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## Three phase transient model of wet coal pyrolysis

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### ABSTRACT

A one-dimensional transient mathematical model was developed to describe the thermal and flow phenomena during coal pyrolysis in a coke oven. The model was solved numerically using partly implicit methods for gas flow and heat transfer problems. It was successfully validated with industrial-scale measurements of temperature change in the middle-plane of the coke oven chamber. The evolution of temperature and pressure, distributions of gas and steam generation rates were presented and analyzed. Special emphasis is put on the progress of vaporization and condensation fronts and their impact on the moisture levels within the coal charge. The obtained results show that moisture content determines the coking process dynamics, lagging the temperature increase above the boiling temperature and in consequence the start up of pyrolysis. The effect of low permeability of coal in its plastic stage on the internal pressure peaks in a coke oven is discussed.

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### 1. Introduction

Pyrolysis is a key stage in a variety of thermal conversion processes of solid fuels. Coal, being one of them, has its own specific features, but like the woody biomass and organic wastes undergoes thermal decomposition when heated up. Physical and chemical properties of coal, unlike those of other organics, are relatively well recognized. It thus provides accessibility to measurement data and material databases, which is the necessity in describing physico-chemical phenomena accompanying pyrolysis and in predicting the flow and thermal behavior during the process.

A common known example of industrial application of slow pyrolysis process (carbonization) is coal coking which aims at producing coke to be further used for steel and iron production or to cover heating requirements. Although having been known for decades, the coal coking still generally bases on empirical development. The main reason is the complexity of the process, which comprises a set of multi-scale physical and chemical phenomena, including heat transfer, hetero- and homogeneous chemical reactions, gas flow through porous media, phase transitions and mechanical stresses, all occurring simultaneously. Hence, modeling

of coal pyrolysis is crucial from practical point of view. Apart from coke quality and the pressure change dynamics in a coke oven, the reduction in carbonization heat consumption is of general importance. It is believed that moisture content is the parameter that is responsible for delaying the total coking time, and so decreasing the efficiency of the process. The reason for this is the energy consumed for vaporization of water agglomerated in coal particles and transported through the coal charge during the process. Many efforts have been done by researchers to develop mathematical models able to describe thermal and flow phenomena in an oven and to predict the change dynamics of the main coking parameters. One of the first was Millard [1], who proposed a one-dimensional model of heat transfer accounting for coal decomposition, evaporation and condensation. Water phase changes were also of general interest in another approach reported in [2–6], which was based on various sub-models of thermal decomposition of coal, including the release of volatile matter, thermo-physical properties, heat transfer and gas flow. The two-dimensional mathematical model of gas flow in a coke oven chamber focusing on the analysis of flow behavior of steam and pyrolysis gas, with special emphasis on the effect of steam transport on the carbonization rate was proposed by Miura et al. [7]. The influence of moisture content on the temperature increase within the coal charge was studied also in [8]. Authors of papers [9–11] have successfully developed two-dimensional model of heat and gas flow in a coke oven, solving one-dimensional problem of a moving isothermal phase transformation for water evaporation and condensation.

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**Nomenclature**

$a$	Propagation speed of sound ( $\text{m s}^{-1}$ )
$a_l$	Specific surface area ( $\text{m}^{-1}$ )
$c_p$	Specific heat ( $\text{J kg}^{-1} \text{K}^{-1}$ )
$h$	Specific enthalpy ( $\text{J kg}^{-1}$ )
$k$	Devolatilization rate ( $\text{s}^{-1}$ )
$K$	Permeability ( $\text{m}^2$ )
$L$	Coke oven width (m)
$m$	Mass (kg)
$p$	Pressure (Pa)
$t$	Time (s)
$T$	Temperature (K)
$v$	Velocity ( $\text{m s}^{-1}$ )
$\dot{W}$	Volumetric mass source ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$x$	Distance (m)
$Y$	Mass fraction ( $\text{kg kg}^{-1}$ )

**Greek letters**

$\epsilon$	Volume fraction, porosity ( $\text{m}^3 \text{m}^{-3}$ )
$\lambda$	Thermal conductivity ( $\text{W m}^{-1} \text{K}^{-1}$ )
$\mu$	Dynamic viscosity (Pa s)
$\rho$	Density ( $\text{kg m}^{-3}$ )

**Subscripts**

0	Initial value
s	Solid (coal/coke)
sg	Solid to gas (pyrolysis)
w	Water
g	Gas
V	Volatiles
wg	Water to gas (vaporization)
w,g	Water (vapor) in gas mixture
$\infty$	Maximum/limit value

The goal of presented work was to investigate the dynamics of coal pyrolysis and to analyze the effect of phase change phenomena – moisture evaporation and condensation – on temperature change within the porous coal bed during the process. The general idea of the study is to develop the model of wet coal pyrolysis and to validate it using measurement data regarding temperature distribution in a real scale coke oven. The proposed model of coal carbonization is one-dimensional and enables to predict the distribution of temperature, pyrolysis gas and vapor yields, as well as pressure inside the coal charge.

