DEVELOPMENT OF OXIDATION HEAT OF THE COAL LEFT IN THE MINED-OUT AREA OF A LONGWALL FACE – MODELLING USING THE FLUENT SOFTWARE

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Dedicated to Professor Jaroslav Šesták on the occasion of his 70th birthday

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Abstract

A commercial CFD software program, Fluent, was used to study oxidation processes in the longwall mined-out (gob) area. A three-dimensional model of the gob area with an advancing coal face has been developed. For the model, typical oxidation behaviour of a bituminous coal from the Ostrava-Karviná District was incorporated as resulted from laboratory investigations. The longwall gob area was designed on the basis of the actual longwall face district. Detailed measurements in the district then enabled re-verification of the model outputs with actual data in situ.

The main attention was paid to modelling the effect of grain size of the coal left in the mined-out area on the oxidation heat and gases evolution. Numerical simulations confirmed the existence of an “optimal” zone for intense development of the spontaneous heating process in the gob area.

Key words: Coal oxidation, spontaneous heating, numerical modelling.

1. Introduction

Despite a decrease in coal mining activities in the Czech Republic, the process of spontaneous combustion of coal continues to be a serious problem. One of the possibilities for better understanding of this process for in situ conditions is mathematical modelling [5, 7, 8]. A modern approach from this point of view is represented by CFD
(Computational Fluid Dynamics) programming enabling simulation of physico-chemical processes in (virtual), time-dynamic space [2, 8].

In the contribution, the commercial CFD software, Fluent, was used to study oxidation processes in the longwall gob area. A 3D model of the mined-out area with advancing longwall coal face has been developed. For the model, typical oxidation behaviour of a bituminous coal from the Ostrava-Karviná District was taken into account, as resulted from laboratory investigations. The longwall gob area was designed on the basis of the real longwall face district. The main attention was paid to modelling the effect of grain size of the coal left in the mined-out area on the oxidation heat and gases evolution.

2. Typical oxidation behaviour of bituminous coal

For simulating the oxidation process, the typical behaviour of bituminous coals to oxygen was taken into account. As “typical” there are denoted the average values of the parameters quantifying the reaction between oxygen and bituminous coals as ascertained from laboratory measurements [10, 11].

Bituminous coal samples for the laboratory examinations were taken from the Ostrava & Karviná coal mining district (OKD). According to coalification degree, the coals fall within the range from approximately 24 to 35 % of volatile matter content (VMdaf).

2.1 Temperature dependence

The effect of temperature on the rate of coal oxidation was quantified using the ARRHENIUS relationship:

\[ k = A e^{-E/(RT)} \]  

where \( k \) – rate constant of coal oxidation, (s\(^{-1}\)),
\( A \) – pre-exponential factor (s\(^{-1}\)),
\( E \) – activation energy, (J/mol)
\( R \) – gas constant, (8.314 J/[mol.K])
\( T \) – temperature, (K).

Basic experimental data were obtained from laboratory investigations by the aerial oxidation of coal in the continuous flow reactor [11]. Calculation of the rate constant \( k \) was done on the assumption that coal oxidation is a first order reaction [4, 12]. The development of the Arrhenius dependencies (\( \ln(k) \) vs. 1/T) as obtained for bituminous coals from the OKD is displayed in Fig. 1.

![Figure 1: Dependence of oxidation rate k (min\(^{-1}\)) on temperature in the Arrhenius coordinates; „typical“ bituminous coal; error bars indicate the scatter of values determined for coal samples from the OKD; \( T_{\text{tsc}} \) – threshold temperature of spontaneous combustion.](image-url)
Figure 1 gives evidence of the threshold temperature of spontaneous combustion $T_{tsc}$, when the linear course in the coordinates $\ln(k)$ vs. $1/T$ breaks and the dependence then acquires a more pronounced character [11]. From the slopes of the linear parts, it is possible to quantify the values of the activation energies of coal oxidation, $E$. 

For the purpose of simulation, the following data were chosen as typical:

- Threshold temperature of spontaneous combustion $T_{tsc} = 95°C$;
- Activation energy of coal oxidation $E$ up to the level of $T_{tsc} = 25 \text{ kJ/mol}$;
- Activation energy of coal oxidation $E$ above the level of $T_{tsc} = 50 \text{ kJ/mol}$;

The values of the rate constant $k$ used in the model then correspond to the average values from the scatter of $k$ values at individual temperatures as shown in Fig. 1.

### 2.2 Effect of time

The dependence of the oxidation rate on time was not (explicitly) taken into account for the numerical simulations. This simplification was accepted as a result of the three supporting aspects:

1) As confirmed experimental observations under isothermic conditions [12], oxidation rate of fresh coal slows down relatively soon and the process reaches a “quasi-stationary” state when the rate of the oxidation is more or less steady.

