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Marian BOJKO***MATHEMATICAL MODEL OF THE LOW-TEMPERATURE OXIDATION
OF COAL IN COAL STOCKPILES AND DUMPS****MATEMATICKÝ MODEL NÍZKOTEPLTNÍ OXIDACE UHLÍ V UHELNÝCH
SKLÁDKÁCH A ODVALECH****Abstract**

Article define mathematical model of the low-temperature oxidation of coal, when it is spontaneously combustion. Process of spontaneously combustion can be initialization inside the coal stockpile by specific atmospheric conditions by reason of air flow through store of coal. Problem of low-temperature oxidation of coal is defined as wall surface reactions of adsorbed carbon in porous zone, which is presented as store of coal. Influence of water vapour product is neglected in definition of reaction mechanism and in stoichiometric equation of combustion. Thus defined mathematical model is applied on the simple geometry as porous zone. Then software FLUENT 12 is used for numerical simulation.

Abstrakt

Tento příspěvek definuje matematický model nízkoteplotní oxidace uhlí, kdy dochází k tzv. samovznícování. K samovznícování uhlí v uhelných skládek může docházet za určitých atmosférických podmínek v důsledku účinku proudícího vzduchu skrz uhelnou hromadu. Problematika nízkoteplotní oxidace uhlí je definována jako povrchové spalování adsorbovaného uhlíku v porézní oblasti, která představuje uhelnou hromadu. V definici reakčního mechanismu a stechiometrické rovnice je zanedbán vliv produkce vodní páry v důsledku spalování. Takto nedefinovaný matematický model je aplikován na jednoduchou geometrii porézní oblasti. Následně k numerické simulaci je použit software FLUENT 12.

1 INTRODUCTION

The low-temperature oxidation of coal we think process of spontaneously combustion e.g. coal stockpile in consequence of air flow through coal material, when coal is oxidation by oxygen. Problem of spontaneous of coal stockpiles and dumps are presented as dangerous risk with respect to environment, when by influence of specific atmospheric conditions can occur to spontaneous ignition of coal stockpile. With low-temperature oxidation of coal is burned with production of carbon dioxide (CO_2), carbon monoxide (CO) and water vapour (H_2O) in temperature range $<0^\circ C \div 200^\circ C>$. Especially mass of water vapour production is important. Result of heterogeneous reaction is oxy-coal in solid phase and gaseous products by low-temperature oxidation.

Basic reaction scheme of low-temperature oxidation can be defined as:



Problem of numerical modeling of the low-temperature oxidation of coal presents difficult process in term of definition the reaction mechanism of spontaneous, because it's combustion of solid particle with creation of gaseous species and solid rest (oxy-coal) – heterogeneous reaction [3]. Final mathematical model of spontaneous of coal will take into account flow of gaseous species, heat trans-

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fer and definition of reaction mechanism for chemical reaction of low-temperature oxidation. Above definition problem will solve by method of finite volume with use program FLUENT.

Procedure the low-temperature oxidation of coal is defined as wall surface reaction of carbon adsorbed inside porous zone in program FLUENT. Porous zone is as coal dump in which the wall surface reaction of carbon (C) can run. Then products of gaseous species flow inside the porous zone and surroundings of dump. Porous zone is characterized by porosity and physical properties of individual type of coal. Next important parameter is definition of permeability of zone. Final flow through coal dump can be characterization as flow through porous zone in which wall surface reaction of adsorbed carbon can defined.

For compressible and steady state flow mathematical model defines basic equations [1], [2]:

The Mass Conservation Equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \bar{u}_j)}{\partial x_j} = 0 \quad (2)$$

Momentum Conservation Equations

$$\frac{\partial (\rho \bar{u}_i)}{\partial t} + \frac{\partial (\rho \bar{u}_i \bar{u}_j)}{\partial x_j} = - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left((\mu + \mu_t) \frac{\partial \bar{u}_i}{\partial x_j} \right) + \rho f_i \quad (3)$$

Species Transport Equations

$$\frac{\partial (\rho Y_r)}{\partial t} + \frac{\partial (\rho \bar{u}_j Y_r)}{\partial x_j} = - \frac{\partial}{\partial x_i} J_{j,i} + R_r + S_r \quad (4)$$

