PREDICTION OF COKING DYNAMICS FOR WET COAL CHARGE

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A one-dimensional transient mathematical model describing thermal and flow phenomena during coal coking in an oven chamber was studied in the paper. It also accounts for heat conduction in the ceramic oven wall when assuming a constant temperature at the heating channel side. The model was solved numerically using partly implicit methods for gas flow and heat transfer problems. The histories of temperature, gas evolution and internal pressure were presented and analysed. The theoretical predictions of temperature change in the centre plane of the coke oven were compared with industrial-scale measurements. Both, the experimental data and obtained numerical results show that moisture content determines the coking process dynamics, lagging the temperature increase above the water steam evaporation temperature and in consequence the total coking time. The phenomenon of internal pressure generation in the context of overlapping effects of simultaneously occurring coal transitions – devolatilisation and coal permeability decrease under plastic stage – was also discussed.

Keywords: pyrolysis, devolatilisation, vaporisation, internal gas pressure

1. INTRODUCTION

The behaviour of coal during thermal decomposition in a coke oven is of general interest in coke making technology, which provides metallurgical coke for steel and iron production industry. The quality of coke is determined not only by physicochemical properties of used coal charge, but it results to a large extent from the thermal regime of the process, i.e. heating rate and final temperature of the process. The evolution of temperature and pressure distributions inside the coal/coke charge are mostly driven by physical and chemical transformations proceeding during the process. As proved by measurement data (Alvarez et al., 1996; Miura et al., 1991; Nomura and Arima, 2000), free moisture in initial coal charge is responsible for delaying the temperature increase above the level of 373 K when undergoing evaporation and in consequence delays the thermo-chemical decomposition, and prolongs the total coking time. Furthermore, transport of evolved steam and gases through the coal/coke charge is ruled by its structure change with increasing temperature. With heating progress, dry degasifying coal charge first transforms from a porous gas permeable medium into a substantially non-permeable plastic form (typically for temperature ranging between 623 and 773 K) that blocks the gas flow, and subsequently re-solidifies turning back into a cracked porous type medium letting the gas to flow through. The appearance of a plastic coal layer that traps inside released gases, results in internal gas pressure increase which, combined with mechanical stresses transferred through the coal charge, is considered as a source of oven wall pressure (coking pressure). It is suggested that the volume increase of softening and simultaneously degasifying coal grains decreases the intra-particle voids, which means a decrease in layer permeability and thus limited gas flow. This results in a pressure peak in

the layer which when expanding exerts the pressure on the walls through the coke and semi-coke layers (Barriocanal et al., 1998; Jenkins, 2001; Karcz and Strugała, 2001; Nomura and Arima, 2000).

To fully understand the mechanisms which drive the process of coal coking in a full scale oven, numerical simulations must be conducted. Quantification of thermal and flow effects requires fundamental study of coupled physical and chemical phenomena, such as heat transfer, phase transitions (evaporation and condensation of moisture and tars), devolatilisation, transport of steam and released volatiles, and coal structure change. In this context, also the thermo-physical properties of coal and coke, mainly thermal conductivity and permeability, having their strong impact on the temperature and pressure change within the oven -charge are of general importance for modelling procedure. Many mathematical models have been developed to describe the phenomena taking place during coal coking and to predict the change dynamics of main process characteristics. An extensive experimental and one-dimensional theoretical analysis of temperature field in a coke oven with special emphasis on the influence of coal charge properties on the coal/ coke charge heating dynamics was carried out by Witos (1977). Atkinson and Merrick (1983), Merrick et al. (1983a-1983c), and Voller et al. (1983) proposed a number of one-dimensional sub-models for transport phenomena associated with thermal decomposition of coal, including heat transfer, devolatilisation or steam and gas flow, and put special emphasis on the determination of changes in the thermo-physical properties of a coal charge. A simplified one-dimensional model of heat transfer and internal gas pressure in a coke oven was demonstrated by Jenkins (2001). A study of thermal and flow behaviour of wet coal charge during decomposition, based on a two-dimensional model was performed by Miura et al. (1991). Barr et al. (1994) and Osinski et al. (1993a, 1993b) developed a two-dimensional integrated model for heat transfer and gas flow within the individual coke oven. The transient two-dimensional model of thermal and flow processes accounting for moisture evaporation, implemented in ANSYS Fluent, was studied lately by Słupik et al. (2015). One of the latest works to be mentioned is the work by Jin et al. (2013) in which a three-dimensional transient model for coupled coking and combustion chambers, developed to simulate transport phenomena using CFX code was presented.

