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MATHEMATICAL MODELLING OF UTILIZATION WASTE GASES FROM INDUSTRIAL FURNACES

ABSTRACT

Combustible waste gases are by-products of many technological processes. They vary in their calorific value and are used to decrease the usage of gases whose calorific value is higher. Coke oven gas from the coking process and process gases from an electric furnace in a copper plant are examples of such gases. Composition and calorific value of coke oven gas depend on coking parameters as well as on the type and quality of coal. The most common process where the coke oven gas is used is the process of heating combustion air in a heat regenerator. The gases from the electric furnace (due to low calorific value) require post combustion at the beginning of their disposal process. The paper addresses mathematical modelling of a coke oven battery regenerator as well as mathematical modelling of post combustion and cooling the electric furnace process gases. The regenerator mathematical model was elaborated for the simplified geometry of a real object making the assumptions for the heat transfer equations. The post combustion and cooling processes of the electric furnace gases are modelled with the aid of the Ansys software. This software was used for both elaborate simplified geometry of the analysed object and carry out the simulations. Mathematical description of occurring processes includes in this case combustion, turbulence and heat transfer.

Keywords: *mathematical modelling, waste gases, heat recovery, post combustion*

MODELOWANIE MATEMATYCZNE ZAGOSPODAROWANIA GAZÓW TECHNOLOGICZNYCH Z PIECÓW PRZEMYSŁOWYCH

W wielu procesach technologicznych produktem ubocznym są palne gazy technologiczne o zróżnicowanej wartości opałowej. Gazy te wykorzystuje się w instalacjach przemysłowych, zmniejszając zużycie paliw wysokokalorycznych. Do tego typu gazów należy gaz koksowniczy będący produktem ubocznym w procesie koksowania oraz niskokaloryczny gaz z pieca elektrycznego w hutnictwie miedzi. Skład i wartość opałowa gazu koksowniczego zależą od parametrów procesu koksowania oraz typu i jakości węgla. Podstawowym procesem jego wykorzystania jest regenerator ciepła służący do podgrzewania powietrza do spalania. Gaz technologiczny z pieca elektrycznego z uwagi na niską wartość opałową wymaga dopalenia przed jego wykorzystaniem. W artykule przedstawiono modelowanie matematyczne regeneratorów baterii koksowniczej oraz modelowanie dopalania i schładzania gazu technologicznego z pieca elektrycznego. Model matematyczny regeneratora opracowano, dokonując uproszczeń rzeczywistej geometrii przy założeniach upraszczających i rozwiązując układ równań przepływu ciepła. Dla modelowania matematycznego dopalania i schładzania gazów z pieca elektrycznego opracowano uproszczoną geometrię obliczeniową i przeprowadzono obliczenia symulacyjne przy wykorzystaniu pakietu oprogramowania Ansys. Opis matematyczny zachodzących procesów obejmuje w tym przypadku spalanie, turbulencje i wymianę ciepła.

Słowa kluczowe: *modelowanie matematyczne, gazy technologiczne, odzysk ciepła, dopalanie*

1. INTRODUCTION

In many industrial furnaces the technological gases can be considered as a secondary product. Depending on the process heating value of the technological gases can vary between 1.2 MJ/Nm^3 and 18 MJ/Nm^3. Gases with the heating value below 2 MJ/Nm^3 should be burned in the process installation. Technological gases with the heating value higher than 4 MJ/Nm^3 can be considered as an independent fuel. The most common technological waste gases are coke-oven gas, blast-furnace gas, converter gas (in ironworks), throat gas (in nonferrous metal plants) and waste gases from refinery, distillation and petrochemical processes.

A coke-oven gas is a secondary product in the coking process carrying out in coke oven batteries (Karcz 1987). Coke oven battery is an industrial furnace installed in coking plants to produce coke from hard coal (in an airless process of heating coal up to 1200 °C). The coke-oven gas has a heating value in the range between 17 and 18 MJ/Nm^3 and it contains around 60 percent of hydrogen and significant amount of hydrocarbons. Around 50 percent of the produced gas is consumed in a coking plant to fire the coke ovens. Very important construction element of the coking oven is a regenerative heat exchanger, which allows one to decrease significantly consumption of a coke-oven gas and hence increase energy efficiency of the process. The main task of that regenerative heat exchanger is a recovery of the physical enthalpy of the flue gases from the coking oven (Project 2008–2014). It is carried out by the accumulation of this excess energy in the ceramic filling frame and transferring it later to the air supplied to the combustion chamber.