The Energy Equation

$$\frac{\partial}{\partial t} (\rho c_p T) + \frac{\partial}{\partial x_j} (\rho \bar{u}_j c_p T) = \rho \bar{u}_j f_j + \frac{\partial (\tau_{ji} \bar{u}_j)}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\lambda_{eff} \frac{\partial \bar{T}}{\partial x_j} \right) \quad (5)$$

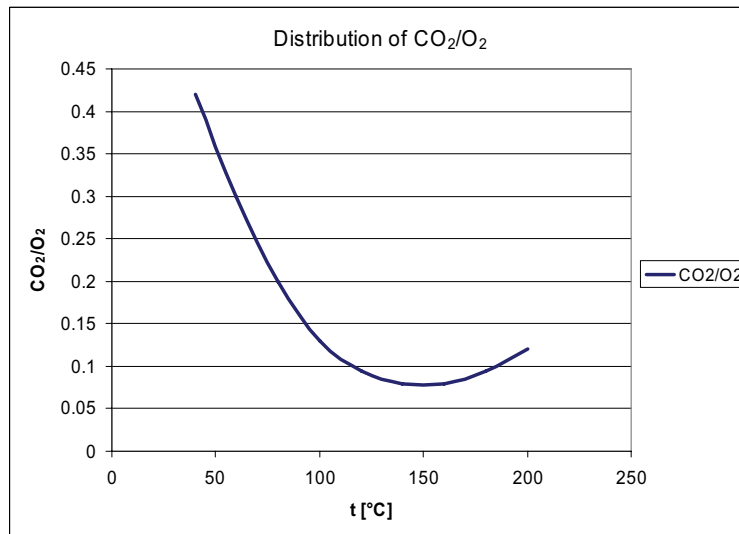


Fig. 1.1 – Course of production CO_2/O_2

Process of the low-temperature oxidation of hard coal can divide on the basis of experimental results of production CO_2/O_2 into the two processes, Fig. 1.1 On the basis of experimental results is

necessary definite reaction mechanism of the low-temperature in two temperature intervals ($<50^{\circ}\text{C} \div 150^{\circ}\text{C}>$; $<150^{\circ}\text{C} \div 200^{\circ}\text{C}>$) with respect to course of production CO_2/O_2 . The low-temperature oxidation will define without formation of water vapour in this article. Corresponding results of numerical simulation will high depend on the correct definition of reaction mechanism for wall surface oxidation of carbon with oxygen.

2 DEFINITION OF WALL SURFACE REACTION IN POROUS ZONE

Porous zone is defines by parameters as porosity (γ) of medium (coal), physical properties (density - ρ_s , specific heat - c_{ps} , thermal conductivity - λ_s) and permeability - α . With regard to non-isothermal flow, when we define energy equation (5), then in porous zone this equation is modification to equation:

$$\frac{\partial T}{\partial t} (\gamma \rho_g c_{pg} + (1-\gamma) \rho_s c_{ps}) + \frac{\partial}{\partial x_j} (\rho c_p \bar{u}_j T) = \rho \bar{u}_j f_j + \frac{\partial}{\partial x_i} (\tau_{ji} \bar{u}_j) + \frac{\partial}{\partial x_j} \left(\lambda_{eff} \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} (c_p T J_{j,i'}) \quad (6)$$

where the effective thermal conductivity is defined:

$$\lambda_{eff} = \gamma \lambda_g + (1-\gamma) \lambda_s \quad (7)$$

and λ_g is thermal conductivity of gaseous phase and λ_s is thermal conductivity of solid medium. Detailed description of definition equations is described in [2].