In the work presented here, a one-dimensional transient model was proposed to predict the change dynamics of temperature, internal gas pressure and the evolution of volatiles during coal coking. Contrary to the previous authors' work (Polesek-Karczewska et al., 2015), the temperature field was calculated for the system including an oven ceramic wall. The model utilises the correlations for temperature-dependent specific heat and thermal conductivity of coal taken from literature. The model was verified using measurement data from a real scale coke oven, showing a considerable influence of assumed thermal conductivity on the predicted temperature history.

2. MATHEMATICAL DESCRIPTION OF TRANSPORT PHENOMENA IN COAL CHARGE

Although the phenomena taking place during coal coking are at least two dimensional, due to their complexity some simplifications have to be made in order to simulate the process in reasonable time. A typical industrial scale coke oven chamber is about 0.4 m in width, 5 m in height and 15 m in depth and is heated from both sides with heating channels. The total duration time of the coking process reaches 18-20 hours. As the heating proceeds from the wall to the centre of the coke oven, the coal charge is first dried and afterwards, when it achieves temperature higher than 623 K it undergoes devolatilisation. The temperature range within which volatile release is the most intensive coincides with the range of coal softening. For temperatures above ca. 773 K the plastic zone turns into the semi-coke and then into coke.

2.1. Model details

In general, the coking process is three-dimensional. In real conditions, the heat transfer and gas flow phenomena are at least two-dimensional in the wall vicinity and in the upper and lower part of a coke oven.

Also, transport processes are recognised as multidimensional at the center of the charge at the end stage of the process, when a large vertical crack appears and the upward gas flow becomes significant. In other charge zones, which occupy most of a coke oven volume, transport processes may be essentially treated as one-dimensional. The one-dimensional approach simplifies the process description allowing to predict its crucial parameters with reasonable accuracy and, simultaneously, reduced time and cost of computations. As the literature on the coking process shows, one-dimensional models in this area of research are very often used as providing satisfactory agreement with real scale measurement data.

To simulate the coal coking process the following hypotheses were introduced:
1) the problem is symmetric due to heating from both sides,
2) regarding the high aspect ratio of the coke oven, the heat transfer and gas flow are one-dimensional (transfer in *x*-direction from the wall to the mid-plane, Fig. 1),
3) the released volatiles are non-condensable (the formation and transport of tars are neglected),
4) thermo-physical properties of coal/coke charge are effective (bulk) properties dependent on temperature,
5) the presence of fissures and cracks is not taken into account when considering the gas flow problem.

According to the one-dimensional approach proposed the flow of gases is driven by pressure difference. Gas is assumed to flow out of the charge at the centre plane being under atmospheric pressure, which is intended to represent the coke oven gas escape in the upwards vertical direction at the mid-plane. In this approach the gas mass balance is conserved in each analysed cross-section and each time step. Also, the total mass balance of gas released in the whole coke oven volume, which is equal to the integral of the mass flux of gas flowing out of the calculation domain, is conserved.
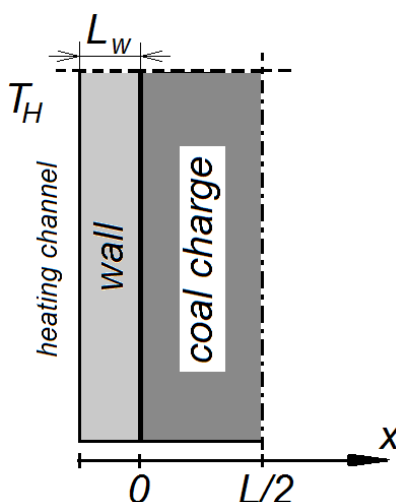

Fig. 1. A schematic of a coke oven chamber

Thus, the model is built on balance equations as follows:
- solid phase mass balance

$$\frac{\partial(\varepsilon_s \rho_s)}{\partial t} = -\dot{W}_{sg},\qquad(1)$$

- moisture mass balance

$$\frac{\partial(\varepsilon_w \rho_w)}{\partial t} = -\dot{W}_{wg},\qquad(2)$$

- water steam mass balance

$$\frac{\partial(\varepsilon_g Y_{w,g} \rho_g)}{\partial t} + \frac{\partial(\varepsilon_g Y_{w,g} \rho_g v_g)}{\partial x} = \dot{W}_{wg},\qquad(3)$$

- mass balance for gas mixture

$$\frac{\partial(\varepsilon_g \rho_g)}{\partial t} + \frac{\partial(\varepsilon_g \rho_g v_g)}{\partial x} = \dot{W}_{sg} + \dot{W}_{wg},$$ (4)

