CFD model of coupled thermal processes within coke oven battery as an example of complex industrial application

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This paper describes results of the mathematical modelling of steady-state and transient physical phenomena taking place in the heating channels of a coke oven battery. A formulated system of standard Computational Fluid Dynamics (CFD) equations coupled with User Defined Functions is solved numerically using commercial software Ansys Fluent. Finally, the developed 3-D model is used to examine the influence of selected operating parameters on the resulting temperature, velocity and concentration fields within considered object. The obtained results are briefly discussed considering their physical correctness related to industrial measurements.

Keywords: computational fluid dynamics, coupled thermal problems, coke oven battery, combustion, radiative heat transfer.

1. INTRODUCTION

CFD has made recently a substantial progress and can nowadays be effectively used not only for direct modelling of coupled heat transfer problems but also for optimization of processes. Taking this fact into account, a numerical analysis of heat and fluid flow processes occurring within the coke oven heating channels is undertaken. A selection of this problem was made because of a lack of advanced knowledge related to process, its importance for engineering practice and also because of model complexity.

The principal advantages of the mentioned methodology can be summarised as follows:

- CFD offers a numerical solution of the fluid flow and conjugate heat transfer problems;

- fluids can chemically react with each other as well as they can react with surfaces of solids;

- flows can be laminar, turbulent or in transition regime;

- there are no limitations in terms of geometrical complexity of the chambers/channels;

- accuracy of the numerical solutions can generally be very high;

- developed mathematical models allow one to run the number of computer simulations helping to understand the process and to minimise the number of measurements and/or prototypes.

At the same time, when applying CFD to modelling of combustion of the gaseous fuel within heating channels in the coke oven battery, one has to be aware of the following difficulties:

- geometry of the channels is fairly complex causing that resulting numerical grid consists of substantial number of elements. As a consequence, the size of the final set of equations is huge and obtaining solution is really time consuming;

- in all boundary conditions, defining behaviour of the solution on the external surfaces and interfaces within the computational domain, there are always uncertainties and discrepancies leading to some solution errors;

- combustion as well as turbulent models always need some experimental validation;

- due to an elevated level of temperatures within considered object, a thermal radiation has to be taken into account.

The advanced mathematical modelling of the heat and fluid flow processes occurring within the coke ovens started only recently when CFD analysis became more popular. The first works have been published by H. Tang, Z. Guo and X. Guo [1, 2]. The authors reported about their mathematical model developed using PHENICS [1].

A commercial software Ansys Fluent was first applied to build advanced models of combustion processes within heating channels by A.J. Nowak and J. Smołka [3]. The same authors, together with A. Fic and L. Kosyrczyk, extended their steady-state model to transient processes occurring within coke oven battery [4]. Similar results were also obtained by M.W. Isajew and I.A. Sultanguzin [5].

The mathematical model proposed in this work consists of geometrical model as well as the system of governing equations describing steady-state and transient processes. The main assumptions and the geometrical model are discussed in Secs. 2 and 3. Next, the fundamental governing equations are discussed in Sec. 3. This system is then solved numerically using commercial software Ansys Fluent with its User Defined Functions capability [6]. Finally, the developed model is used to examine the influence of selected operating parameters on the resulting temperature, velocity and concentration fields for both steady-state and transient processes. The obtained results can be useful for a more precise control of the coking process in the coke oven battery.

2. Basic assumptions

The basic assumptions adopted at the stage of building mathematical model of the fluid flow and heat transfer processes in the coke oven are as follows:

- the subject of consideration is a single heating chamber (also known as heating channel) of the PWR-63 coke oven battery. This chamber provides heat to two neighbouring coking chambers as it is schematically shown in Fig. 1a;

- interaction of the heating channel with those two coking chambers is, in this work, simulated either by convective boundary condition (what is schematically demonstrated in Fig. 1b) or by the heat flux having a profile taken from the technical literature. Within next stages of the conducted project these boundary conditions will be replaced by a detailed mathematical model of coking processes taking place in neighbouring chambers;

- coke oven battery is fired with a coke oven gas being burned in the air preheated up to 1000–1100°C;

- the cycle consisting of a loading of coal, heating it and producing a coke lasts 15 hours. During that period both heating walls deliver heat into two neighbouring coking chambers with a phase shift equal to 7.5 hours;

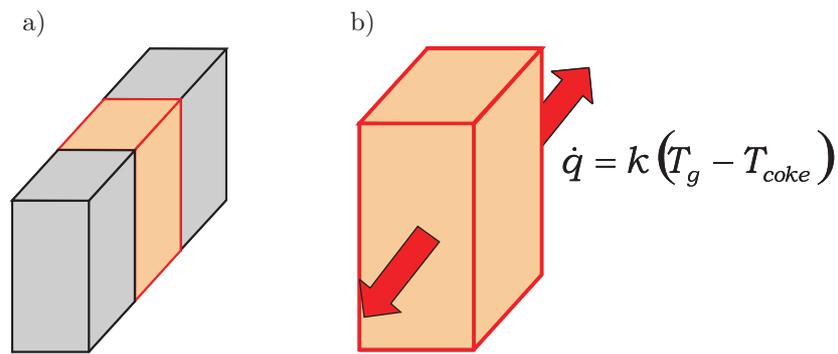- during each coking cycle reversal of gas, air and flue gasses takes place every 21 minutes;

a) b)

$$\dot{q} = k\left(T_g - T_{coke}\right)$$

Fig. 1. a) Heating channels with two neighbouring coking chambers, b) interaction of selected heating channels with the neighbouring coking chambers.