3 REACTION SCHEME OF WALL SURFACE REACTION

Rate of consumption (R_r) for adsorbed i' solid phase (e.g. carbon) on the wall by influence chemical reaction (low-temperature of wall surface oxidation) in equation (3) is defined in FLUENT [2]:

$$R_r = M_{\omega,i'} \sum_{r=1}^{N_R} (s'_{i',r}) k_r \prod_{i=1}^{N_S} [\rho_{site}]^{s'_{i',r}} \quad (8)$$

where $M_{\omega,i'}$ is the molecular weight of species i' solid phase $\left[\frac{\text{kg}}{\text{kmol}} \right]$, N_R - number of chemical species in the system, $s'_{i',r}$ is stoichiometric coefficient for reactant (adsorbed i' solid phase), k_r - rate constant, N_S - number of species adsorbed, ρ_{site} site density $\left[\frac{\text{kmol}}{\text{m}^2} \right]$.

where

k_r - rate constant is computed using the Arrhenius expression :

$$k_r = A_r T^{\beta_r} \exp\left(-\frac{E_r}{RT}\right) \quad (9)$$

where A_r is pre-exponential factor (s^{-1}), β_r is temperature exponent, E_r is activate energy $\left[\frac{\text{J}}{\text{kmol}} \right]$

and R is universal gas constant $\left[\frac{\text{J}}{\text{kmol} \cdot \text{K}} \right]$.

On the basis of course concentration CO_2/O_2 (Fig.1) is necessary to define two Arrhenius equations for two ranges of temperature intervals. We have to define constant A_r , β_r , E_r , R . Next input parameter is site density ρ_{site} $\left[\frac{kmol}{m^2} \right]$.

Site density of wall ρ_{site} defines density of active center (areas which can react with oxygen) on the wall of coal. Surface of coal available for molecules of oxygen is substantiated and real to include microspores. It is obvious, that oxygen can get to minimal pores during oxidation. From introduction interval of surface S for hard coal we defined average value $S = 150 \left[\frac{m^2}{g} \right]$. We calculated limited case of site density of wall that every adsorbed place on the surface of coal is at the same time place enable react with oxygen. Limited value of site density issue from adsorbed data for one molecule is $0.162 \left[nm^2 \right]$. Then we can write following condition.

*Surface = adsorb quantity in " monovrstvě " * surface of constant molecule * Avogadrova const.*

$$150 \left[\frac{m^2}{g} \right] = n_m \left[\frac{mol}{g} \right] \cdot 0.162 \cdot 10^{-18} \left[m^2 \right] \cdot 6.023 \cdot 10^{23} \left[\frac{1}{mol} \right] \Rightarrow n_m = 1.54 \cdot 10^{-3} \left[\frac{mol}{g} \right] = 1.54 \cdot 10^{-6} \left[\frac{kmol}{g} \right] \quad (10)$$

Then limit resulting of site density wall is defined:

$$\rho_{site} = \frac{n_m}{S} = 1.10^{-8} (kmol / m^2) \quad (11)$$

4 NUMERICAL SOLUTION OF WALL SURFACE REACTION IN POROUS ZONE

Mathematical model of wall surface reaction oxidation was defined inside porous zone on the easy model of hexahedron with size $l[m]$ **Fig. 4.1**, where the hexahedron was located in territory. Hexahedron will simulate coal dump where is adsorbed carbon inside. Air comes to zone from left side vertically to surface, bottom surface is adiabatic and other surfaces are defined by boundary conditions pressure-outlet, where we define zero gauge pressure **Fig. 4.1**. In this article I define wall surface reaction of oxidation coal with oxygen in porous zone without production of water vapour by research [4]. Then stoichiometric equation is defined as:



Porosity of porous zone of coal dump defines by value $\gamma = 0.4$. Then define reciprocal value of permeability $\frac{1}{\alpha} = 400000 \left[\frac{1}{m^2} \right]$.