- momentum balance for gas mixture

$$\frac{\partial(\varepsilon_g \rho_g v_g)}{\partial t} + \frac{\partial(\varepsilon_g \rho_g v_g^2)}{\partial x} = -\frac{\partial(\varepsilon_g p_g)}{\partial x} - \frac{\mu \varepsilon_g v_g}{K} + \varepsilon_g \mu \frac{\partial^2 v_g}{\partial x^2},$$ (5)

- energy balance for the coal charge

$$\rho c_v \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} - \dot{W}_{sg} h_{sg} - \dot{W}_{wg} h_{wg},$$ (6)

- energy balance for the coking chamber wall

$$\rho_{cw} c_{v,cw} \frac{\partial T}{\partial t} = \lambda_{cw} \frac{\partial^2 T}{\partial x^2}.$$ (7)

Quantity $\dot{W}_{sg}$ appearing in Eqs. (1), (4) and (6) represents mass source resulting from thermal decomposition of coal and is determined by relation:

$$\dot{W}_{sg} = k \varepsilon_{s,0} \rho_{s,0} (Z - Z_\infty)$$ (8)

where Z denotes pyrolysis progress defined as $Z = m_s/m_{s,0}$. Subscript ∞ refers to the maximum devolatilisation, which means the mass loss value for very slow pyrolysis. To describe the value of Z_∞, the approximation of thermogravimetric data for Zofiowka coal ($Y_V = 22\%$) is adopted (see Tab. 1). Devolatilisation rate k [1/s] is calculated using correlation dependent on volatile content proposed by Postrzednik (1994).

Since the model does not account for detailed gas composition, for the purposes of internal gas pressure computations that require the data on molar mass, gas mixture was assumed to be characterised by an average approximate composition of coke oven gas, i.e. 55% H_2, 23% CH_4, 7% CO, 3% CO_2, 3% C_mH_n, 8% N_2 and 1% O_2. (Sultanguzin, 2007).

The volumetric mass source of moisture $\dot{W}_{wg}$, introduced into the Eqs. (2)-(4) and (6) is described as follows:

$$\dot{W}_{wg} = j_{wg} \times a_I$$ (9)

with the net mass flux j_{wg} dependent on the difference between the water vapour pressure above the liquid surface ($p_{w,g}$) and water pressure at the fluid-particle interface (p_w^{sat}), which may be written in the form:

$$j_{wg} = \sqrt{\frac{M_w}{2\pi RT}} \frac{\sigma}{2-\sigma} \left(p_w^{sat}(T) - p_{w,g}\right).$$ (10)

The details and discussion regarding the vaporisation/condensation model are given elsewhere (Polesek-Karczewska et al., 2015). Also, similarly as in the mentioned work, the values of steam convection parameter σ and specific surface area a_I were set to 0.01, 11.0 (for vaporisation) and 550.0 (for condensation), respectively.

2.2. Boundary and initial conditions

The initial conditions are the ambient temperature and pressure uniformity and zero gas velocity, (see Fig. 1):

$$T(x,0) = T_0$$ (11a)

$$p_g(x,0) = p_0 \tag{11b}$$

$$v_g(x,0) = 0 \tag{11c}$$

The temperature at the charge-side of the inter-wall between the heating channel and the coking chamber was calculated by solving heat conduction problem in the wall, setting its width to $L_{cw} = 0.1$ m and temperature on the heating channel side to a constant value $T_H = 1373$ K. The thermo-physical properties of the wall were assumed to be constant, i.e. $\rho_{cw} = 2.0 \times 10^3$ [kg/m³], $c_{v,cw} = 2.5 \times 10^3$ [J/(kg K)] and $\lambda_{cw} = 2.0$ [(W/(m K)].

The boundary conditions at the refractory wall are the wavy-like pressure change:

$$p_g(0,t) = p_g(0, t-\Delta t) + a \frac{p_g(\Delta x, t - \Delta t) - p_g(0, t - \Delta t)}{\Delta x / \Delta t}, \quad a = \sqrt{\frac{\partial p_g}{\partial \rho_g}} \tag{12a}$$

and the wall non-permeability

$$v_g(0,t) = 0 \tag{12b}$$

At the centre-plane of a coke oven, i.e. at $x = L/2$, the symmetry boundary conditions for temperature and velocity are assumed, respectively:

$$\left.\frac{\partial T}{\partial x}\right|_{(L/2, t)} = 0 \tag{13a}$$

$$\left.\frac{\partial v_g}{\partial x}\right|_{(L/2, t)} = 0 \tag{13b}$$

and the ambient pressure

$$p_g(L/2, t) = p_0 \tag{13c}$$

3. RESULTS AND DISCUSSION

To solve the problems of gas flow and heat transfer, partly implicit numerical schemes were applied. During the carbonisation process the porosity of coal/coke changes due to its thermal decomposition, which results in charge porosity and thus bulk density change. However, the variety of structures to which the decomposing coal charge converts, leads to difficulties in the estimation of these parameters in the full temperature range, and consequently, to the lack of complete experimental data that could provide the continuous temperature-dependent functions to describe them. Strugała (2000) reported experimental data on true density of coal chars derived from various coal blends at temperatures ranging between 823 K and 1273 K. On the other hand, he analysed experimentally true density of Polish bituminous coals for temperatures up to 773 K (Strugała, 2002a) and provided data on the volume of pores for a temperature range from 658 to 1273 K (Strugała, 2002b). The model proposed herein requires the introduction of either the charge porosity or the coal apparent density as an input parameter in the whole temperature range. Therefore, for the purposes of the present study an apparent density of coal ρ_s in the form of a temperature-dependent function was implemented. In order to express somehow the structure change, the test results for simultaneous thermogravimetric analysis and measurement of the shape of coal grains (IChPW, 2007) were utilised (see Fig. 2). For permeability the temperature-dependent function, approximating experimental data of Miura and Nishioka (Mertas et al.,2013), was employed (see Fig. 3). Gas density ρ_g is calculated using

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the ideal gas equation. Other physicochemical parameters of coal, gas and water, assumed for numerical calculations are summarised in Table 1.
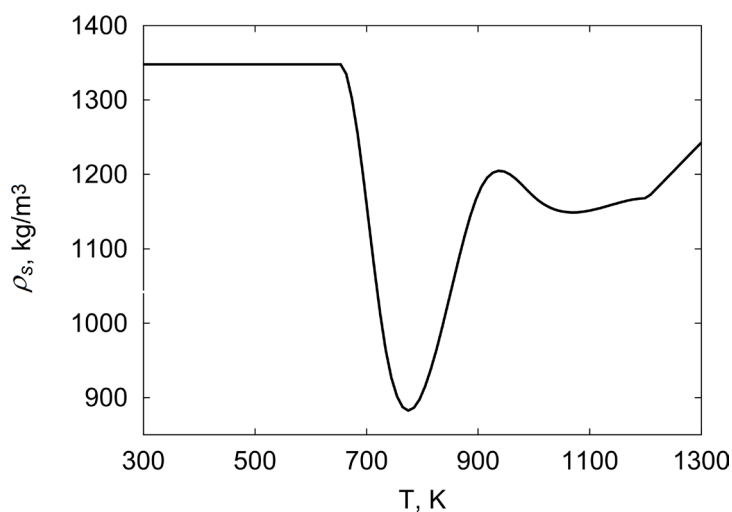

Fig. 2. Apparent density of coal/coke

Table 1. Input parameters for numerical simulation

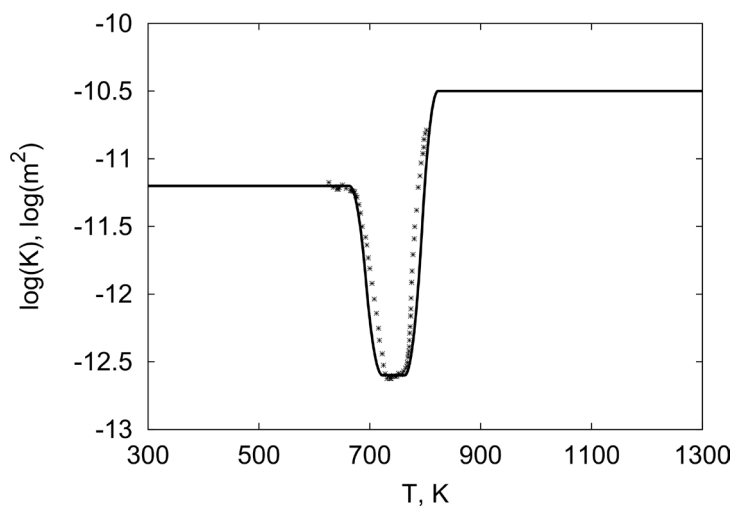| Parameter	Value	Ref.
$c_{v,s}$, J/(kg K)	$a+b(T\text{-}273)+c(T\text{-}273)^2+d(T\text{-}273)^3+e(T\text{-}273)^4$, for T[K] $a = 1.08\times10^3$, $b = 3.81$, $c = 5.48\times10^{-4}$, $d = -7.83\times10^{-6}$, $e = 3.99\times10^{-9}$	Tomeczek and Palugniok (1996)
$c_{v,g}$, J/(kg K)	$-1.3268\cdot10^{-7}T^3+3.2135\cdot10^{-4}\,T^2-0.0926T+0.7192$	tabulated data
ρ_w, kg/m^3	1000.0	
$c_{v,w}$, J/(kg K)	4200.0	
λ_w, W/(m·K)	0.60	
μ, Pa·s	10^{-5}	
Z_∞	$\begin{cases} \dfrac{a_1}{2}\left(1+\mathrm{erf}\left(\dfrac{T-b_1}{c_1\sqrt{2}}\right)\right), & 273\,\mathrm{K} < T \leq 573\,\mathrm{K} \\[2ex] \left(d\sqrt{T}-a_2\right)\left(1+\mathrm{erf}\left(\dfrac{T-b_2}{c_2\sqrt{2}}\right)\right)+a_1, & 573\,\mathrm{K} < T \leq 1273\,\mathrm{K} \end{cases}$ $a_1 = 1.52298$, $a_2 = 17.8652$ $b_1 = 413.794$, $b_2 = 780.823$ $c_1 = 39.55$, $c_2 = 49.2996$ $d = 0.8253$	Polesek-Karczewska (2008)
L, m	0.4	
L_w, m	0.1	
h_{sg}, MJ/kg	0.20	
h_{wg}, MJ/kg	2.20	
T_0, K	300.0	
p_0, Pa	10^5	
$\varepsilon_{s,0}$	0.55	
$\varepsilon_{w,0}$	0.1	