In cooper plants the waste gases have rather small and very floating heating value. Moreover those gases are heavily polluted with dust. Usually, those gases are burned out in the

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chambers located just after the technological furnaces. Produced flue gases are cooled down and dust is removed in the sack filers. An example of a technological waste gas in the cooper plant is a gas produced in the electric furnace. Problems with recycling of the waste technological gases undergo continuous research focused on the mathematical modelling and optimisation of the operation of the recycling units.

In this paper mathematical models of the regenerative heat exchanger of the coke-oven and post combustion chamber of the waste gases from the electric furnace are presented.

2. MATHEMATICAL MODELLING OF THE COKE-OVEN REGENERATIVE HEAT EXCHANGER

In the presented mathematical model of the regenerative heat exchanger, the complicated geometry of the ceramic filling (fig. 1) is replaced with the equivalent flat plate with the same volume and heat transfer surface (Imer and Hofman 1975, Rusinowski 1995, Rusinowski 2003, Willmot 1969).

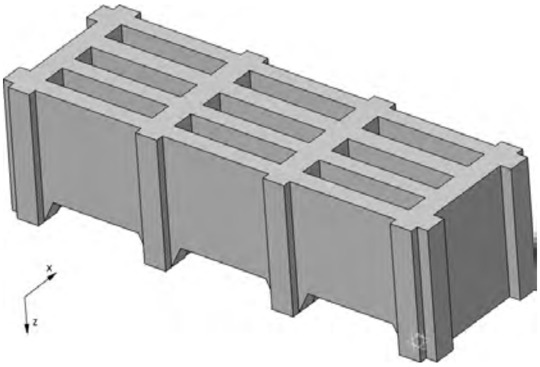

Fig. 1. The ceramic block HR151 of a coke oven battery filling

Due to complicated shape of the flow passages inside the heat exchanger filling it is difficult to define appropriate boundary conditions and solve the problem analytically. That is why geometry simplification was applied. Further the simplified heat exchanger filling is discretised spatially along its height and depth (fig. 2), keeping the time continuous. As the time is not discretised, spatial discretisation of the heat transfer equations results in the set of first order ordinary differential equations. Great advantage of such an approach is obtaining quasi-steady solution without calculation all the previous time steps. This significantly reduces the calculation time.

The operation cycle of the regenerative heat exchanger contains heating up phase of the heat exchanger filling (flue gases phase) and cooling phase of the heat exchanger filling (air phase). To take under consideration variations of the parameters of the inflowing gases (air and flue gases) with time, a single phase of the operation cycle is divided into a number of time periods. Moreover, it is more and more common to carry out so called channel ventilation during the initial 40 to 90 seconds of the each operation phase. During the air phase the channel ventilation is done by choking the air flow rate. While in the flue gas phase the channel ventilation is carried out by passing decreased air flow instead of the flue gases. The operation cycle of the regenerative heat exchanger is shown in figure 3.

Developed mathematical model of the heat transfer in the regenerative heat exchanger is based on the three-dimensional model of the Cowper stove (Rusinowski 1995, 2003). This model was adapted to the construction and operation parameters of the regenerative heat exchangers of the PWR coke-oven.

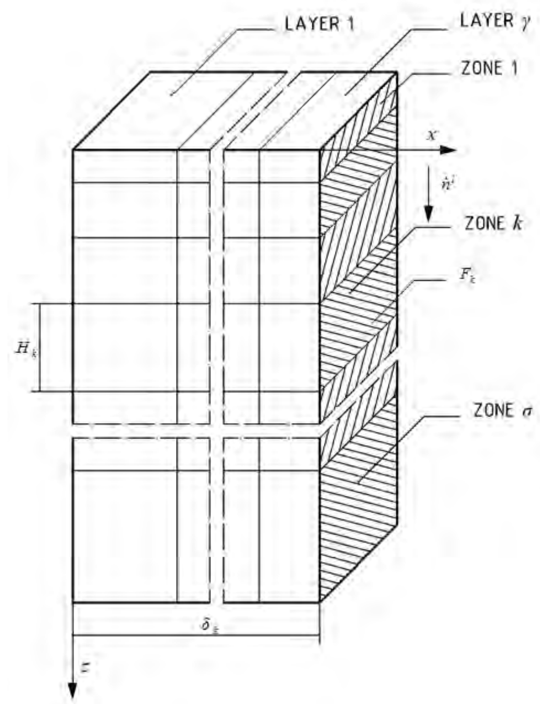

Fig. 2. Division of the regenerator into zones and substitute plate filling into layers

