

NUMERICAL MODEL OF AIR-STAGING AND OFA IN PC BOILER

ROBERT STRAKA* AND JINDŘICH MAKOVIČKA, MICHAL BENEŠ

Abstract. We describe behavior of the air-coal mixture using the Navier-Stokes equations accompanied by a k - ϵ turbulence model. The undergoing chemical reactions are described by the Arrhenian kinetics. We also consider the heat transfer via conduction and radiation. The system of PDEs is discretized using the finite volume method (FVM) and an advection upstream splitting method as the Riemann solver. The resulting ODEs are solved using the 4th-order Runge-Kutta method. After appropriate setup we use this model to simulate NO_x reduction techniques of air-staging and OFA (over-fire air) for the pulverized coal (PC) boiler.

Key words. pulverized coal combustion, staged combustion, NO_x formation

AMS subject classifications. 76N15, 80A32, 80A20

1. Introduction. Our main motivation of the combustion model research is its use for design of the combustion chamber geometry and other important parameters needed for the boiler operation. In this paper we deal with NO_x reduction techniques called air-staging and over-fire air (OFA). Both techniques were successfully used and proved good ability of pollutants reduction. Production of the nitrogen oxides, which strongly depends on the temperature distribution, can be controlled by intelligent distribution of fuel and oxygen into the burners. Because the experiments on a real device are prohibitively cumbersome and expensive, in extreme cases even hazardous, the only way to test the behavior of the furnace is mathematical modeling.

An industrial pulverized coal furnace is basically a vertical channel with square cross-section. The dimensions are determined by the power generation requirements from the order of meters to tens of meters. In the case we model, the furnace has 35 meters in height and 7 meters in width, 49 m^2 cross-section. Power production of such a furnace is about 90 MW, and the furnace coupled with a steam generator is capable of producing about 100 tons of pressurized superheated steam per hour.

In the bottom of the channel walls, there are several burners — jets where the mixture of the air and coal powder is injected. The mixture then flows up and burns, while it transfers some of the combustion heat to the walls containing the water pipes. Above burners there are several OFA slots used as over-fire air inlets.

At the top, the heated flue gas continues to flow to the superheater channel where further heat exchange occurs, and this has already been covered by [6]. Our main concern is now modeling of the processes in the area, where the coal gets burnt and nitric oxides are produced.

2. Mathematical model. The mathematical model of combustion is based on the Navier-Stokes equations for a mixture of multiple components where the coal particle are treated as one of the phases. Unlike e.g. in [1], where the gas particles are treated separately and use separate equations of momentum, we chose to use this approach, as it simplifies the model especially when dealing with turbulence, and also removes several empirical relations and constants. Currently, the following components of the mixture are considered:

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- chemical compounds engaged in major thermal and fuel NOx reactions: nitrogen (N_2), oxygen (O_2), nitric oxide (NO), hydrogen cyanide (HCN), ammonia (NH_3), and water (H_2O);
- char and volatile part of the coal particles;

The gas phase is described by the following equations. As stated above, the mass balance is described by equations of mass balance of each subcomponent (the Einstein summation is used)

$$\frac{\partial}{\partial t}(\rho Y_i) + \frac{\partial}{\partial x_j}(\rho Y_i u_j) = \nabla \cdot \vec{J}_i + R_i, \quad (2.1)$$

where ρ is the flue gas mass density, Y_i concentration of the component, and u_j are the gas velocity components. The right-hand side terms describe the laminar and turbulent diffusion of the components and either production or consumption due to chemical reactions within the R_i term.

The above equations of component mass balance are accompanied by the equation of total mass balance

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0. \quad (2.2)$$

Equations of momentum conservation are as follows

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu_{\text{eff}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_l}{\partial x_l} \right) \right] + g_i, \quad (2.3)$$

where $\vec{g} = [g_1, g_2, g_3]$ is the external force acting on the fluid, in our case the gravity. The effective friction coefficient μ_{eff} is calculated from the turbulence model as

$$\mu_{\text{eff}} = \mu + \mu_t = \mu + \rho C_\mu \frac{k^2}{\epsilon},$$

where μ is the laminar viscosity, k the turbulent kinetic energy, and ϵ the turbulent energy dissipation rate. Constant C_μ , like additional constants mentioned later in the description of the turbulence model, has to be chosen empirically for the particular problem, in our case we use $C_\mu = 0.09$, which appears to give satisfactory results. All empirical constants in the turbulence model stated here are taken from [18].