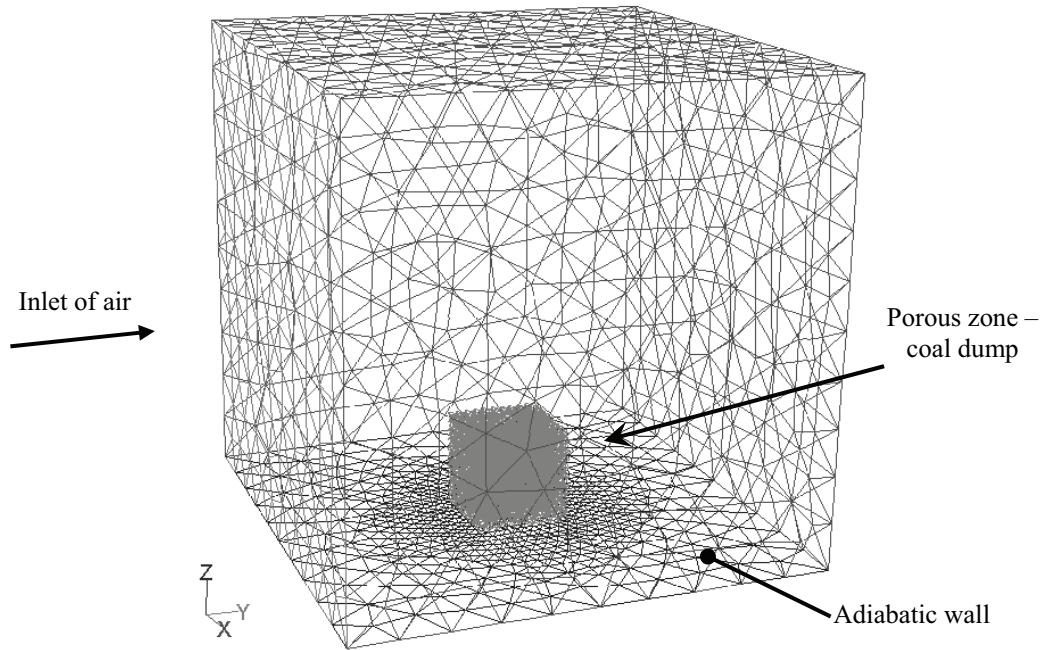


Fig. 4.1 – Geometry of computational zone

Define of boundary conditions and physical properties

Air comes to zone by constant value of $v = 1\text{m/s}$ and by mass fraction of oxygen $O_2 = 0.23$ and nitrogen $N_2 = 0.77$. Physical properties of coal and kinetic parameters [4] for definition of rate constant (Arrhenius equation (8)) are released in **Tab. .**

Tab. 3.1 – Physical and kinetic properties of the coal

	Value	Units
Coal density	1300	$\left[\frac{kg}{m^3} \right]$
Coal specific heat	1003.2	$\left[\frac{J}{kg \cdot K} \right]$
Coal thermal conductivity	0.1998	$\left[\frac{W}{m \cdot K} \right]$
Activation energy	90	$\left[\frac{J}{kmol} \right]$
Pre-exponential factor	60000	s^{-1}
Porosity	0.4	

Physical properties (density, viscosity, specific heat, thermal conductivity) mixture of gaseous species is calculated by equation of ideal gas, or by ideal gas mixing law for ideal gas [5].

5 RESULTS OF THE NUMERICAL SIMULATION OF SPONTANEOUS COMBUSTION IN POROUS ZONE

Results of numerical simulation of the low-temperature oxidation of coal in porous zone are evaluated in plane which is passed in direction of air flow, which is passed through center of porous

zone. Vectors of velocity, field of temperature and concentration of gaseous species (CO_2 , CO) by distribution of mass fractions are evaluated in this plane for various time interval.

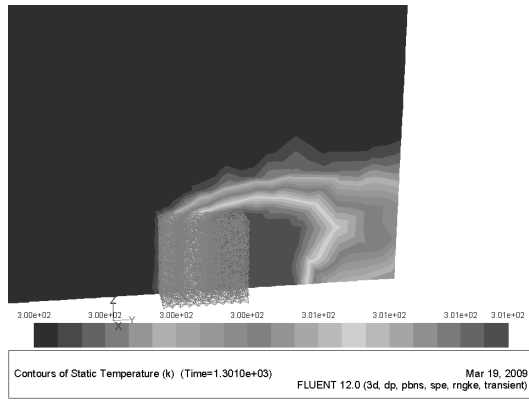


Fig.5.1 – Distribution of temperature in time $t=21\text{min } 41\text{s}$ in plane through porous zone and surround