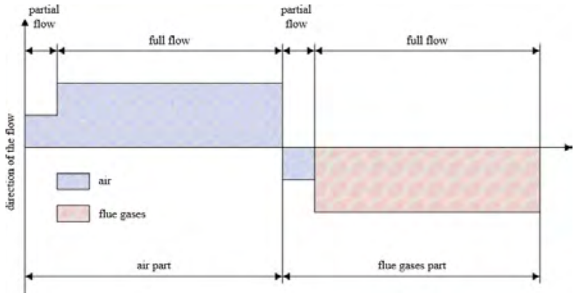

Fig. 3. Operation cycle of the regenerative heat exchanger

The main model assumptions are as follows:

- The regenerator is divided into σ zones, the zone $k = 1$ is the highest temperature zone.
- The real filling of the regenerator is replaced by a plate-filling.
- The substitute plate-filling in the zone of the regenerator is divided into γ layers. The layer $j = \gamma$ is situated adjacent to the surface of the plate.
- The work cycle of the regenerator (the heating and cooling phase of the filling) is divided into l_o time intervals in which the heat flux and preheated flux have a constant value; $l = 1,\ 2,\ \ldots, l_o$.

- The temperature of the blast at its intake to the filling of the regenerator has a constant value T_A.
- The thermal properties of the gases and filling inside the regenerator are constant within the range of the given zone and time interval.
- The temperature of the gas is equalized across the vertical section in relation to its direction of flow.
- The heat conducts in the filling parallelly to the gas flow has been left out of consideration.

This model is used to carry out calculations, i.e. calculations of the temperature of gases leaving the regenerator, the fluxes and parameters of the gases which feed the regenerator being known, as well as its material and structural parameters. The heat transfer problem in the zone k and the time interval l is described by the following equations:

- the energy balance in the gas spaces

$$\begin{aligned} -\dot{n}^l\left(Mc_p\right)_k^l \frac{\partial T_k^l(z,\tau)}{\partial z} = \\ = \alpha_k^l \frac{F_k}{H_k}\left[T_k^l(z,\tau) - \theta_k^l(\delta_k,\tau)\right] \end{aligned} \tag{1}$$

- Fourier-Kirchhoff's equation for the substitute plate-filling

$$c_k^l \rho_k \frac{\partial \theta_k^l(x,\tau)}{\partial \tau} = \frac{\partial}{\partial x}\left(\lambda_k^l \frac{\partial \theta_k^l(x,\tau)}{\partial x}\right) \tag{2}$$

where: T_k^l – temperature of the gas (K), θ_k^l – temperature of the filling (K), $\dot{n}^l$ – gas flux ($kmol/s$), $(Mc_p)_k^l$ – thermal capacity of the gas ($J/(kmol \cdot K)$, c_k^l – thermal capacity of the filling material ($J/(kg \cdot K)$), α_k^l – convective heat-transfer coefficient ($W/(m^2 \cdot K)$), λ_k^l – thermal conductivity ($W/(m \cdot K)$), ρ_k – density of the filling (kg/m^3), H_k, M_k – height and surface area of the zone, δ_k – half the thickness of the substitute plate filling, x, z – coordinates, τ – time (s).

The convective heat transfer coefficient is calculated from individual algorithm belonging to the mathematical model. Equations (1) and (2) are supplemented by the following initial and boundary conditions:

- for the temperature of the gas

$$T_k^l(0,\tau) = T_{dk}^l(\tau) \tag{3}$$

where: $T_{dk}^l(\tau)$ – temperature of the gas supplying to the zone.

- for the temperature of the filling

$$\theta_k^l(x,0) = \theta_0^l(x) \tag{4}$$

where: $\theta_0^l(x)$ – distribution of temperature in the zone at the beginning of the process.

- of the second kind in the symmetry plane of the substitute plate-filling

$$\left.\frac{\partial \theta_k^l(x,\tau)}{\partial x}\right|_{x=0} = 0 \tag{5}$$

- of the third kind in the symmetry plane of the substitute plate-filling

$$\left.-\lambda_k^l \frac{\partial \theta_k^l(x,\tau)}{\partial x}\right|_{x=\delta_k} = \alpha_k^l\left[\theta_k^l(\delta_k,\tau) - T_{mk}^l(\tau)\right] \tag{6}$$

where:

$$T_{mk}^l(\tau) = \frac{1}{H_k}\int_0^{H_k} T_k^l(z,\tau)\,dz \tag{7}$$

In order to solve the problem of unsteady heat conduction in an equivalent plate filling the method of discrete spectral transformation (DST) has been applied. The substitute plate-filling in this zone was divided into γ layers; next, by means of the method of elementary balance, (2) including gas balance equation (1) and boundary conditions (5)–(7), was transformed into a continuous discrete form, obtaining a set of ordinary differential equations which, expressed in the matrix form, looks as follows:

$$\frac{d\theta_k^l(\tau)}{d\tau} = \mathbf{A}_k^l \theta_k^l(\tau) + T_{dk}(\tau)\,\mathbf{b}_k^l \tag{8}$$

where: $\mathbf{A}_k^l$ is the matrix of the coefficients of the set of equations and $\mathbf{b}_k^l$ is a vector of coefficients; the coefficients result from the transformation.