Fig. 3. Assumed permeability function (solid line) based on experimental data by Miura and Nishioka (points) given in Mertas et al.(2013)

Regarding the considerable effect of physicochemical properties of the coal/coke charge on the temperature dynamics in the coke oven, in order to compare the temperature predictions with real scale measurement data, three various correlations for thermal conductivity were taken into consideration. They are listed in Table 2.

Table. 2. Thermal conductivity assumed for dry coal/coke charge, λ [W/(m·K)]

Case	Value	Ref.
1	$0.1043\exp(0.0035(T+273))$	IChPW data
2	$0.003132\exp(0.0063T)$	Kasperczyk and Simonis (1971)
3	$0.23, \qquad\qquad\qquad T \leq 673$ K $0.23+2.24\times10^{-5}(T-673)^{1.8}, \; T > 673$ K	Adesanya and Pham (1995)

The model predictions for the midpoint temperature of a coke bed were compared with industrial measurements conducted in the coke oven of a battery at Przyjaźń coking plant. The thermo-elements were put inside through the coke side about 4.1 m above the sole before charging. One of them was placed near the inter-wall ($x = 0$) and the other in the centre-plane (at $x\sim 20$ cm from the wall). It is obvious that due to the measuring procedure difficulties in industrial scale, the data sets may deviate. The position of temperature sensors may change during the process, for instance, as a result of charge shrinkage. Moreover, heat transfer is strongly affected by local charge heterogeneity, and so by the liquid conductivity, convection and radiation from flowing gas, and the information on such effects is impossible to obtain. However, based on numerous data regarding thermal histories in the charge, it may be assumed that the total measurement error does not exceed 5%.

The evolution of calculated and measured (3 test series) temperatures at the centre of a coke oven is shown in Fig. 4. Both, the experimental and theoretical results show the delay in temperature increase above the boiling point (373 K), which is caused by moisture evaporation and condensation. The steam is transported from the wall to the centre of the oven and condenses in cooler zones of the charge, stabilising temperature at the level of 373 K until all the water is released. Measurements show the total drying process to last, depending on the data set, from 7 to 9 hours. Numerical simulations show longer times of moisture vaporisation, which starts about 2-3 hours from the process beginning and is completed within the next 9 or 11 hours, depending on the thermal conductivity assumed in computations, case 2 and case 3, respectively. In the case studied, the best agreement between model predictions and experimental data was obtained when employing the correlation for thermal conductivity which was experimentally derived at

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IChPW (Zabrze, Poland), (case 1). For other thermal conductivity functions the simulation results show either shorter (case 2) or longer total coking time (case 3).
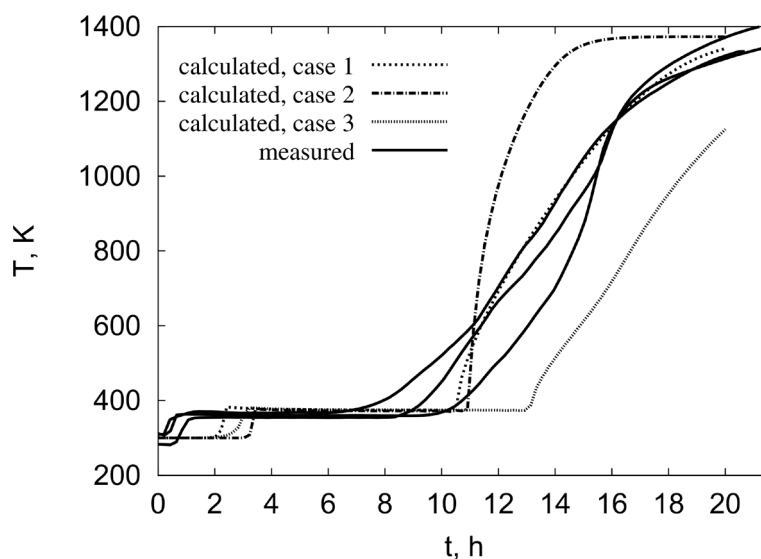