The last equation describes the conservation of energy

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho u_j h) = -n_{\text{coal}} \frac{dm_{\text{coal}}}{dt} h_{\text{comb}} + q_r + q_c + q_s, \quad (2.4)$$

where the right-hand side terms are the heat of combustion, heat transfer by radiation, heat transfer by conduction, and heat source or sink. The heat transfer terms are computed as follows

$$-q_c = \nabla \cdot (\lambda \nabla T),$$

for the transfer by conduction, which is described by the Fourier law of heat conduction, and

$$q_r = \nabla \cdot (cT^3 \nabla T),$$

for the transfer by radiation. The radiation heat transfer is fully described by an integral-differential equation of radiation, which is very computationally expensive to solve. However, as the flue gas can be considered an optically thick matter, the above approximation of the radiation flux called the Rosseland radiation model can be applied [18].

The heat sink term is nonzero only in the edge computation cells and describes the energy exchange with the walls of the furnace via conduction and radiation

$$q_s = -A(T_{\text{gas}} - T_{\text{wall}}) - B(T_{\text{gas}}^4 - T_{\text{wall}}^4),$$

where A and B are constants dependent on the properties of the interface between the modeled region and its surroundings.

The particle mass change rate is currently described by the one-step Arrhenian kinetics, which is used separately for the char and volatile coal components — combustion of the volatiles is more rapid than combustion of the char

$$\frac{dm_p}{dt} = -A_v m_p^\alpha [\text{O}_2]^\beta \exp\left(-\frac{E_v}{RT_p}\right),$$

where m_p is the particle combustible mass, A_v , E_v are empirical constants, $[\text{O}_2]$ oxygen concentration T_p is the particle temperature and R is universal gas constant.

These equations are accompanied by the equation of state, as usual

$$p = (\kappa - 1)\rho_{\text{gas}} \left(e_{\text{gas}} - \frac{1}{2}v_{\text{gas}}^2 \right).$$

Here, κ is the Poisson constant and e_{gas} is the gas energy per unit mass.

For the turbulence modeling, we use the standard k - ϵ model, which describes the evolution of turbulence using two equations — first one for the turbulent kinetic energy

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k - \rho \epsilon, \quad (2.5)$$

and the second one for the turbulent kinetic energy dissipation rate

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_j}(\rho \epsilon u_j) = \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + C_{1\epsilon} \frac{\epsilon}{k} G_k - C_{2\epsilon} \rho \frac{\epsilon^2}{k}. \quad (2.6)$$

Constants in this model have again to be determined empirically, in our case we use the following values: $C_{1\epsilon} = 1.44$, $C_{2\epsilon} = 1.92$, $\sigma_k = 1.0$, $\sigma_\epsilon = 1.3$.

Left hand sides of the equations describe passive advection of the respective quantities by the advection velocity \vec{u} . Right hand sides describe their spatial diffusion, their production and dissipation.

The term G_k , which describes the production of turbulence, can be derived from the Reynolds averaging process and written in the terms of the fluctuating part of the velocity as

$$G_k = \tau_{jl} \frac{\partial u_j}{\partial x_l} = -\overline{\rho u'_j u'_l} \frac{\partial u_j}{\partial x_l},$$

where τ_{jl} is the Reynolds stress tensor. However during practical computation, fluctuations u'_j and u'_l are unknown. Using the Boussinesq hypothesis that the Reynolds

stress is proportional to the mean strain rate

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right),$$

one can write turbulent production in a closed form

$$G_k = \mu_t S^2, \quad S = (2S_{jl}S_{jl})^{1/2}.$$

Diffusion of the species consists of two processes — laminar and turbulent, and the diffusion term in Eq. (2.1) can be written in the form

$$\vec{J}_i = - \left(\rho D_{i,m} + \frac{\mu_t}{Sc_t} \right) \nabla Y_i.$$

First term corresponds to linear laminar diffusion, the second one to turbulent diffusion. Given the fact that the turbulent diffusion generally predominates the laminar one, and the term $D_{i,m}$ is difficult to determine, the laminar diffusion can be usually ignored. The coefficient Sc_t is the turbulent Schmidt number and we put $Sc_t = 0.7$.