In the case of the DTS method the set of differential equations is transformed into a set of independent differential equations, applying a diagonalization of the matrix $\mathbf{A}$. Heaving got the solution and after retransformation we obtain equations which describe the change of temperature in time of the differential elements of the filling in the given zone, as well as the temperature of the gas leaving the zone of the regenerator:

$$\theta_k^l(\tau) = \mathbf{H}_k^l(\tau)\,\theta_{0k}^l + \left[\mathbf{H}_k^l(\tau)\right] \cdot \left[T_{dk}^l(\tau)\right]\mathbf{b}_k^l \tag{9}$$

$$\begin{aligned} T_{wk}^l(\tau)\,\mathbf{n} = d_k^l \mathbf{I} \cdot \mathbf{H}_k^l(\tau)\,\theta_{0k}^l + \\ + \left[\left(1 - d_k^l\right) + b_{k\gamma}^l d_k^l H_{k\gamma\gamma}^l(\tau)\right] \cdot \left[T_{wk-1}^l(\tau)\right]\mathbf{n} \end{aligned} \tag{10}$$

where:

$$H_{kmp}^l(\tau) = \sum_{s=1}^{y} g_{kms}^l \tilde{g}_{ksp}^l \exp\left(\lambda_{ks}^l \tau\right) \tag{11}$$

where: g_{kms}^1, $\tilde{g}_{ksp}^1$ – elements of the transformation matrix $\mathbf{G}_k^1$ formed by the own vectors of the matrix $\mathbf{A}$ and the elements of the inverse matrix to the transformation matrix; λ_{ks}^1 – eigenvalues of the matrix $\mathbf{A}$.

Making use of the condition of the continuity of the gas–temperature function in the regenerator and basing on the (9) and (10) we get:

$$T_{wk}^l(\tau) = \sum_{i=1}^{k}\sum_{p=1}^{\gamma} U_{ki\gamma i}^l(\tau)\,\theta_{0ip}^l + \left[\varphi_k^l(\tau)\right] \cdot \left[T_{Sd}^l(\tau)\right] \tag{12}$$

$$\theta_{\mathbf{k}}^{\mathbf{l}}(\tau) = \sum_{i=1}^{k} \mathbf{W}_{ki}^l(\tau)\,\theta_{0i}^l + \left[\Psi_k^l(\tau)\right] \cdot \left[T_{Sd}^l(\tau)\right] \tag{13}$$

where:

$$U_{ki\gamma p}^{l}\left(\tau\right)=\sum_{r=i}^{k}\sum_{s=1}^{y}A_{ki\gamma prs}^{l}\exp\left(\lambda_{rs}^{l}\tau\right) \tag{14}$$

$$W_{kimp}^{l}\left(\tau\right)=\sum_{r=i}^{k}\sum_{s=1}^{y}C_{kimprs}^{l}\exp\left(\lambda_{rs}^{l}\tau\right) \tag{15}$$

$$\varphi_{k}^{l}\left(\tau\right)=B_{k0}^{l}+\sum_{r=i}^{k}\sum_{s=1}^{y}B_{krs}^{l}\exp\left(\lambda_{rs}^{l}\tau\right) \tag{16}$$

$$\psi_{km}^{l}\left(\tau\right)=\sum_{r=i}^{k}\sum_{s=1}^{y}D_{kmrs}^{l}\exp\left(\lambda_{rs}^{l}\tau\right) \tag{17}$$

where: A, B, C, D – coefficients.

The measurements of the medium temperatures inside the regenerative heat exchanger were carried out to verify the mathematical model (Project 2008–2014). Localization of the measuring points is presented in figure 4.