Fig. 4. Temperature change in the centreline of the coke oven – measured (3 test series) and calculated assuming various thermal conductivity for the charge

Thermal histories in the coal charge (case 1) at various distances from the wall, including wall temperature ($x = 0$), are shown in Fig. 5. It is clearly seen that wall temperature decreases down to about 650 K in the first stage of the process and starts to increase afterwards. The difference in duration of drying is also observed. It lasts about 1.5 h at $x = 5$ cm, 3 h at $x = 10$ cm, 6 h at $x = 15$ cm and 9 h at $x = 20$ cm.
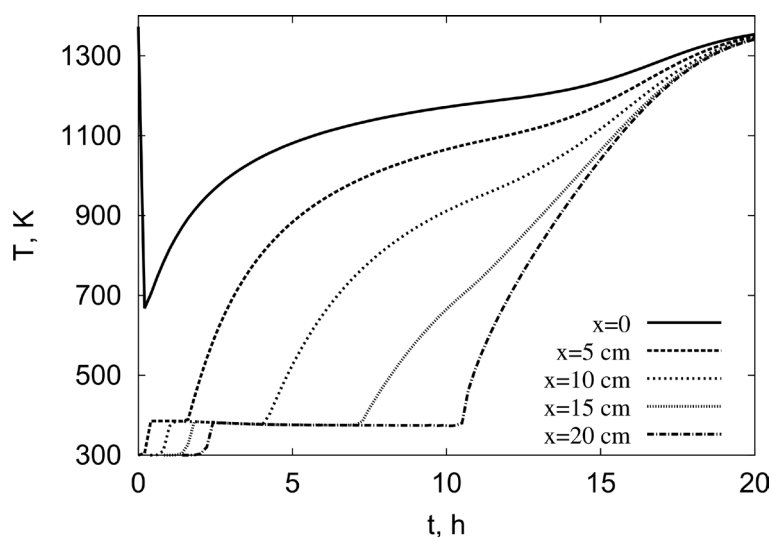

Fig. 5. Predicted temperature evolution within the coal/coke charge during coking

The temperature evolution corresponds with the change dynamics of gas generation within the charge, which is shown in Fig. 6. It may be observed that the rate of gas volatile release increases when the temperature is locally within the range of intensive devolatilisation, which is between ~ 673 and 823 K. Hence, for instance, at the distance of $x = 5$ cm the volumetric mass flux of gases rises up immediately between 3rd and 6th hour of the coking cycle and between 6th and 10th hour at $x = 10$ cm. Further increase in gas mass rate observed after about 11 hours of the process follows from the fact that at this stage of the cycle the zones of more and less intensive devolatilisation are distributed along the whole charge at a temperature above 673 K.
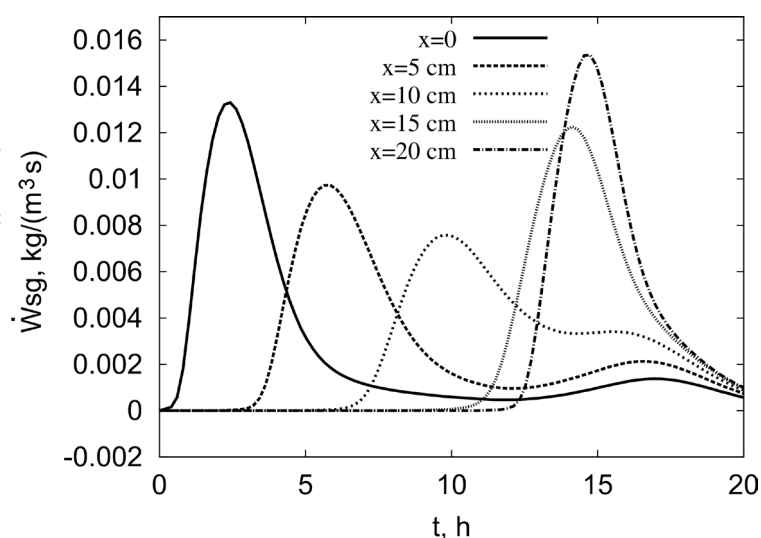
Fig. 6. Predicted evolution of gas release within the coal/coke charge during coking