- to analyse, in a very systematic way, an influence of the selected parameters on the fluid flow and heat transfer within considered chamber, the so-called reference case is determined. Then, the time evolution of the heating chamber outputs is found and presented;

- finally, behaviour of the heating channels due to fuel and flue gasses reversal is analysed.

3. GEOMETRICAL MODEL OF THE HEATING CHANNELS

As already mentioned, the considered geometrical model consists of one heating chamber with both upward and downward channels. The two channels are connected by three windows. Two of them are located symmetrically at the bottom level, while the third one connects channels at the ceiling level (sort of fire bridge). That makes the domain of the heating channels fairly complex. Figure 2 shows 3-D view of the main elements of the heating channels as well as their cross-section at the bottom level.
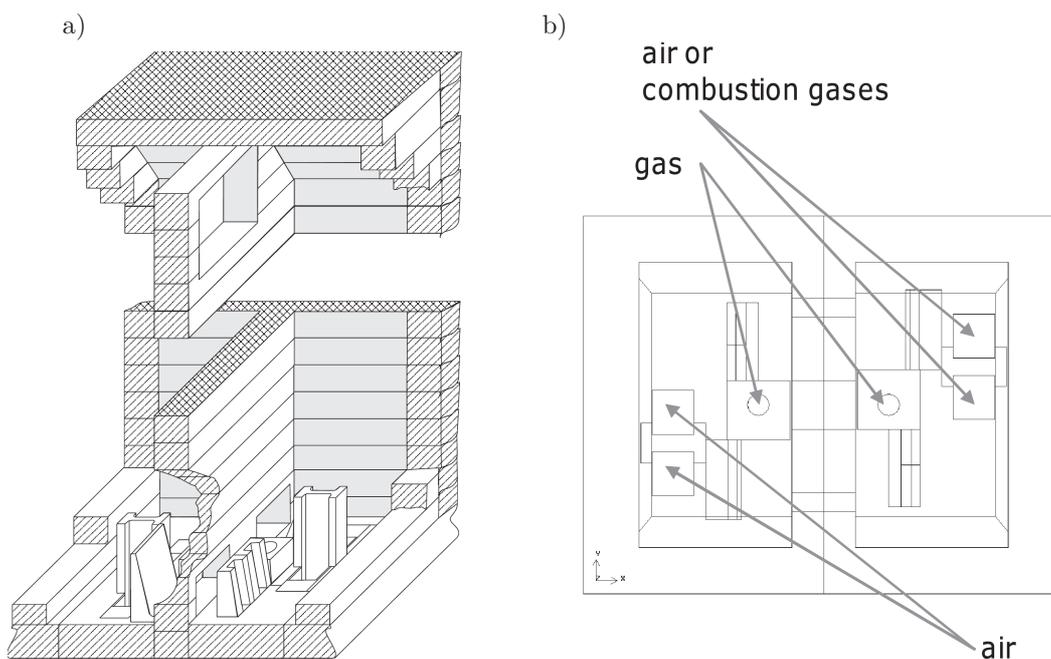
a) b)

air or
combustion gases

gas

air

Fig. 2. a) 3-D view of the main elements of the heating channels, b) horizontal cross-section of the heating channels at the bottom level.
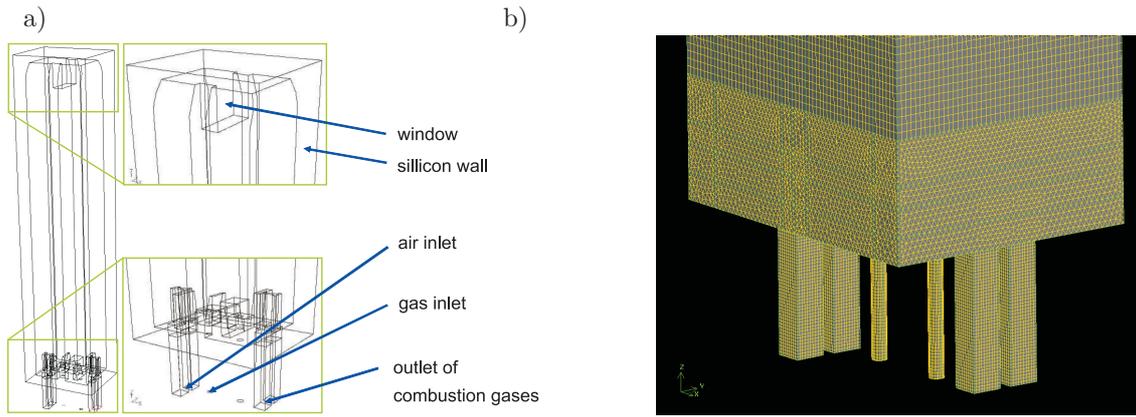
a)
b)

Fig. 3. a) 3-D view of the main geometrical elements of the heating channels, b) numerical grid in the vicinity of inlets and outlets.