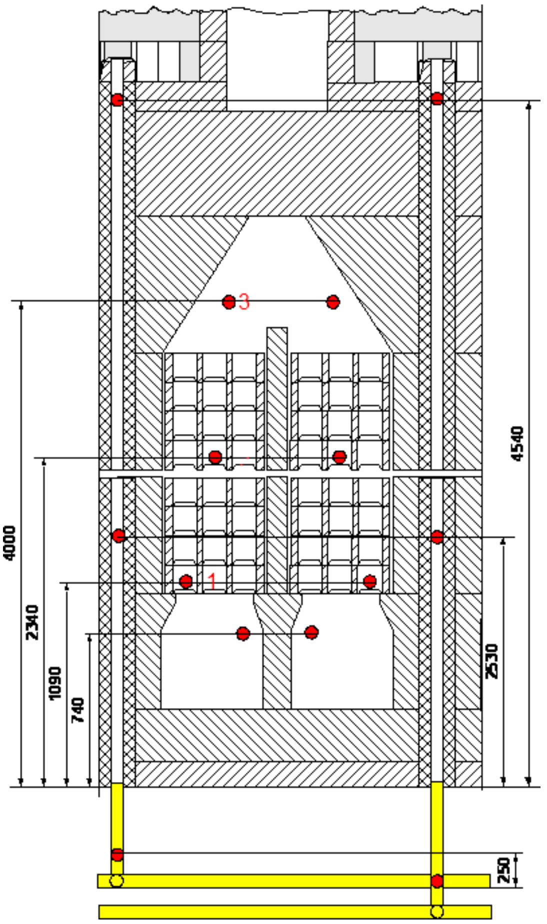

Fig. 4. Location of the measuring points for analysis of temperature distribution in heating system of the PWR-63 battery

Figures 5 and 6 show the time course of the gases temperature in the points 1 and 3 during analyzed operation cycles of the regenerative heat exchanger as well as the variation range at the standard deviation level.

The variation range about 30 K of the measured flue gases temperature is observed. It occurs during the heating up phase at the point located above the heat exchanger filling. This variation is a consequence of both measuring temperature with the aid of a traditional thermocouple instead of an aspirated thermocouple as well as time-varying parameters (unsteady process). A measured quantity in the case of measuring high temperature gases is significantly disturbed by radiation of the surfaces surrounding thermocouple if a traditional thermocouple is used. It may strongly overestimate the measured air temperature value at the beginning of the heat exchanger cooling phase and underrate the value of the flue gases temperature at the beginning of the heating up phase of the heat exchanger filling.

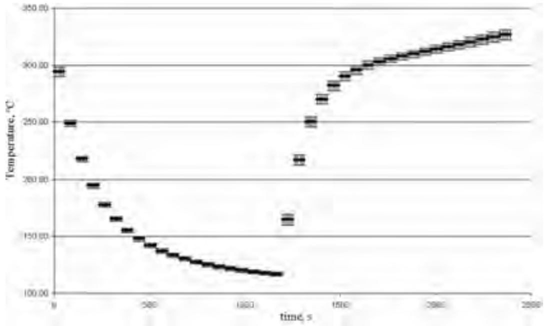

Fig. 5. Time distribution of the gases temperature under the regenerative heat exchanger filling

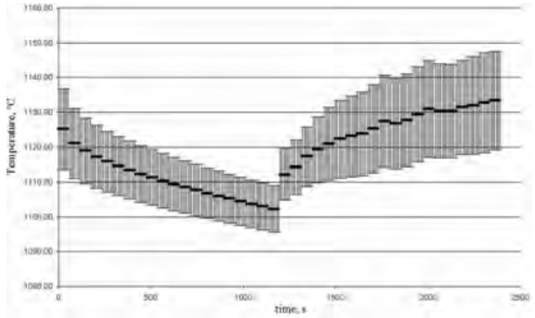

Fig. 6. Time distribution of the gases temperature above the regenerative heat exchanger filling

Comparison of the computation results with the experimental data for the point 1 located in the lower part of the filling (1090 mm from the bottom of the heat exchanger) and the point 3 located above the filling (placed at the height 4000 mm from the heat exchanger bottom) is presented in figures 7 and 8.

During the measurements the most important parameters of the coke-oven were recorded, namely flow rate and composition of the supplied coke-oven gas, temperature of the gas and air supplied for combustion (Project 2008–2014). Comparison of the computation results with the measurements data shows reasonably good agreement. It should be noticed that it is extremely difficult to carry out measurements in conditions prevailing inside the coke-oven installation. Hence, obtained results have rather significant measurement uncertainty. The best agreement can be noticed at points 1 and 3, i.e. in the lower and upper region of the regenerative heat exchanger. Significant discrepancy of the flue gases and air temperature is observed in the middle of the heat exchanger filling. The measurements were carried out with use of traditional thermocouples, which in case of high temperatures may result in the significant error due to very intense radiative heat transfer.