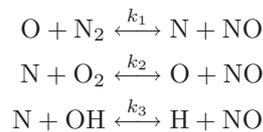
To be able to model the particle phase, especially surface area of the particles, we still have to track the numerical density of the particles using the equation similar to the mass balance equation

$$\frac{\partial n_{\text{coal}}}{\partial t} + \frac{\partial(n_{\text{coal}}u_{\text{coal}})}{\partial x_1} + \frac{\partial(n_{\text{coal}}v_{\text{coal}})}{\partial x_2} = 0. \quad (2.7)$$

3. Simplified model of NOx chemistry. This model has been developed to approximately describe the amounts of NOx emissions leaving a coal combustion furnace. The real mechanism of coal flue gas production seems to be very complicated, so that just the most important phenomena and reaction paths were considered to provide maximum possibility of using this model in real-time control and operation systems.

In most cases, NOx is interpreted as a group of NO and nitrogen dioxide (NO₂), which strongly pollute our living environment. There are two major processes attributing to the total NOx. The former is known as *Thermal NOx* or *Zeldovich* and simply consists of oxidation of atmospheric nitrogen at high temperature conditions. The latter is called *Fuel NOx* and describes NOx creation from nitrogen, which is chemically bounded in coal fuel. Fuel NOx is usually the major source of NOx emissions. These are the only mechanisms involved, although a few more could be considered (such as *Prompt NOx (Fenimore)* or *Nitrous oxide (N₂O) intermediate* mechanisms).

3.1. Thermal NO. Thermal NO generation mechanism attributes only at high temperature conditions ($\sim 1800\text{K}$) and is represented by a set of three equations, introduced by Zeldovich [7] and extended by Bowman [8]

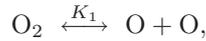


All these reactions are considered to be reversible. Rate constants were taken from [12].

In order to compute the NO concentration, concentrations of nitrogen radical [N], oxygen radical [O] and hydroxyl radical [OH] must be known. It is useful to assume [N] to be in a quasi-steady state according to its nearly immediate conservation after creation. In fact, this N-radical formation is the rate limiting factor for thermal NO production, due to an extremely high activation energy of nitrogen molecule, which is caused by a triple bond between two nitrogen atoms. Hence, the NO formation rate can be stated as

$$\frac{d[\text{NO}]}{dt} = 2k_1^+ \cdot [\text{O}] \cdot [\text{N}_2] \cdot \frac{1 - \frac{k_1^- k_2^- [\text{NO}]^2}{k_1^+ [\text{N}_2] k_2^+ [\text{O}_2]}}{1 + \frac{k_1^- [\text{NO}]}{k_2^+ [\text{O}_2] + k_3^+ [\text{OH}]}}.$$

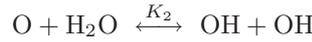
Under certain conditions, the oxygen molecule splits and recombines cyclically



which can be profitably described by following partial equilibrium approach [9]

$$[\text{O}] = K_1 \cdot [\text{O}_2]^{1/2} \cdot T^{1/2}.$$

As for OH radical, a similar partial equilibrium approach can be made, according to next reaction



and the approach is [10]

$$[\text{OH}] = K_2 \cdot [\text{O}]^{1/2} \cdot [\text{H}_2\text{O}]^{1/2} \cdot T^{-0.57}.$$

Equilibrium constants K_1 and K_2 are as follows

$$K_1 = 36.64 \cdot \exp\left(\frac{-27123}{T}\right), \quad K_2 = 2.129 \cdot 10^2 \cdot \exp\left(\frac{-4595}{T}\right).$$