Dimensions of the object were set on the basis of the technical documentation provided by a coke oven plant. Within presented geometry, a mesh of a very high quality was applied. This operation was carried out by means of Gambit, which is Ansys Fluent package pre-processor [5]. The final grid contained mainly hexahedral elements and a certain number of the tetrahedral cells in the vicinity of inlets. The total number of elements was over 1 500 000. The computational domain also contained additional air and fuel channels at the inlet and outlet in order to simulate a developed velocity profiles at the inlet of the combustion chamber and to properly define outflow boundary condition for combustion gasses leaving heating channels (*c.f.* Fig. 3).

4. FUNDAMENTAL GOVERNING EQUATIONS OF THE MATHEMATICAL MODEL

The details of the mathematical model are not explained here because of a very limited space. Details on the governing equations adopted in the model reader can be easily found in the CFD textbooks, *e.g.* [7, 8]. Nevertheless, the most fundamental governing equations are listed below together with the brief information which physical unknown is calculated when solving particular equation. Hence:

- The Fourier-Kirchhoff equation is solved for the temperature in both fluid (combustion gasses) and solid walls. In fluid this equation reads:

$$
\frac{\partial(\rho\,h - p)}{\partial t} + \nabla \cdot (\rho\,\boldsymbol{v}\,h) = \nabla \cdot (k\,\nabla T) + (\tau : \nabla\boldsymbol{v}) - \nabla \cdot \left(\sum_i h_i\,J_i\right) + S_h,
$$

(1)

$$
J_i = -\rho\,D_i\,\nabla m_i, \qquad h = \sum_i h_i\,m_i, \qquad h_i = \int_{T_{ref}}^{T} c_{pi}\,\mathrm{d}T,
$$

where ρ is the density, h represents the specific enthalpy, t is time, $\boldsymbol{v}$ is the velocity, T represents temperature, k stands for the thermal conductivity, τ is the stress tensor, J represents the diffusion mass flux and S stands for the source term in transport equation of scalar quantity. The mass diffusion coefficient is noted by D while m represents the mass fraction. Finally, symbol c_p stands for the isobaric specific heat.

In solid walls, the above equation is considerably simplified, *i.e.*, some terms are just dropped,

$$
\frac{\partial(\rho\,h)}{\partial t} = \nabla \cdot (k\,\nabla T),
$$

(2)

- momentum equation is solved for velocity vector only in fluids,

$$\frac{\partial(\rho\,\boldsymbol{v})}{\partial t} + \nabla \cdot (\rho\,\boldsymbol{v}\,\boldsymbol{v}) = -\nabla p + \nabla \cdot \tau + \rho\,\boldsymbol{g} + \boldsymbol{S}, \tag{3}$$

where p is the pressure and $\boldsymbol{S}$ stands for the source term in transport equation of vector quantity;

- continuity equation is solved for pressure only in fluids,

$$\frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\,\boldsymbol{v}) = \sum_i S_{mi}; \tag{4}$$

- transport equations for all chemical species are solved for their concentrations. In those equations volumetric heat sources resulted from combustion chemical reactions are also considered,

$$\frac{\partial(\rho\,m_i)}{\partial t} + \nabla \cdot (\rho\,\boldsymbol{v}\,m_i) = \nabla \cdot (\rho\,D_i\,\nabla m_i) + S_{mi}; \tag{5}$$

- two-equation $\kappa - \varepsilon$ realizable turbulence model is solved in fluids for turbulent kinetic energy κ and dissipation of turbulence kinetic energy ε,

$$\frac{\partial(\rho\kappa)}{\partial t} + \nabla \cdot (\rho\nu\kappa) = \nabla \cdot [(\mu + \mu_T/\mathrm{Pr}_k)\,\nabla\kappa] + S\,(\mu_T,\,\kappa,\,\boldsymbol{v}) - \rho\,\varepsilon,$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla \cdot (\rho\nu\varepsilon) = \nabla \cdot [(\mu + \mu_T/\mathrm{Pr}_\varepsilon)\,\nabla\varepsilon] + C_{\varepsilon 1}\,\frac{\varepsilon}{\kappa}S\,(\mu_T,\,\kappa,\,\boldsymbol{v}) - C_{\varepsilon 2}\,\rho\,\frac{\varepsilon^2}{\kappa}, \tag{6}$$

where μ is the dynamic viscosity and Pr stands for Prandtl number;