Fig. 7 depicts a comparison between the predicted change in global volumetric gas rate during the coking process and the data from literature (Trefny, 1951) . It shows that in case of model simulations the gas generation rises during the first 3-4 hours into the process to the level of approximately 200 Nm^3/h, then remains almost constant for the next 7 hours, and rises again achieving its maximum of about 450 Nm^3/h at about 14th hour of process duration.
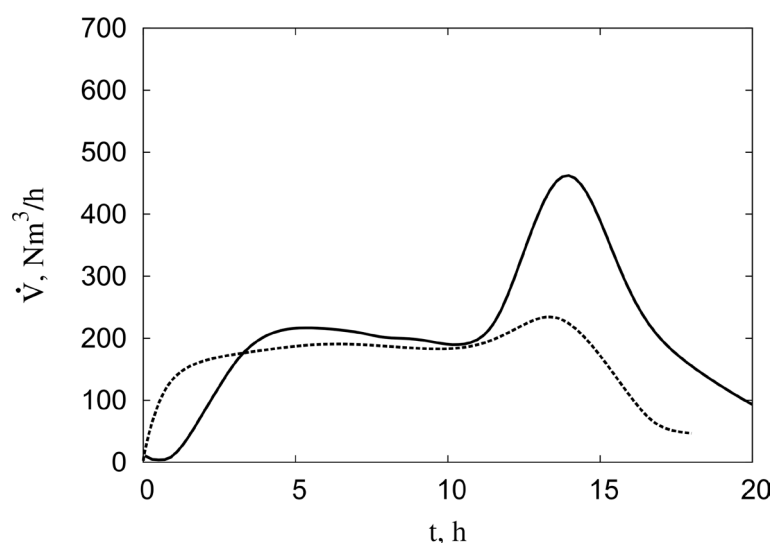

Fig. 7. Global coke oven gas (dry) release rate vs. time – results of model calculations (solid line) and literature data (dotted line, Trefny, 1951)

Finally, after 20 hours, the amount of gas released from the coke oven decreases to the level of approximately 100 Nm^3/h. The obtained function of gas rate, particularly as regards the time when the maximum of gas release appears, is in good qualitative agreement with typical characteristics of gas yield.

Evolving steam and volatiles, when they meet or are trapped in the plastic zone, result in the increase in the internal gas pressure in a coke oven. The change dynamics of internal gas pressure is plotted in Fig. 8. The local rapid pressure increase is observed at the distance where the temperature is at the level of coal softening, i.e. about 700 K, which means a decrease of coal permeability. In the case considered, the plastic zone begins at $x = 10$ cm at about 6h into the process, whereas at $x = 15$ cm at the time of approximately 10 h (compare with Fig. 5). The maximum pressure achieving the level of about 8 kPa is observed in about 12.5 hour of the coking cycle, which is due to the thickness of the plastic layer that blocks the

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flow of gases. In general, its extent (for the typical temperature range of 623 – 773 K) increases as the process is in progress. Analysing temperature profiles (Fig. 5) one can see that at the mentioned stage of the process, i.e., 2/3 of the duration time, the predicted plastic layer joins the one formed on the opposite side of the center-plane. Consequently, the plastic zone then occupies the area between $x = 26$ cm and $x = 34$ cm (the area between $x = 0$ and $x = 0.1$ m represents the coke oven wall), approximately, which may clearly be seen from the temperature plot in t-T coordinate system, shown in Fig. 9.

Next, when the charge is being further heated it re-solidifies and the pressure drops down to the ambient.
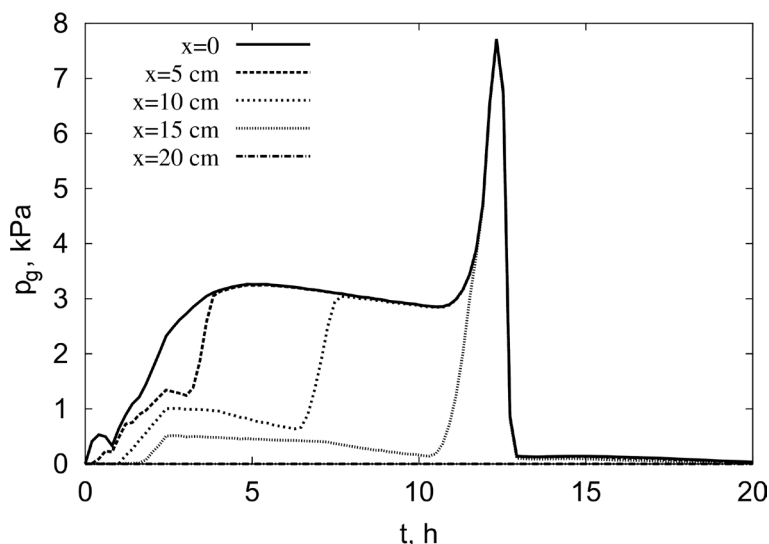