2) Coal in the mined-out area in situ is not quite fresh and, thus, the “quasi-stationary” stage of the oxidation process can be assumed.

3) The method of aerial oxidation of coal in the continuous flow reactor, using which the values of the oxidation rate $k$ were obtained, describes the coal oxidation behaviour at this “quasi-stationary” oxidation stage rather than that of fresh coal.

### 2.3 Effect of grain size

The dependence of oxidation rate $k$ on grain size (usually characterized by mean diameter of coal grain $d$) is frequently expressed in the form:

$$k \sim d^{-D},$$  \hspace{1cm} (2)

where $D$ is an exponent quantifying the dependence of the oxidation rate on grain size.

For the purpose of numerical simulations, the exponent $D = 0.45$ was accepted as a typical value for bituminous coal of grain size less than 2 mm [10]. In the case of coal fractions with a diameter greater than 2 mm, the value $D = 1$ was taken into consideration representing the direct proportion between the oxidation rate and the geometrical surface of the coal lump.

### 2.4 Evolution of gases during coal oxidation

Carbon dioxide and carbon monoxide were considered as basic (“macro”) gases released from coal during its oxidation. Figure 2 shows the temperature dependence of carbon monoxide evolution for coals from the OKR as was obtained from measurement using aerial oxidation of coal in continuous flow reactor.

For numerical simulations, equations of regression curves expressing the course of mean values of the gas/temperature dependencies (e.g. from Figure 2) were used for the evolution of CO and CO$_2$ respectively.
In addition to oxidation gases, methane emission was taken into account. Methane was supposed to be released at the bottom and on the top of the mined-out area. Maximal evolution of methane reached 7 m$^3$/min and it exponentially decreased towards the depth of the mined-out area.

2.5 Evolution of oxidation heat

The constant value of oxidation heat $H=11$ J/ml $O_2$ (= 250 kJ/mol $O_2$) was used as the mean value of the heat effect accompanying the chemical action of oxygen on coal. This value of $H$ resulted from numerous calorimetric examinations and is typical both for bituminous and subbituminous coal types [10].

3. Modelling the longwall district

3.1 Longwall face at the Lazy mine (OKD), parameters of the modelled district

Geometry of the longwall face with the caving method of mining was used in the numerical simulations. As a “pattern”, the longwall district No. 138 202 situated at the Lazy mine (OKD) was applied. In the district, long-term experimental measurements were carried out with monitoring of the composition of the air in the intake and return side of the mined-out area [2]. For the monitoring, “lost” pipes were used with apertures enabling the taking of air samples. The distance between sampling apertures in the pipes was 50 m on both sides. The natural state of the gob area was monitored for nine months, i.e. from the start-line of the longwall face up to the stage when the depth of the gob was about 350 m.

Input parameters for the numerical model correspond to these of longwall district No 138 202: length of the face =170 m, thickness of the extracted coal seam = 4 m; (virgin) temperature of the rocks =$27^\circ$C; “U” ventilation system with air flow rate at the intake =$25$ m$^3$/s; pressure drop at gob area =$7$ Pa; air leakage into the gob =$25$–$35\%$.

It was considered that a 20 cm layer of coal seam was left in the gob floor for technological reasons. In addition, a 40 cm layer of coal from the roof of the extracted seam was available in three discrete sites in the gob because of tectonics and irregular development of the seam. The sites are denoted as I, II and III, cf. Figs. 4 and 5.

The size of the modelled gob increased
depending on the daily advance of the longwall face, ranging from 0.16 to 2.6 m/day. The permeability of the gob depended on the location of the site in the area. In the longitudinal axis (perpendicular to the longwall face) permeability followed the course ascertained by Slazak [9] and ranged from $2 \times 10^{-8}$ up to $9 \times 10^{-6}$ m$^2$, see Fig. 3. Porosity of the gob changed linearly in the vertical direction with value of 25% at the floor and 5% on the top of the cave. Using the values of permeability and porosity, the mean grain diameter of the rock (coal) in the mined-out area was estimated. Near the floor, the grain diameter ranged from 2 to 14 cm depending on the gob depth (i.e. distance from the longwall face). The shape of the “grain diameter vs. gob depth” dependence in the longitudinal axis of the gob is very similar to that displayed in Fig. 3 for permeability.

![Figure 3: Permeability as a function of the gob depth.](image)

### 3.2 Basic approach to numerical modelling

A three-dimensional numerical model of the longwall district has been developed with time dependent geometry of the gob area using the commercial CFD software FLUENT, version 6.3. Mesh for the simulation are generated using the mesh generator software, GAMBIT. The cells are the shape of regular hexahedrons with a side length of 2 m. At the longwall face, these cells stretch up to a length of 3 m and then they are divided into cells with a length ratio 1:2. Thus, growth of the gob area as a result of the advancing face can be simulated. The air flow at the longwall and face supports is considered to be turbulent using an RNG k-ε model (FLUENT - User’s Guide, 2006). The air flow in the porous gob is supposed to be laminar with evaluating of the actual flow rate in the gaps among broken rock. The model uses equations of continuity, movement and energy.