3.2. Fuel NO. Composition analysis show, that nitrogen-based species are more or less present in coal, usually in amounts of tenths to units of percent by weight. When the coal is heated, these species are transformed into certain intermediates and then into NO. Fuel itself is therefore a significant source of NO pollutants. When a coal particle is heated, it is presumed, that nitrogen compounds are distributed into volatiles and char. In several studies (e.g. [13]) it is unreasonably told, that half of the coal-bounded nitrogen is distributed to volatiles and half into the char. Since there is no reason for a presupposition like this, a parameter α is introduced to describe the distribution of the coal-bounded nitrogen between the volatiles and char part of the coal particle.

$$\begin{aligned} m_{\text{vol}}^{\text{N}} &= \alpha \cdot m_{\text{tot}}^{\text{N}}, \\ m_{\text{char}}^{\text{N}} &= (1 - \alpha) \cdot m_{\text{tot}}^{\text{N}}, \end{aligned}$$

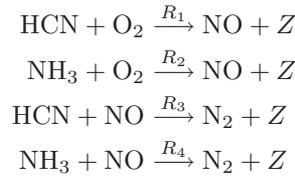
where $\alpha \in \langle 0, 1 \rangle$, $m_{\text{tot}}^{\text{N}}$ is the total mass of nitrogen, $m_{\text{vol}}^{\text{N}}$ is the mass of bounded nitrogen in volatiles and $m_{\text{char}}^{\text{N}}$ is the mass of bounded nitrogen in char.

As already mentioned, nitrogen transforms to pollutants via intermediates, which usually are ammonia NH_3 and hydrocyanide HCN . To proceed further, we must define four parameters to describe complex partitioning of the fuel bound nitrogen.

- β is amount of volatile bounded nitrogen which converts to HCN.
- δ_1 is distribution of char bounded nitrogen which converts to HCN.
- δ_2 is distribution of char bounded nitrogen which converts to NH_3 .
- δ_3 is distribution of char bounded nitrogen which converts to NO.
- $\beta \in < 0, 1 >$, $\delta_1 + \delta_2 + \delta_3 = 1$.

Different parametric studies should be carried out to find the best values of α , β , δ_1 , δ_2 and δ_3 suitable for specific type of coal. Five overall reactions of either NO formation or depletion were incorporated in the combustion part of the numerical code.

3.2.1. NO, HCN, NH_3 reactions. According to [16], formation rates of reactions

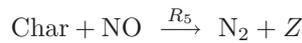


are given as

$$\begin{aligned} R_1 &= 1.0 \cdot 10^{10} \cdot X_{\text{HCN}} \cdot X_{\text{O}_2}^a \cdot \exp\left(\frac{-33732.5}{T}\right), \\ R_2 &= 4.0 \cdot 10^6 \cdot X_{\text{NH}_3} \cdot X_{\text{O}_2}^a \cdot \exp\left(\frac{-16111.0}{T}\right), \\ R_3 &= -3.0 \cdot 10^{12} \cdot X_{\text{HCN}} \cdot X_{\text{NO}} \cdot \exp\left(\frac{-30208.2}{T}\right), \\ R_4 &= -1.8 \cdot 10^8 \cdot X_{\text{NH}_3} \cdot X_{\text{NO}} \cdot \exp\left(\frac{-13593.7}{T}\right), \end{aligned}$$

where X is the mole fraction, a is the oxygen reaction order and Z are other products we simply neglect.

3.2.2. Heterogeneous NO reduction on char. Present char allows following adsorption process to occur



Levy [17] uses pore surface area (BET) to define NO source term

$$S_{\text{ads}}^{\text{NO}} = k_5 \cdot c_s \cdot A_{\text{BET}} \cdot M_{\text{NO}} \cdot p_{\text{NO}},$$

where $k_5 = 2.27 \cdot 10^{-3} \cdot \exp\left(\frac{-17168.33}{T}\right)$ is the rate constant, $S_{\text{ads}}^{\text{NO}}$ is the NO source term, c_s is the concentration of particles, A_{BET} is the pore surface area and p_{NO} is the partial pressure of NO.