- radiative transfer equation (Discrete Ordinate model [7]) is solved for radiative heat sources in fluids and for radiative heat fluxes on the surfaces of solid walls,

$$\frac{\mathrm{d}i(\boldsymbol{r},\xi)}{\mathrm{d}\xi} = -a\,i(\boldsymbol{r},\xi) + a\,i_b(\boldsymbol{r},\xi),$$

$$\dot{q}_r = a \int\limits_{\omega=4\pi} (i - i_b)\,\mathrm{d}\omega, \qquad \dot{q}_{v,r} = -\nabla \cdot \dot{q}_r, \tag{7}$$

where i is the intensity, a represents absorption coefficient and ω stands for solid angle.

In the developed mathematical model the $\kappa - \varepsilon$ realizable turbulence model is adopted and it is assumed that the combustion is generally limited by the process of mixing gaseous fuel with oxygen. Bearing this in mind, Magnussen and Hjertager proposed turbulence-chemistry interaction model (known as the eddy-dissipation model) [6, 9]. In this model the following two-stage oxidation chemical reactions of methane, carbon oxide and hydrogen are considered:

$$\left.\begin{aligned} &CH_4 + 1.5O_2 = CO + 2H_2O \\ &CO + 0.5O_2 = CO_2 \\ &H_2 + 0.5O_2 = H_2O \end{aligned}\right\} \tag{8}$$

To obtain the numerical solution of the above discussed set of equations, the appropriate boundary conditions are required [7, 8]. The most important of these conditions formulated in the model are presented in Fig. 4.

It is also worth mentioning that the computational domain consists of two types of materials, which were walls of the coke oven battery and flue gasses. Thermal properties of the wall materials were set based on the producers' information and they were temperature dependent. The flue gasses were results of combustion of the coke oven gas. Its chemical composition is given in Table 1.
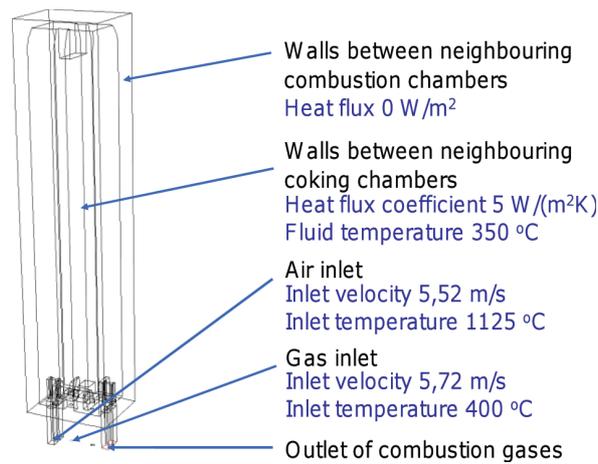
Walls between neighbouring
combustion chambers
Heat flux 0 W/m²

Walls between neighbouring
coking chambers
Heat flux coefficient 5 W/(m²K)
Fluid temperature 350 ºC

Air inlet
Inlet velocity 5,52 m/s
Inlet temperature 1125 ºC

Gas inlet
Inlet velocity 5,72 m/s
Inlet temperature 400 ºC

Outlet of combustion gases

Fig. 4. Main adopted boundary conditions.

Table 1. Chemical composition of the fuel (coke oven gas).

compound	dry gas mole fraction	moist gas mole fraction	mole mass	moist gas mass fraction
H_2	0.5420	0.5297	2	0.0920
CH_4	0.2650	0.2590	16	0.3597
CO	0.1010	0.0987	28	0.2399
CO_2	0.0380	0.0371	44	0.1418
N_2	0.0460	0.0450	28	0.1093
O_2	0.0080	0.0078	32	0.0217
H_2O	0.0233	0.0228	18	0.0356
sum	1.0233	1.0000		1.0000

5. Results of selected simulations and their discussion

The described above mathematical model of the heat transfer and fluid flow processes allows one to carry out numerous computer simulations applying commercial code Ansys Fluent. Results of selected simulations are presented in this paper.

In Fig. 5, dependence of the temperature on height of the heating channels at three different locations B, D and G as a result of steady-state process is shown. It is clearly visible that temperature
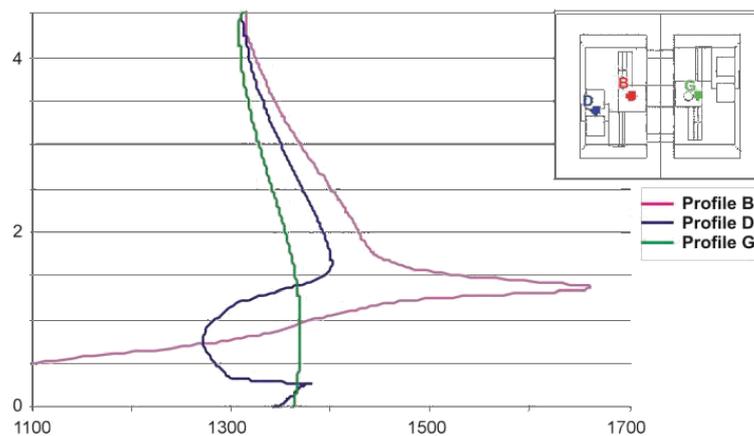
Fig. 5. Temperature profiles (in °C) along the height of the channels at selected locations B, D and G.