## 2. Mathematical model of transport phenomena in a coke oven

The single coke oven chamber, being in general a part of coke battery is heated from both sides by heating channels. A schematic of a single coke oven is presented in Fig. 1. Typically, an industrial coke oven is up to 0.5 m in width ( $x$ -direction), about 5 m in height ( $z$ -direction) and up to several meters in depth ( $y$ -direction). A typical linear size of coal particle in a coke oven chamber is around  $2 \div 3 \text{ mm}$ .

Being consisted of various mass and flow phenomena, differing in both, time and space scales, coal coking process is of very complex nature. Perturbations in gases propagate with the velocity of an order of  $10^2 \text{ m s}^{-1}$ , whereas the mass flow of gases is about  $10^{-3} \text{ m s}^{-1}$ . On the other hand, the heat is transported with the velocity  $10^{-6} \text{ m s}^{-1}$ . The time of chemical reaction is of an order of  $10^{-10} \text{ s}$  and the coking process takes about 20 h. Therefore, detailed description of the full scale process would require

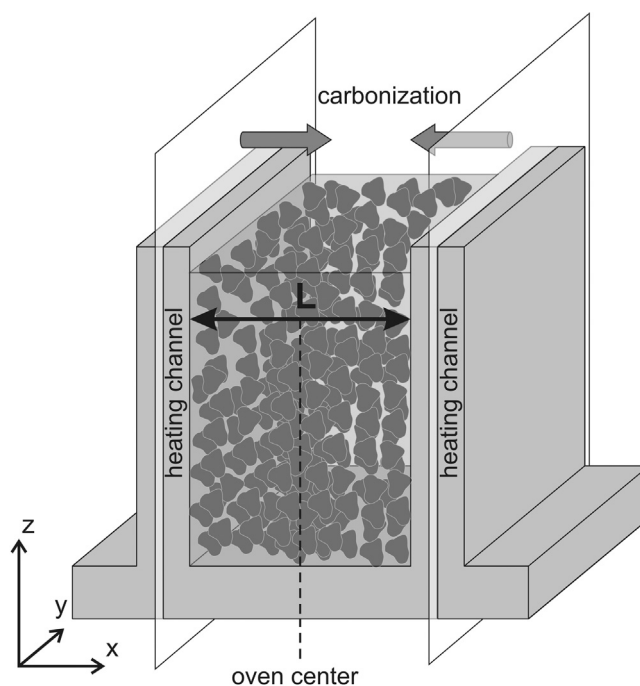


Fig. 1. The schematic of a coke oven.

sophisticated two- or three-dimensional transient mathematical models and time-consuming numerical calculations. And this is beyond current computing possibilities and seems to be useless for practical issue.

Regarding the small aspect ratio of coke oven chamber and assuming the uniformity of temperature distribution at both heating walls, the problem of heat and mass transfer in this case may be considered as one-dimensional and symmetric.

After being placed inside the hot coke oven (typically at maximum temperature 1273 K), the heated wet coal charge undergoes physical and chemical transformations. As the heat is transported from the refractory wall to the center of the oven chamber, the free moisture contained in coal particles evaporates in a first place. Further, as the heating continues, the coal charge changes its structure due to thermal decomposition and volatiles are being released. Evolved gases flow through the coal bed to the center and some of them (the heavier hydrocarbons) condense entering the cooler zones of the charge constituting tars. In general, the maximum intensity of coal pyrolysis takes place for temperatures between 673 and 823 K. Within this temperature range, depending on the coal type [12,13], the coal being devolatilized becomes a plastic nearly homogeneous medium. The permeability in the plastic zone, in comparison to the value typical for the coal/coke charge, drastically decreases and blocks the flow of gases, which in extreme situations may lead to the large pressure increase inside the charge. The plastic coal layer resolidifies in temperatures above 823 K and turns into the highly porous lump being called semi-coke. Afterwards, still devolatilizing semi-coke layer fractures, letting the gases to escape through the formed fissures and cracks. It is the last stage of the process giving the final product – coke. Consequently, the heat transferred through the coal bed leaves behind the zones of coke, semi-coke, plastic layer and dry coal, until the whole coal charge is carbonized.

However, as mentioned above, the process stage that has considerable effect on the delay of total coking time is the dehydration and steam transport through the coal bed. To illustrate the mechanism of coal evaporation and condensation, which is important

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