In order to evaluate overall NO source term, single source terms have to be summarized. This overall source term can be further used in transport equations. As for HCN and NH_3 source terms, it is possible to determine them from coal burnout rate. It is assumed, that nitrogen from both char and volatiles transforms to intermediate species quickly and totally.

4. Numerical algorithm. For numerical solution of the equations, finite volume method is used. For left and right hand sides in Eqs. (2.1), (2.2), (2.3), (2.4), (2.5), (2.6), (2.7), advection upstream splitting method (see [2]) is used to approximate fluxes in the FVM formulation, and edge dual-volume approximation is used to approximate the second order derivatives respectively. For detailed description of the solution procedure see [6].

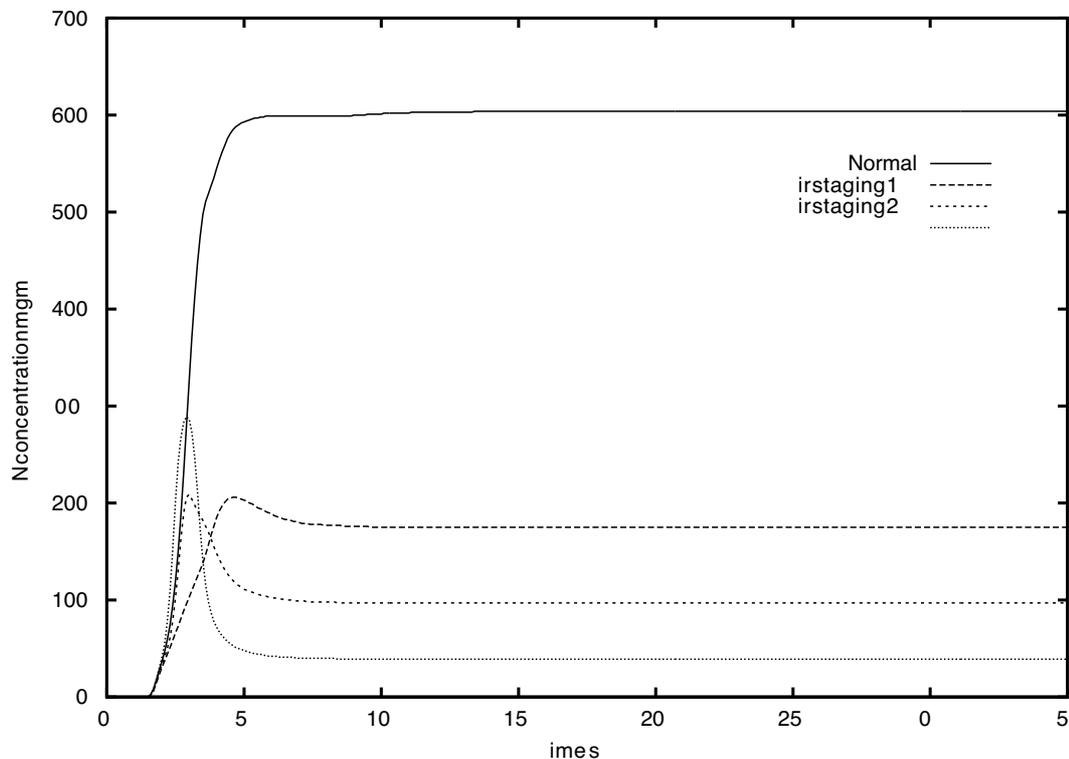


FIG. 4.1. Concentration of NO in the outlet cross-section of the boiler.

5. Air-staging and OFA. Often called staged combustion methods, relying on the reduction of the total air at the burners in one of the following two ways.