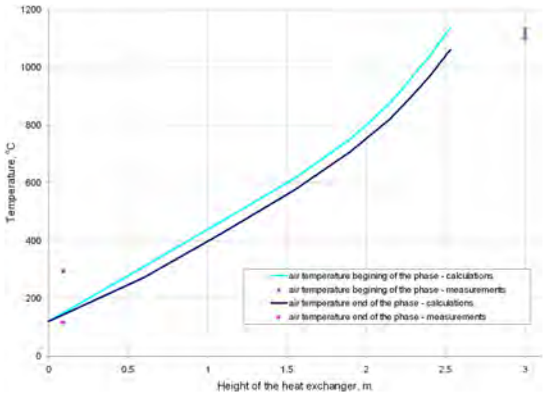

Fig. 7. Distribution of air temperature along the heat exchanger height

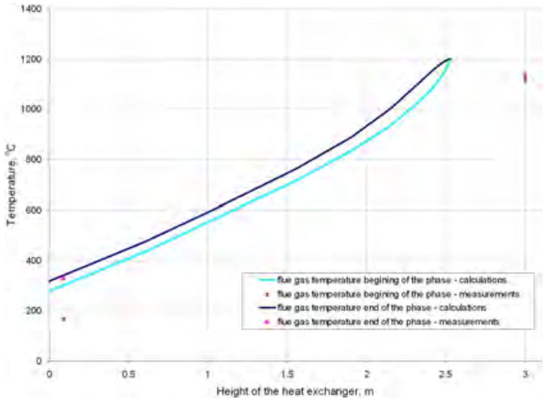

Fig. 8. Distribution of flue gases temperature along the heat exchanger height

3. MATHEMATICAL MODELING OF POST COMBUSTION AND COOLING OF THE ELECTRIC FURNACE OFF-GASES

The post combustion of the electric furnace process gases occurs in a post combustion chamber located behind the furnace. This chamber is in the shape of vertical cylinder that has an internal diameter of 2.644 m and height of 44.2 m and it is divided into 9 segments (fig. 9).

The connector and oblique pipe are used to supply and lead out the gases respectively. The combustion air is supplied by 10 nozzles surrounding the lower part of the chamber (at the height of the first and the second segment of the chamber). The whole lower part of the post combustion chamber (segments 1–3) is surrounded by water coolers. These coolers are in the shape of coil pipes embedded in a layer of refractory concrete. They are divided into 11 water sections in the case of the first and the second chamber segments and into 13 water sections in the case of the third chamber segment. In addition to cooling off-gases in water coolers they are also cooled by additional cooling air which is supplied by 12 nozzles surrounding upper part of the chamber (at the fifth segment height). The whole upper part (segments 4–9) of the chamber is lined with fireproofed materials.