in upward channel changes rapidly with height along vertical lines located at points B and D. This is a result of the combustion processes occurring in this channel. In downward channel, changes of the temperature along vertical line located at point G are considerably smaller. Nevertheless, close to the bottom of the channel, the temperature is slightly higher than the temperature close to the ceiling.

The steady-state temperature fields in two selected cross-sections A and B of the heating channels are presented in Fig. 6. Left figure (cross-section A) shows also the vertical wall separating upward and downward channels together with window linking both channels. In both cross-sections, a flame is visible in the upward channel. In addition, because of a lack of symmetry in locations of gas and air inlets, the flame in the right cross-section is pushed to the left wall by the inflowing air.
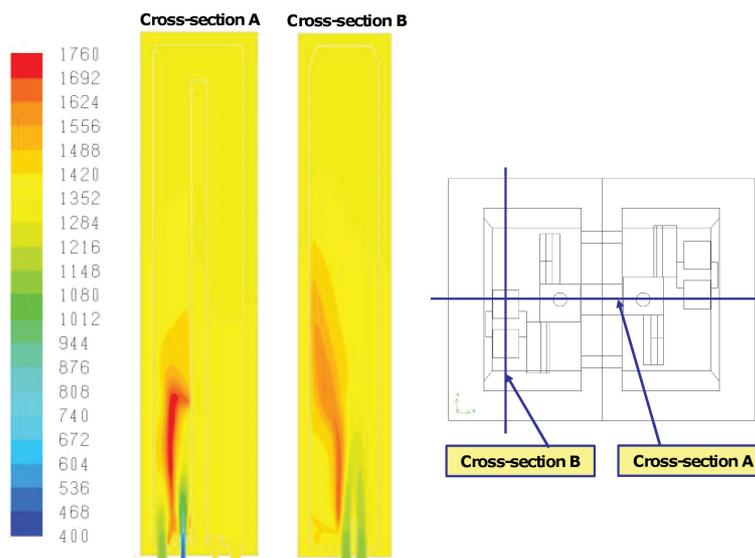
Fig. 6. Maps of steady-state temperature fields (in °C) in two cross-sections.

The above discussed phenomena are confirmed in Fig. 7. It shows the steady-state velocity fields in the same two cross-sections. The resulting velocity contours, particularly in the right cross-section, coincide very well with temperature profiles measured experimentally.
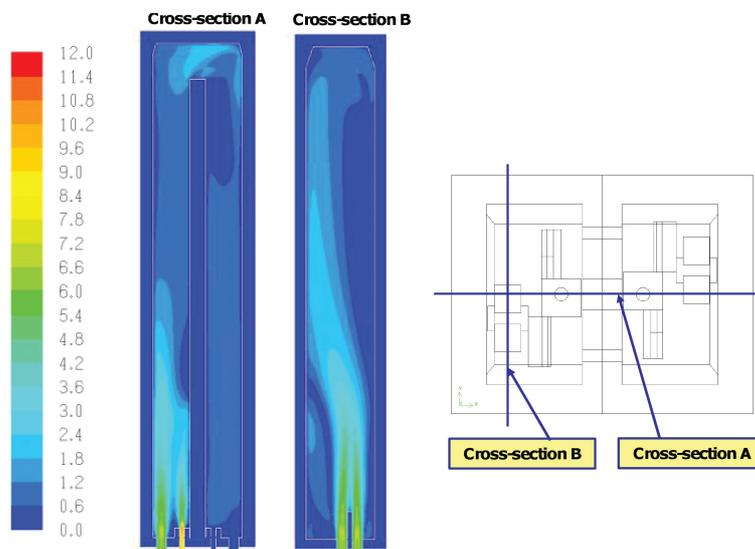
Fig. 7. Maps of velocity fields (in m/s) in two cross-sections.