5.1. Over-fire air. The excess air coefficient in the burner is about 0.8 – 0.9 for coal. This region is called the primary combustion region. The remaining combustion air is injected into the furnace between 1.5m and 3m above the upper edge of the top active nozzles. This part of air is called secondary air or over-fire air. The ratio of the OFA and the total air is usually in the range of 0.1 – 0.2 in the PC boiler. In this method, because of the insufficient air in the primary combustion region, the fuel cannot burn completely and the temperature is too low. The temperature being low, the thermal NO_x is low. As air is insufficient, fuel NO_x formation decreases too. The method is able to reduce not only high-temperature NO_x but also fuel NO_x .

5.2. Air-staging. In this method, total air is distributed among burners, so several burners are under fuel-rich condition and several are under fuel-lean condition. This allows staged char burnout and reduction of NO_x because air is designed to mix into the flame gradually.

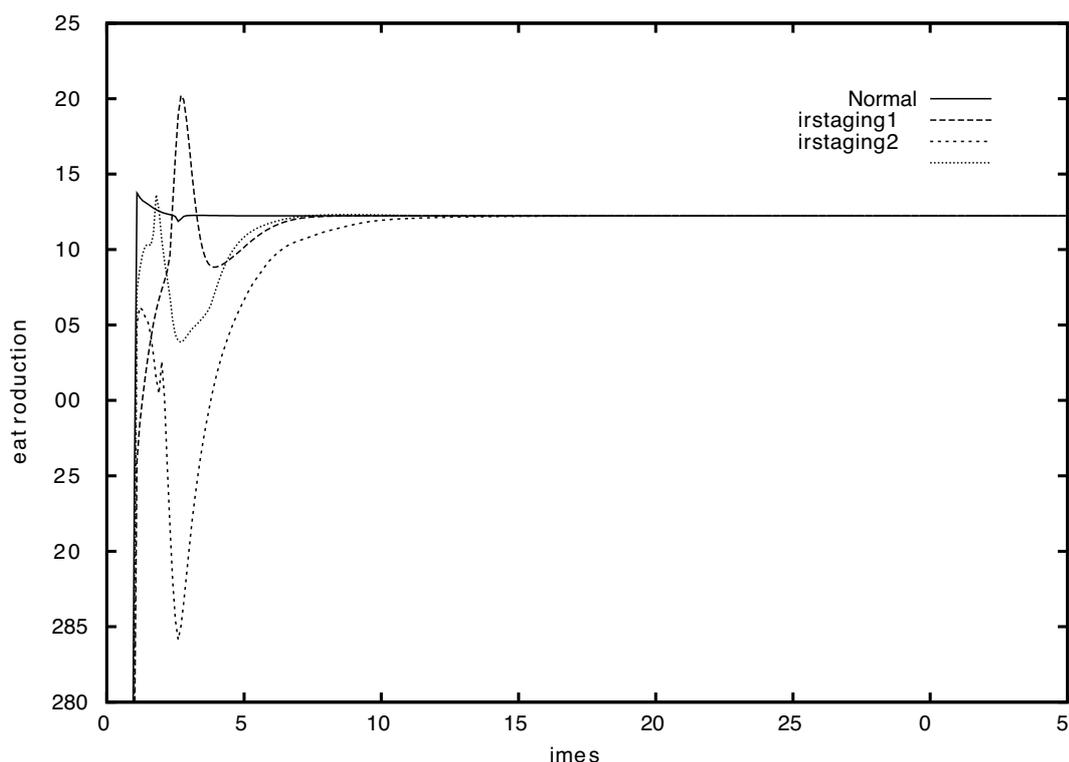


FIG. 4.2. Heat production in the whole volume of the boiler.

6. Results. Here we will present computed profiles of the following parameters of the boiler:

1. Concentration of NO at the outlet cross-section of the boiler (in mg/m^3).
2. Total heat production in the boiler (in MW).
3. Total heat transfer to the walls of the boiler (in MW).

Properties of the coal and boiler setup used in simulations are given in the Tab. 6.1. Those parameters are consistent with lignite, with medium volume of volatile matter. Operating parameters for studied cases are given in Tab. 6.2, we investigated numerically four cases, the first case is the normal operation with air distributed equally among burners. In the second case the part of total air is fetched to the OFA slot. In third and fourth case, air-staging method is used and air is distributed among burners as indicated in Tab. 6.2. Comparison of the studied cases are depicted at Fig. 4.1, 4.2, 4.3.