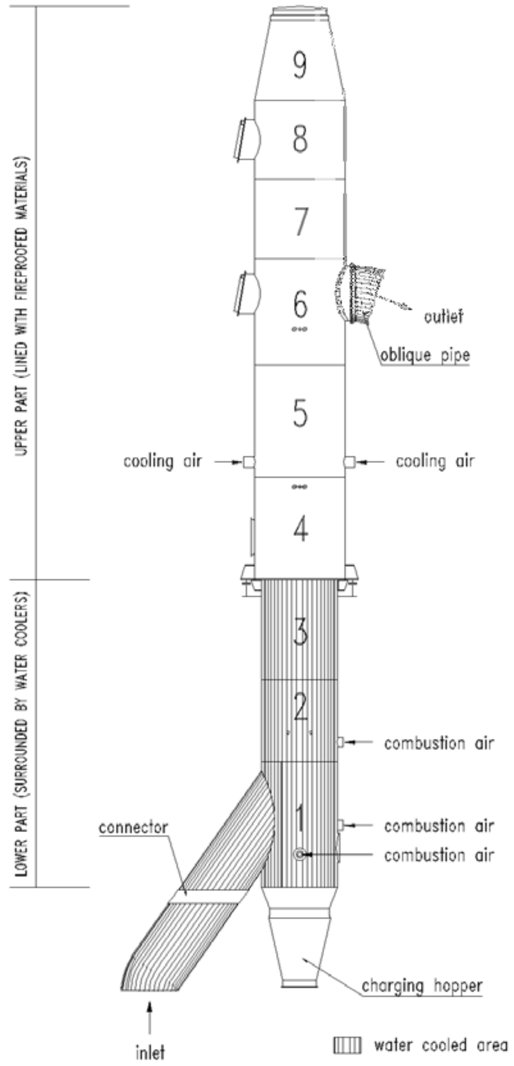

Fig. 9. Post combustion chamber of the electric furnace off-gases

A numerical model of post combustion and cooling of the off-gases from the electric furnace was elaborated. The Ansys Gambit and Fluent (Ansys, Inc. 2010) software were used to this end. Gambit was applied to build geometry of the post combustion chamber, generate numerical mesh and to define boundary conditions whereas Fluent was applied to define the required equations and initial conditions as well as to carry out numerical simulations. Around 5 million numerical cells were adapted in the analyzed domain. Hex/Wedge – Cooper algorithm was used to obtain 5 and 6 wall elements. The k-ε turbulence model, the Eddy Dissipation combustion model and the Discrete Ordinates radiation model were applied to describe occurring processes (Ansys, Inc. 2010; Chung 2002, Modest 1993, Versteeg and Malalasekera 2007). The dust contained in the gases was treated as discrete phase. The elaborated model allows carrying out numerical simulations for various mass flows, compositions and parameters of the gases as well as the combustion and cooling air. It was used to perform simulation of the post combustion and cooling process for the data presented in table 1.

Table 1

Parameters of the off-gases, combustion and cooling air as well as cooling water assumed in calculations

Medium	Mass flow (kg/s)	Temperature (K)	Composition (mole fractions)				
			CO	CO_2	O_2	H_20	N_2
Process gas	11.66	1400	0.27	0.21	0	0	rest
Combustion air (I row of nozzles – 2 nozzles)	3.64	343	0	0	0.21	0.01	rest
Combustion air (II row of nozzles – 2 nozzles)	3.64	343	0	0	0.22	0.02	rest
Combustion air (III row of nozzles – 6 nozzles)	7.26	343	0	0	0.23	0.03	rest
Cooling air (12 nozzles)	17.76	343	0	0	0.24	0.04	rest
Cooling water (I segment – 11 water sections)	23.54	303	–	–	–	–	–
Cooling water (II segment – 11 water sections)	15.73	303	–	–	–	–	–
Cooling water (III segment – 13 water sections)	18.59	303	–	–	–	–	–

The presented data concern the gases, air and water inlet cross-sections. The mass flows of the air and cooling water presented in table 1 are the total mass flows which are supplied to the particular air nozzles rows or water sections. The equal division of these mass flows between particular air nozzles and water sections was assumed in the simulations. The external wall surfaces of the connector, oblique pipe and air nozzles are treated as being adiabatic. The gases temperature in the inlet cross-section is assumed to be equal to the gases temperature in cross-section behind the connector. In the case of the external surfaces of other walls (charging hopper and segments 1–9 walls – fig. 9) the heat flux is determined on the basis of information included in (Kostowski 2000; Milejski and Rusinowski 2012).

Simulations of the post combustion and cooling processes were carried out until the residuals for the defined equations were lower than 1e-06 (energy equation), 1e-05 (radiation model equation) or 1e-03 (rest equations). It required more than 15,000 iterations. No oscillations in the calculated values (e.g. temperature, species concentrations) were observed before the simulations were stopped which indicates on convergence of the final solution. In order to verify the obtained results the mass and energy balances were checked for the whole numerical domain. Due to high temperature and dust concentration in the gas from electric furnace it is currently impossible to get data required for more detailed validation (there is no appropriate measuring apparatus in the system). Such a validation, however, should be performed in the future to confirm if the model produces correct results.

The calculation results are shown in figures 10–12. These figures show the distributions of carbon monoxide and oxygen concentrations (fig. 10–11) and the distribution of temperature (fig. 12) in the selected longitudinal sections of the post combustion chamber.

The figure 12 shows that the maximum temperature reached by the gases is between the segments 1 and 2 in the region next to the chamber walls (in front of the gases inlet). It amounts there about 1700 °C. The temperature in the opposite site at the third segment height is slightly lower. The highest temperature in these regions affects the air nozzles spacing. This spacing causes that the oxygen concentration in the region next to the chamber walls is significantly higher than the oxygen concentration in the middle of the chamber. The opposite occurs in the upper part of the chamber. This is the result of supplying the cooling air at the height of the segment 5 (fig. 9).

The applied cooling system allows decreasing the average temperature from about 1200 °C in the highest temperature regions to about 800 °C in the gases outlet cross-section. An important is the fact that complete combustion of carbon monoxide requires supplying the additional air by the air nozzles surrounding the segment 2. Before that the concentration of carbon monoxide is still high (fig. 10). Comparing results shown in figures 10–11, it should be noted that in the regions where the concentration of oxygen is highest there is the lowest concentration of carbon monoxide. It indicates that the elaborated model gives correct data.