Combustion requires inflow of oxygen and its presence in the combustion reactions zone. The oxygen concentration, represented by the mole fraction, within the same two cross-sections, is presented in Fig. 8. Analyzing these results one can easily find a location and shape of the flame. Its height and local temperatures are very important parameters affecting the local heat fluxes on the channel walls.
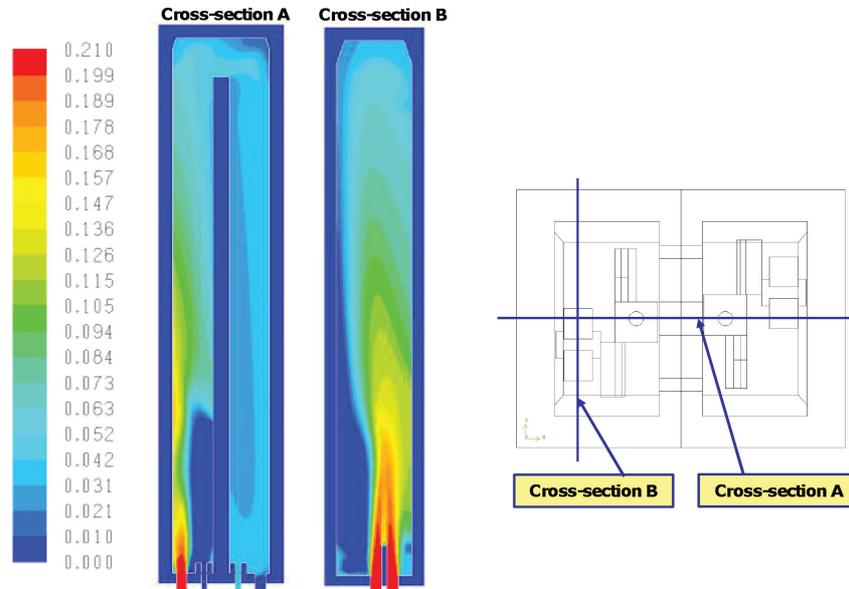
Fig. 8. Mole fraction field of oxygen (O_2) within two cross-sections of heating channels.

Figure 9 presents results of the heat flux step jump on the external surface of the wall separating heating channels from the coking chamber. Particularly, Fig. 9a shows temperature field (in °C) on external surfaces of both heating walls. Interaction of these surfaces with upward and downward channels is clearly visible. Calculations were carried out for constant heat flux equal to 6 kW/m^2. The shapes of the isotherms on external surfaces of both heating walls are generally fairly similar.
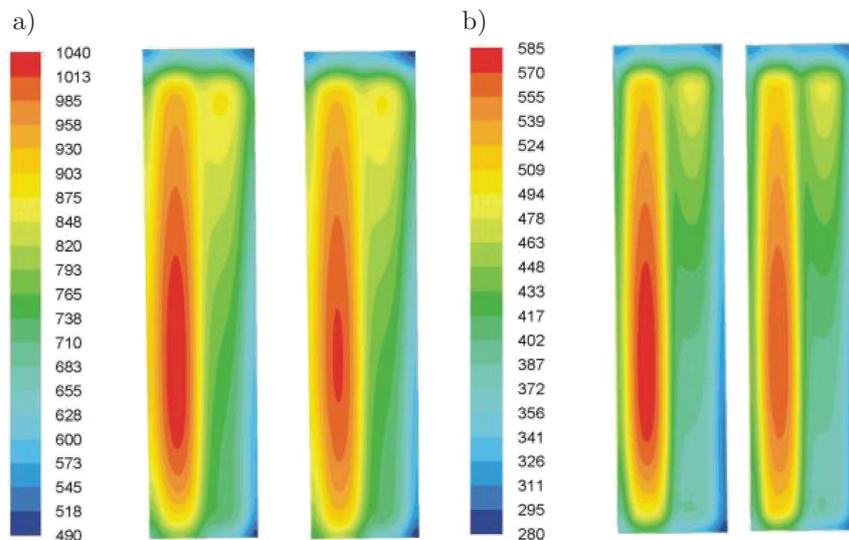
Fig. 9. a) Temperature field (in °C) on external surfaces of both walls of heating channels in steady-state with uniform heat flux of 6 kW/m^2, and b) temperature field (in °C) on external surfaces of both walls of heating channels in transient state after 1 hour when heat flux has jumped from 6 up to 15 kW/m^2.

It should be noted, however, that temperature of the left-hand-side wall, situated closer to the flame, is slightly higher.

Figure 9b shows the temperature field (in °C) on the same external surfaces 1 hour after the heat flux step jumped from 6 kW/m^2 up to 15 kW/m^2. Such a jump of heat flux can be caused for instance by loading into the coking chamber a fresh cold coal. It should be stressed that in spite of the fact that shapes of the isotherms have not been considerably changed, the range of wall temperatures changed dramatically. This dramatic drop of the wall temperature can mainly be observed on the external surface of the wall (the one which is in contact with cold coal). Temperatures of the internal surface of the wall (interface to the heating channels) do change, but not that much. To explain that phenomenon it should be noted that during the whole cycle of coking, heat is first accumulated in the wall and then it is released when the cold coal is placed in the coking chamber. It should also be noted that there is some asymmetry between left-hand-side and right-hand-side walls. That asymmetry should be considerably weakened by reversal in firing.