7. Conclusion. We have developed a mathematical model, which approximates the combustion process in an industrial furnace¹, while being affordable from the computational complexity standpoint. We show the effects of air-staging and OFA on the most important parameters of the boiler as heat production, heat transfer to the walls and NO_x concentration at the outlet of the boiler. It can be seen at the above figures that the NO_x concentrations are severely affected by the air-staging techniques. Such results are in good agreement with an experimentally observed reduction of the

¹See Appendix for design details

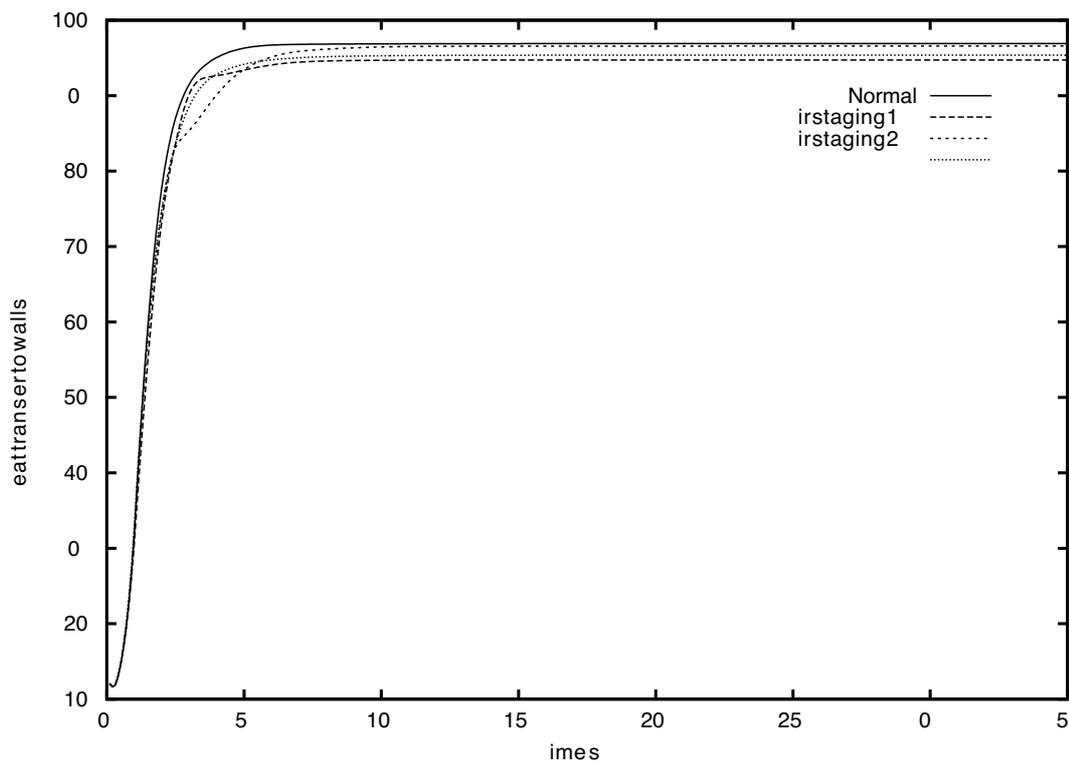


FIG. 4.3. Heat transferred to the walls of the boiler.

TABLE 6.1

Thermochemical and chemical properties of coal, consistent with lignite and furnace design setup.