Using the model, air flow, temperature and gas conditions in the gob area could be simulated from the starting line of the longwall up to the stage when the depth of the gob exceeds 350 m.

### 4. Simulation of the oxidation process in the gob area

#### 4.1 Model outputs verification

The basic simulation was set up with the above-mentioned parameters. Basic grain size of the coal left in the sites I, II and III of the gob was set to be one fifth of the mean grain diameter of the surrounding rocks. The reason for the diminishing of coal grain size in the sites I, II and III draws from experimental observations that coal passing to the gob area on the roof of the extracted seam is crushed with more marked intensity than coal left at the bottom of the seam [3].
Verification of the model was enabled by comparison of the simulation outputs with the actual conditions in the district 138202 as were ascertained during monitoring in situ. Such a comparison for contents of methane, oxygen and carbon monoxide is shown in Figure 4, experimental values of CH$_4$, O$_2$ and/or CO concentrations being written at the positions of sampling points in the gob. The Figure confirms a correspondence between experimental and numerically simulated data giving identical trends in the content changes of all the gases with respect to location of the site in the gob area. In addition, it is worth mentioning that the state of the gob presented in Fig. 4 was generated

![Figure 4: Comparison of experimental and numerically simulated concentrations of CH$_4$, O$_2$ and CO in the gob area (experimental values are represented by numbers on the intake and return sides of the gob; depth of the gob is 350 m).](image-url)
following simulations of the face advancing from the starting line up to the given development of the gob (i.e. when the distance of the longwall face from the starting line is 350 m).

4.2 Effect of grain size on the process of spontaneous heating of coal in the gob area

The situation with coal at sites I, II and III was used for a more detailed analysis of the effect of coal crushing on the character of the oxidation process in the gob area. After the numerical simulation with the basic grain size, crushing of coal at sites I – III was simulated to grain size of 20, 40 and 50 times smaller, respectively, than that of the rock in their surroundings.

Figure 5, representing the gob with a depth of 350 m, then compares the differences between distribution of the temperatures for the basic grain size (Fig. 5a) and that of 40 times smaller (Fig. 5b). In both cases, there is an obvious increase in temperatures at sites I–III. However, for the basic grain size, the temperature increase is by around 10°C while for 40-times finer coal the rise is by 30–50°C.

From Fig. 5, one can further read that for basic grain size (Fig. 5a) the maximal temperature is reached in the farthest site I. On the other hand, for a 40-times finer coal, site III is the hottest, which lies closest to the coal face (Fig. 5b).

![Figure 5: Temperature profiles in the gob area as a function of the grain size of the coal at the sites I, II and III; a- basic grain size; b – the grain size 40 x finer; depth of the gob is 350 m.](image)
We tried to investigate this interesting finding in more detail. For different degrees of coal crushing (5–50 times), the highest temperature of site I was examined as a function of the distance from the longwall face. Thus, in principle, the temperature of site I was “scanned” with the advancing face – up to its position at the depth of approximately 300 m in the gob. Results are summarized in Figure 6. From the Figure, courses of the temperature with local maxima are evident. Simultaneously, it is obvious that the position of the maximal temperature “moves” towards the coal face when the coal grain size decreases. Thus, for the basic grain size, the maximal temperature is reached at a depth of the gob of around 200 m, while for a 40-times smaller grain size, it is approximately at 110 metres. When coal is crushed to a fraction 50 times smaller (than the grain size of surrounding rock), the temperature rise is so marked that site I passes into open flame at a depth of the gob of 70 m, see Fig. 6.

The finding of the maximal temperatures confirms the existence of “optimal” conditions for the development of the oxidation process [1] Thus, at the “optimal” depth of the gob, air flow is sufficient to supply the oxidizing coal with oxygen, and, simultaneously, minimal cooling effect of the flowing air occurs. After the heated site passes through this “optimal” position to a greater depth of the gob, the coal deposit begins to dampen, because of insufficient supply of O₂.

5. Conclusion

Numerical simulations confirmed the existence of an “optimal” zone for intense development of the spontaneous heating

![Figure 6: Dependence of the temperature of the site I on its position in the gob - as a function of coal fragmentation.](image)
process in the gob area. Based on the simulations, it is possible to specify that the position of the “optimal” zone is not constant as it shifts towards the longwall face if the coal grain size in the gob decreases. For coal crushed to a grain size of approximately 0.5–1 mm it can be expected (under conditions comparable to the model gob area) that the greatest risk of a spontaneous combustion incident is at a depth of the gob of around 70 ± 20 metres.

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References