The last computer simulation reported in this work refers to the reversal of the fuel and flue gasses. This periodic process taking place every 21 minutes is overlapped with the periodicity of the coke production lasting 15 hours. Temperature evolution is observed at selected locations which are as follows: burner (point 1), point 3 in upward and downward channels and fire bridge (point 5). They are the same points where temperature is measured (using pyrometer) on industrial plant. Those locations are also schematically shown for two exemplary heating channels in Fig. 10 while the time evolution of temperature at those locations is presented in Fig. 11 and 12.

Instead of changing direction of flows when modelling the reversal of the fuel and combustion gasses, only 3-D temperature field within walls was transformed with respect to two symmetry planes.
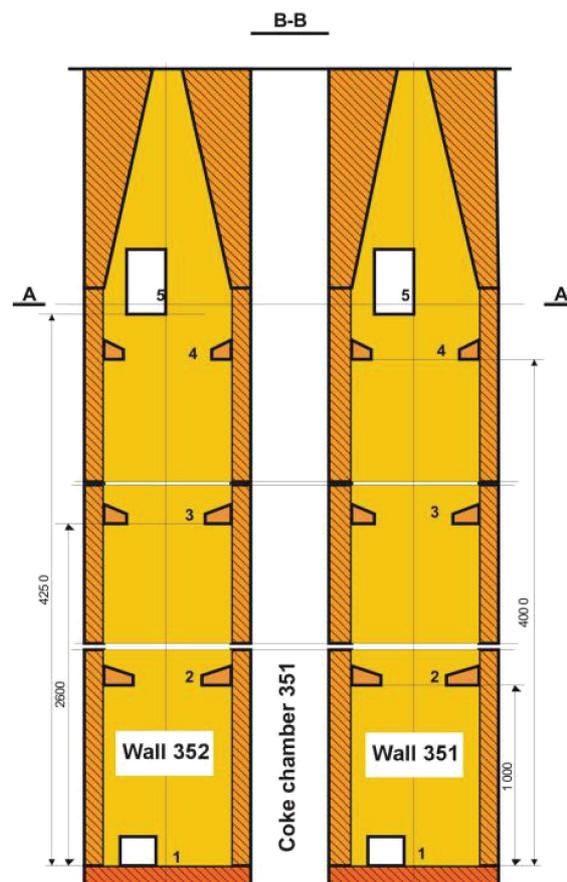

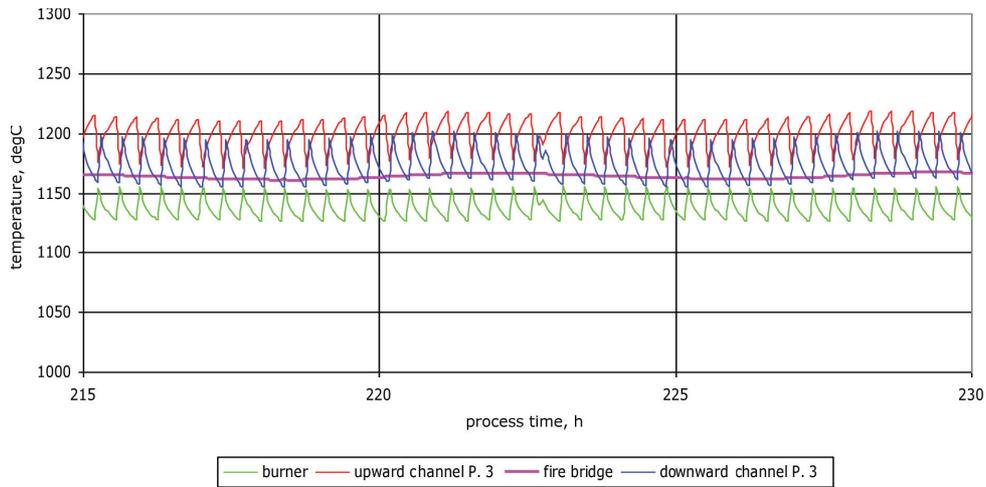**Fig. 10.** Measurement points 1–5 inside the heating channels.

Fig. 11. Time evolution of temperature at burner (point 1), in upward and downward channels (point 3) and fire bridge (point 5).
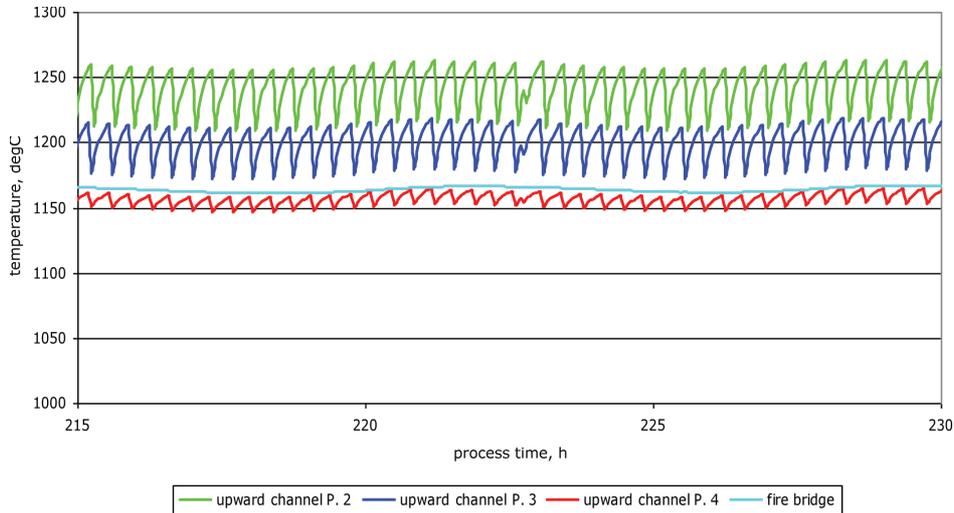