Parameter	Symbol	Value	Unit
Ultimate analysis:			
Ash	A	0.095	-
Moisture	M	0.3	-
Carbon	C	0.4572	-
Hydrogen	H	0.0369	-
Sulfur	S	0.0116	-
Nitrogen	N	0.0051	-
Oxygen	O	0.0942	-
Volatile matter	VM	0.54	-
Lower heating value	LHV	17.922	MJ/kg
Oxygen per 1kg fuel	$O_{2,min}$	0.999	m^3/kg
Air excess coefficient	α	1.3	-
Mixture temperature	T_{in}	400	K
Inlet coal mass flux	m_{coal}	16.4	kg/s
Inlet air mass flux	m_{air}	121.4867	kg/s
Burner diameter	D_{hb}	0.8	m
OFA slot diameter	D_{OFA}	0.4	m
First burner row position	B_1	4.0	m
Second burner row position	B_2	5.6	m
Third burner row position	B_3	7.2	m
Fourth burner row position	B_4	8.8	m
OFA slot position	B_{OFA}	12.2	m

TABLE 6.2

Boiler air setup for studied cases. Total air is distributed among rows of burners, percentage distribution is indicated in the table.

Case	Air percentage for burners				
	B_1	B_2	B_3	B_4	OFA
Normal operation	25	25	25	25	0
Air-staging1	50	20	20	10	0
Air-staging2	10	20	20	50	0
Over fire air	20	20	20	20	20

concentration of NO_x by air-staging [21]. At the Fig. 4.3 one can see that maximum heat is transferred to the walls for the Normal operation mode and for Air-staging 2 mode (which is consistent with creating fuel-rich and fuel-lean zones in order to decrease NO_x concentration and make the char burnout complete). In every case the char burnout was complete which one can observe at the Fig. 4.2 (same production level indicates complete burnout of the fuel). We can conclude that OFA technique is the best possible for reduction of the NO_x concentration even if some heat transfer to the water-wall is lost (due to lower temperature of the region above the OFA slots), but the overall heat escaping with flue gases can be utilised in other parts of the flue-gas duct which are not modeled here. As an outlook to the future, mainly the following improvement possibilities are being considered:

1. Further refining of the coal combustion model.
2. Heat transfer by radiation improvement.
3. 3D model.

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We also would like to acknowledge the help of the HPC-Europa project, and extraordinary hospitality of the crew of CINECA supercomputer center in Bologna (Italy), where the work on the parallelization has been done. This part of the work has been performed under the Project HPC-EUROPA (RII3-CT-2003-506079), with the support of the European Community — Research Infrastructure Action under the FP6 "Structuring the European Research Area" Program.

Appendix. Here we will provide simplified geometry design of the industrial furnace.

An industrial pulverized coal furnace (for schematics, see Figure 7.1) is basically a vertical channel with square cross-section. The dimensions are determined by the power generation requirements from the order of meters to tens of meters. In the case we model, the furnace has 30 meters in height and 7 meters in width, 49 m² cross-section. Outlet area of the furnace is 24.5 m² (3.5*7). Power production of such a furnace is about 90 MW, and the furnace coupled with a steam generator is capable of producing about 100 tons of pressurized superheated steam per hour.

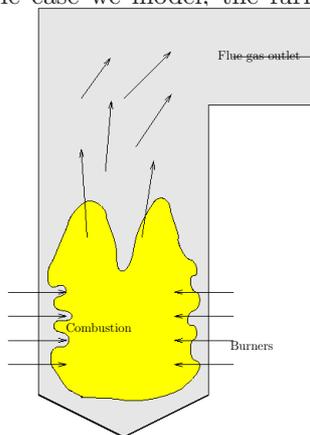


Fig. 7.1: Schematics of a coal furnace

In the bottom of the channel walls, there are two wind-boxes with several burners — jets where the mixture of the air and coal powder is injected. In our model we have 4 burners in each row and 4 rows of burners at opposite sides of the furnace. So we have 2x16 burners of the diameter D_{hb} and one row of the Over-Fire-Air ports with diameter of D_{OFA} through which heated air is blown in to the furnace. Positions B_1, B_2, B_3, B_4 and B_{OFA} are the distances from the bottom of the furnace's ash hopper. The mixture then flows up and burns, while it transfers some of the combustion heat

to the walls containing the water pipes.

At the top, the heated flue gas continues to flow to the superheater channel where further heat exchange occurs, and this has already been covered by [6]. Our main concern is now modelling of the processes in the area, where the coal gets burnt and nitric oxides are produced.

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