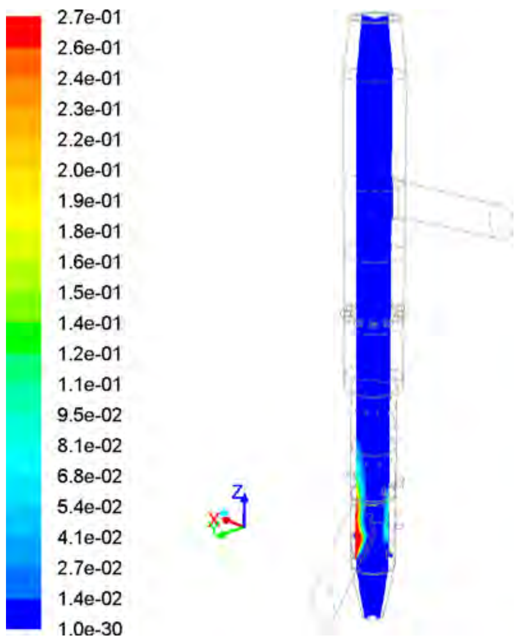

Fig. 10. Distribution of CO (molar fraction) in longitudinal sections

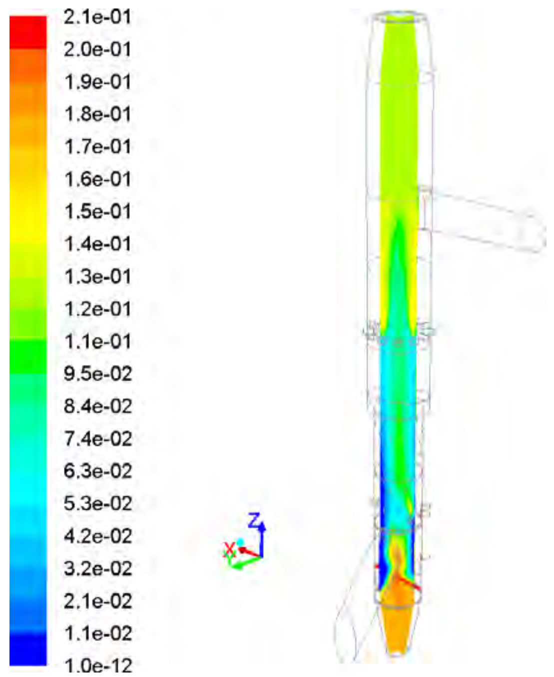

Fig. 11. Distribution of O_2 (molar fraction) in longitudinal sections

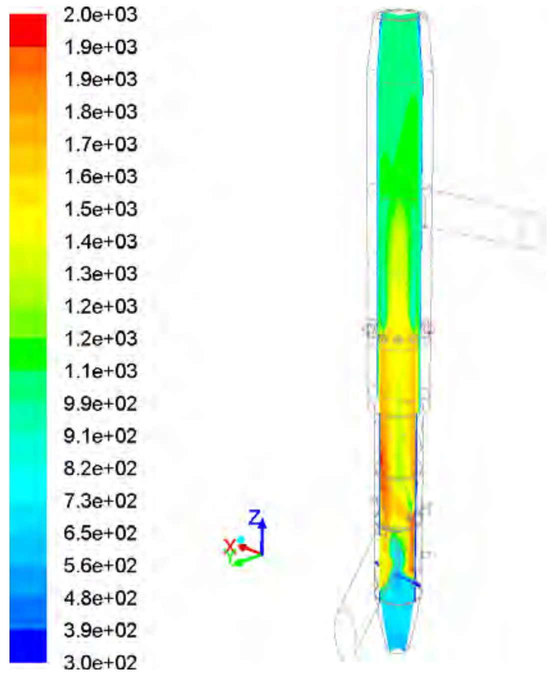

Fig. 12. Distribution of temperature (K) in longitudinal sections

4. CONCLUSIONS

The paper addresses two models: the mathematical model of the coke-oven regenerative heat exchanger and the numerical model describing post combustion and cooling of the process gases from the electric furnace in copper metallurgy. The heat regenerator model was elaborated by solving the differential equations describing conductive heat transfer in its filling. It was applied in a coke-oven battery simulator for optimizing the operating parameters (Kosyrczyk 2013). The post combustion and cooling processes numerical model was elaborated by means of the CFD (Computational Fluid Dynamics) software. This model allows optimization of the post combustion and cooling parameters. It may be used for properly design the post combustion and cooling installation.

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