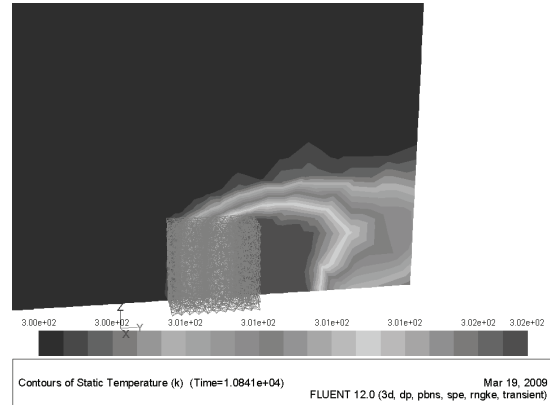


Fig. 5.2 - Distribution of temperature in time $t=3\text{h } 41\text{s}$ in plane through porous zone and surround

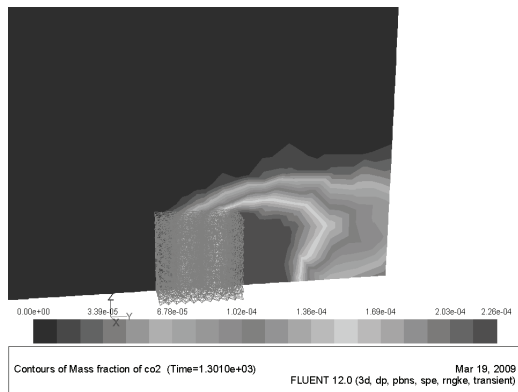


Fig. 5.3 – Distribution of mass fraction CO_2 in time $t=21\text{min } 41\text{s}$ in plane through porous zone and surround

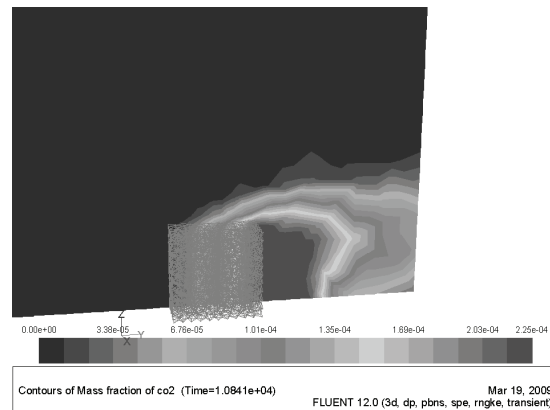


Fig. 5.4 - Distribution of mass fraction CO_2 in $t=3\text{h } 41\text{s}$ in plane through porous zone and surround

Temperatures fields are evaluated in differently time periods (in time $t_1 \sim 21\text{min}$ and then after $\Delta t \sim 2\text{h } 39\text{min}$) in plane through porous zone on the **Fig.5.1** and **Fig.5.2**. Increase to temperature in this time interval is 0.92°C . Differences between temperatures fields evidently from graphic results aren't, because the processes are high time unstable. From results of study [ff] is evidently that after 5 days the changes are significant. Increase to temperature in this interval is only $\sim 25^\circ\text{C}$ and very slowly. Then we can note that we are on the start of process spontaneous from results. Main absence of results is present-day solution capacity for numerical calculation. From production of carbon dioxide (CO_2) are similar conclusions (**Fig5.3**, **Fig.5.4**) as in temperature fields.

6 CONCLUSIONS

Article defines problem of spontaneous oxidation of coal dump in detail, where can be balanced production of water vapour or can be neglected. Appropriate stoichiometric equations of low-temperature oxidation of coal are defined for both variants. Then total mathematical model of spontaneous of dump coal is defined when wall surface reaction of coal is used in porous zone. In detail basic equations of final mathematical model are defined including detailed description of reaction mechanism for wall surface oxidation. Article solve problem of spontaneous coal dump in easy ge-

ometry (hexahedron) without production of water vapour. Parameters of physical properties and kinetic of coal combustion are defined on the basis article [4]. Results of numerical simulation are presented by distribution of temperature and concentration (CO_2) by mass fraction in porous zone and surround. With respect to work time of numerical simulation are evaluated only continuously results and numerical solution running. Next research will define new type of coal and production of water vapour.

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