $m^2/s$
- EPKE - reverse time scale of turbulence,  $1/s$
- FK1 ( $K_1$ ) - reaction constant of thermal nitrogen oxides,  $m^3/kmol \cdot c$
- KOND - thermal conductivity of the gas flow,  $W/m \cdot K$
- MC ( $m_{(C)}$ ) - mass fraction of atomic carbon
- MCFU( $m_{(C)fu}$ ) - mass fraction of carbon in  $C_xH_y$
- MH ( $m_{(H)}$ ) - mass fraction of atomic hydrogen
- MFU( $C_{fu}$ ) - molar fuel concentration,  $kmol/m^3$
- MHFU ( $m_{(H)fu}$ ) - mass fraction of hydrogen in  $C_xH_y$
- MN( $m_{(N)}$ ) - mass fraction of atomic nitrogen
- MN2 ( $C_{N_2}$ ) - molar concentration of nitrogen,  $kmol/m^3$
- MO ( $m_{(O)}$ ) - mass fraction of atomic oxygen
- MOA ( $C_{(O)}$ ) - molar concentration of atomic oxygen,  $kmol/m^3$
- MO2 ( $C_{O_2}$ ) - molar oxygen concentration,  $kmol/m^3$

- OXID - mass fraction of the oxidant (air)
- PMNO ( $n_{NO_x}$ ) - megamolar fraction of nitrogen oxides, *ppm*
- PROD - mass fraction of combustion products
- RATE - spare variable
- RNOP ( $R_{NO,P}$ ) - rate of formation of fuel oxides of nitrogen,  $kg / m^3 \cdot s$
- RNOT ( $R_{NO,T}$ ) - rate of formation of thermal nitrogen oxides,  $kg / m^3 \cdot s$
- RNOX ( $R_{NO_x}$ ) - total rate of formation of nitrogen oxides,  $kg / m^3 \cdot s$
- SUMA - sum of the mass fractions of atomic elements
- SUMC - the sum of the mass fractions of fuel, oxidizer and products
- TMP1 ( $T$ ) - temperature of the gas flow, *K*
- XX ( $x$ ) - number of carbon atoms in  $C_xH_y$
- YCO2 ( $m_{CO_2}$ ) - mass fraction of carbon dioxide
- YFU, FUEL ( $m_{fu}$ ) - mass fraction of fuel
- YH2O ( $m_{H_2O}$ ) - mass fraction of water vapor
- YN2 ( $m_{N_2}$ ) - mass fraction of nitrogen
- YO2 ( $m_{O_2}$ ) - mass fraction of oxygen
- YSUM - sum of the mass fractions of chemical compounds
- YY ( $y$ ) - number of hydrogen atoms in  $C_xH_y$

### Specific Model Formulations

The equation of nitrogen oxides mass conservation YNOX (here  $m_{NO}$ ):

$$\text{div}(\rho \vec{v} m_{NO}) = \text{div}(\Gamma_{\text{eff}} \text{grad} m_{NO}) + R_{NO_x} \quad (1)$$

Mass fraction of carbon in  $C_xH_y$ :

$$m_{(c)fu} = \frac{12x}{12x + y} \quad (2)$$

Mass fraction of hydrogen in  $C_xH_y$ :

$$m_{(H)fu} = \frac{y}{12x + y} \quad (3)$$

Conversion of the mixture fraction, MIXF ( $f$ ), into mass fractions of atomic elements:

$$m_{(C)} = m_{(C)fu} f \quad (4)$$

$$m_{(H)} = m_{(H)fu} f \quad (5)$$

$$m_{(O)} = 0.233(1 - f) \quad (6)$$

$$m_{(N)} = 0.767(1 - f) \quad (7)$$

Mass fractions of chemical compounds:

$$m_{fu} = FUEL \quad (8)$$

$$m_{N_2} = m_{(N)} \quad (9)$$

$$m_{H_2O} = \frac{18}{2} (m_{(H)} - m_{(H)fu} m_{fu}) \quad (10)$$

$$m_{CO_2} = \frac{44}{12} (m_{(C)} - m_{(C)fu} m_{fu}) \quad (11)$$

$$m_{O_2} = m_{(O)} - \frac{16}{18} m_{H_2O} - \frac{32}{44} m_{CO_2} \quad (12)$$

Molar concentrations of nitrogen, oxygen and fuel:

$$C_{O_2} = \frac{m_{O_2} \rho}{32} \quad (13)$$

$$C_{N_2} = \frac{m_{N_2} \rho}{28} \quad (14)$$

$$C_{fu} = \frac{m_{fu} \rho}{12x + y} \quad (15)$$

Molar concentration of atomic oxygen:

$$C_{(O)} = 1.255 \cdot 10^4 (C_{O_2} / T)^{0.5} \exp(-31090/T) \quad (16)$$

The constant of reaction of thermal nitrogen oxides:

$$K_1 = 1.8 \cdot 10^{11} \exp(-38370/T) \quad (17)$$

The rate of thermal nitrogen oxides formation:

$$R_{NO,T} = 2 \cdot 30 \cdot K_1 C_{(O)} C_{N_2} \quad (18)$$

The rate of formation of fuel oxides of nitrogen:

$$R_{NO,P} = 30 \cdot 6.4 \cdot 10^6 \left( \frac{28}{\rho} \right)^{1.5} C_{O_2}^{0.5} C_{N_2} C_{fu} \exp\left( -\frac{36539}{T} \right) \quad (19)$$

The total rate of formation of nitrogen oxides:

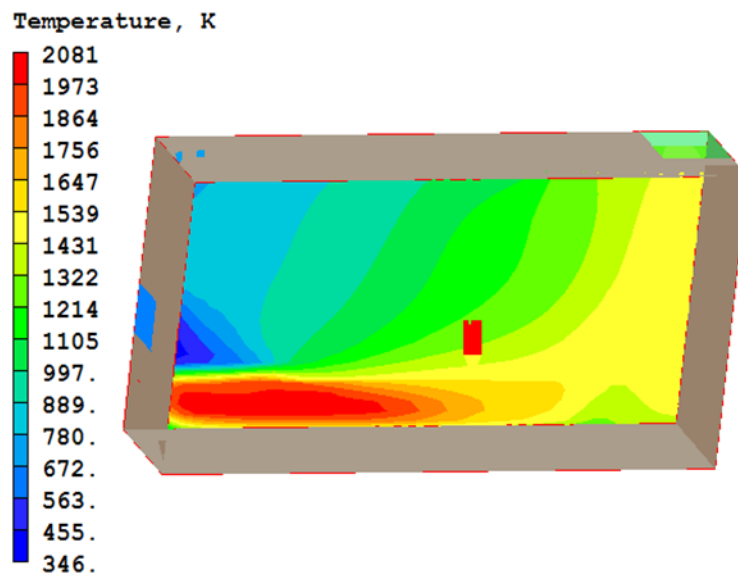
$$R_{NO_x} = R_{NO,T} + R_{NO,P} \quad (20)$$

Megamole fraction of nitrogen oxides:

$$n_{NO_x} = 10^6 m_{NO_x} \frac{28}{30} \quad (21)$$

### Numerical results

Figure 2 shows the distribution of temperatures in the plane of the center of the fuel flow inlet. Investigation of the flow shows that the zone of maximum values is located near the bottom of the furnace chamber in the immediate vicinity of the wall, through which flows of fuel and oxidizer are injected.

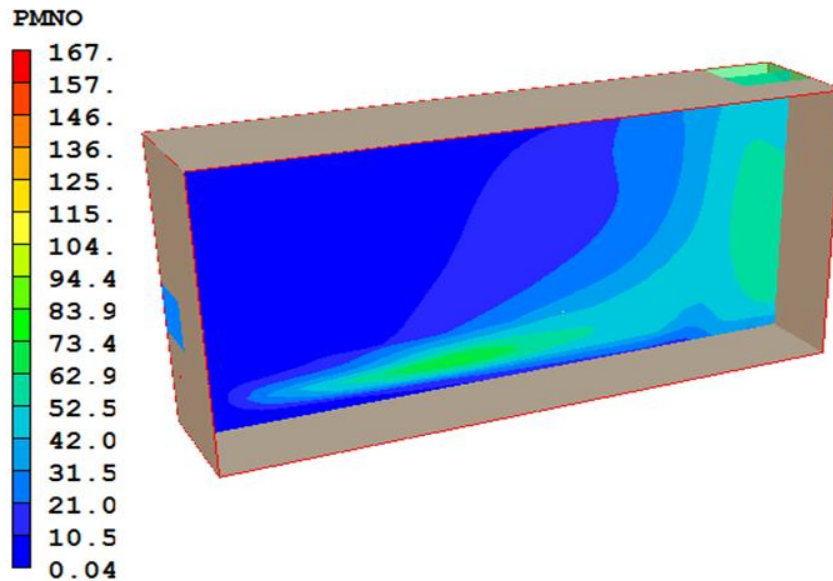


**Figure 2.** Distribution of temperatures in the plane of fuel inlet.

The temperature unevenness over the surface of the hearth is not too pronounced, which is a desirable feature of the furnace operation. This indicates that the organization of the inclined flow inlet in the direction of the bottom reaches the desired effect. As expected, the highest concentrations of combustion products occur in the maximum temperature zone. The temperature of the gases at the outlet from the furnace is 1421.3 K, which corresponds well to the calculations of the total heat and material balances of the burning space.

The distribution of nitrogen oxide concentrations in the plane of the center of the fuel inlet is shown in Figure 3.





**Figure 3.** Distribution of megamolar concentration of nitrogen oxides in the plane of the fuel inlet.

The average megamolous concentration of  $\text{NO}_x$  at the outlet from the furnace is 42.79 ppm. The study of the spatial pattern of formation of nitrogen oxides in the combustion space of the furnace indicates the existence of two zones of the greatest generation of oxides. The first zone is located approximately in the center of the hearth, and the second is placed on the far external surface of the furnace. In this distribution of generation zones, the work of two mechanisms of nitrogen oxide generation is reflected. The fuel mechanism, which is most intensively working closer to the wall with the flow entrances placed on it, makes a noticeable contribution to the upstream part of the combustion space. The subsequent total accumulation of oxides reaches its maximum in the zone of the gas flow turn in the direction of its movement towards the outlet from the furnace.

### Concluding remarks

A description of the partitioned example of the programming and computing suite SCAN developed for the modeling of natural gas combustion accompanied by the generation of nitrogen oxides is presented. The results of the simulation are quantitatively realistic and demonstrate the right qualitative trends.

The instructions given in the description are quite general and, therefore, can be used as a working manual for modeling of combustion processes of gaseous fossil fuels for industrial power boilers in the SCAN environment. All model statements are encoded in the attached source data file, which can be directly used for parametric studies and engineering calculations, as well as for modification in the direction of adjustment and adaptation of the model to the mode-constructive features of specific energy technology devices.

### References

- [1] Garyaev A, Popov S, Glazov V and Zhubrin S 2015 A program complex for the study of installations with thermochemical regeneration of thermal residuals *Industrial Power Engineering* **3** 43 – 8.