Fig. 12. Time evolution of temperature at points 2–5 in upward channel outlets.

The resulting temperatures oscillate considerably with the period equal to 21 minutes and oscillate gently with the period of 7.5 hours. The latter period is due to the phase shift between left-hand-side and right-hand-side walls. This is clearly seen in Fig. 11.

It should be also noted that oscillations of particular temperatures are fairly close to each other but not identical. This is a result of different heights of points where temperatures are monitored. Finally, it is worth stressing that observation point marked as fire bridge (point 5) lies on both symmetry planes and this is why the temperature at this point does not suffer any oscillations due to reversal.

The temperature profile and character of oscillations along the height of the upward channel is even more precisely shown in Fig. 12. It is evident that temperature is decreasing with the height. This was also confirmed by model of steady-state phenomena, $c.f.$ Fig. 5. At the same time, one can say that amplitudes of oscillations also decrease with the height. For instance, oscillations at point 4 are substantially weaker than those at point 3 and particularly at point 2. It was already explained why at point 5 there are no oscillations with shorter period.

Simultaneously with computer simulations some pyrometer temperature measurements on the real coke oven plant have been carried out. Some of these measurements for different time instances in one exemplary heating chamber are presented in Fig. 13.
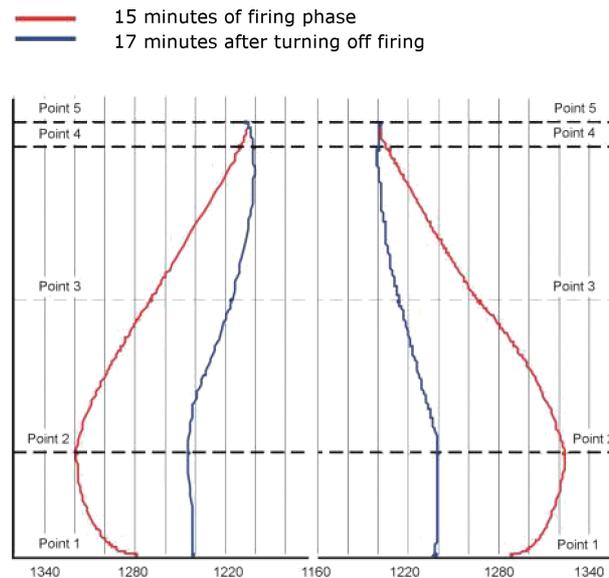
Fig. 13. Pyrometer temperature measurements at points $1-5$ in exemplary heating chamber in two time instants.

It should be noted that although detailed experimental validation of the model was not possible, measured temperatures are at similar range that those obtained from the model. Additionally, the proposed mathematical model offers results which are physically coherent as well as is already demonstrating the main features of the fluid flow and heat transfer processes taking place in the heating channels and heating walls of the coke oven battery. Capabilities of the model should be considerably increased very soon since it is currently being extended by detailed mathematical model of the coking processes taking place in neighbouring chambers. This will allow one to eliminate convective boundary conditions prescribed on external domain boundaries at this stage. Results of this research will be subject of future publications.

6. CONCLUSIONS

The analysis of results included into this work but also the outcomes of many remaining computer simulations, *e.g.*, [3], allowed one to draw the following conclusions:

- developed mathematical model of the heat transfer and fluid flow processes in heating channels produces results which are physically correct and demonstrates properly main stages of the coking process;

- numerical tests with some turbulent models showed [3] that the most appropriate one is the two-equation $\kappa - \varepsilon$ realizable turbulence model. Results of these tests are not included here because of space limitation;

- thermal radiation cannot be neglected during simulations of the gaseous combustion in the heating channels of coke oven. Indeed, a different definitions of the absorption strongly affect the final temperature field. The applied Discrete Ordinate model which takes into account both surface to surface and surface to gas radiation with the Weighted Sum of Grey Gases Model for absorption coefficient produced the most reasonable results. Again results of these tests are not included here because of space limitation but more details can be found in [3];

- developed mathematical model is currently being validated experimentally and results of that validations will be subject of future publications.

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