Fig. 8. Predicted evolution of internal pressure within the coal/coke charge during coking
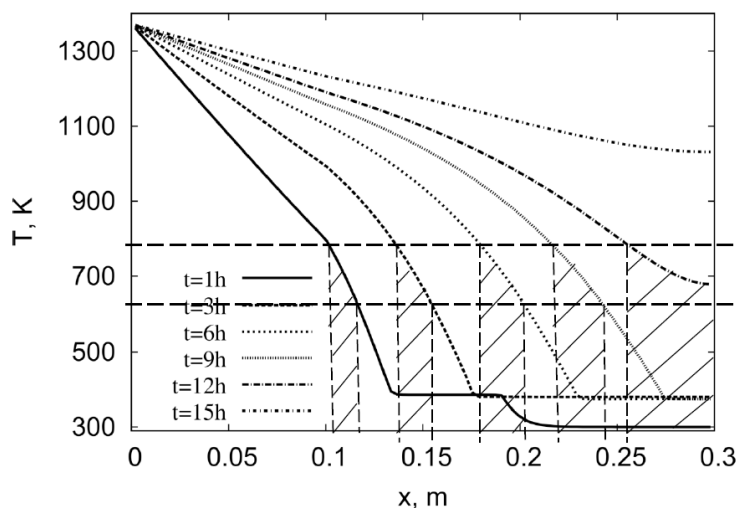

Fig. 9. Predicted temperature distribution within the coke oven (1/2 of the coke oven chamber) with the plastic layer zone marked (hatched areas)

The gas escape from the plastic layer is due to the permeability of the adjacent layers. Coke and semi-coke layers include, apart from pores, fissures and cracks that are developed during the stage of plastic coal re-solidification, which allow the gas outflow and internal pressure release. And, on the opposite side of the plastic layer where the intra-particle voids in coal charge are partly occupied by condensed heavy tars, the gas flow is limited (Barriocanal et al, 1998). As shown, for instance, by studies of Casal et al. (2006) fissure patterns formed in the so-called dangerous coals, i.e., generating higher wall pressures, are far less developed compared to safe coals. However, a quantitative description of the relationship between fissuring structure and pressure peaks is too complex and still remain a challenge.

4. SUMMARY

- The model, although one-dimensional, extends the capability to predict and control the dynamics of coal coking process characteristics, including temperature, pressure, gas and steam release.

- Heat transfer affected by water phase transitions was proved to drive the process of thermo-chemical conversion of coal and showed the vaporisation and condensation of moisture to be responsible for the delay in temperature increase above 373 K and hence for prolonging the duration of the total process.

- The calculation results for temperature in the mid-plane were verified with industrial measurement assuming various temperature-dependent functions for charge thermal conductivity; satisfactory agreement was obtained in case of one of the functions assumed.

- The model predictions regarding the total gas release rate are in good qualitative agreement with data reported in the literature.

- In general, internal pressure peaks correspond with charge devolatilisation inside the coal plastic zone, which is non-permeable and blocks the gas outflow.

SYMBOLS

a_I	specific surface area, m^2/m^3
c_v	specific heat, J/(kg K)
h	enthalpy of transition, J/kg
j	net mass flux, $kg/(m^2 s)$
K	permeability, m^2
M	molar mass, kg/kmol
L	oven width, m
L_{cw}	width of the coking chamber wall, m
p	pressure, Pa
R	universal gas constant, 8.314 J/(mol K)
T	temperature, K
t	time, s
$\dot{W}$	mass rate, $kg/(m^3 s)$
Y	mass fraction, kg/kg
v	velocity, m/s
x	space coordinate, m
Z	pyrolysis progress, $Z = m_s/m_{s,0}$

Greek symbols

ε	volume fraction, m^3/m^3
λ	thermal conductivity, W/(m K)
μ	dynamic viscosity, Pa·s
ρ	density, bulk density, kg/m^3

Superscript

sat	saturation

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Subscripts

l	liquid phase
cw	coking chamber wall
g	gas phase
s	solid phase
sg	solid to gas (pyrolysis)
w	water
wg	water to steam (vaporisation)
w, g	water steam in gas mixture
0	initial state
∞	for $t \rightarrow \infty$

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