Underground Coal Fire Extinction Model using Coupled Reactive Heat and Mass Transfer Model in Porous Media

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Abstract: Green house gases emission associated with natural hazard of underground coal seam fire has been recognized as a worldwide problem leading to global warming threat. Therefore, in this paper a model to study underground coal fire is presented and the results will be devoted to strategic development of coal fire extinction technology within the framework of Sino-German Coal Fire Research Initiative. The developed model consists of five multiphysics models, namely Darcy law, diffusion, conductive heat transfer, coupled convection and conduction, and coupled convection and diffusion models. In addition, some experimental works have been carried out for validation purpose.

Keywords: Reactive heat – mass transfer, underground coal fire, porous media.

1. Introduction

Underground coal fires start to propagate when coal deposit as a combustible material with an adequate supply of oxygen is subjected to enough heat and is able to sustain a chain reaction. Once the coal is ignited, a chain of exothermic reaction takes place. Furthermore, the fire may propagate provided that there is a continuous supply of oxygen in the coal seam. Those fires are typically uncontrolled hot fires and generate potential smoke and fumes and eventually damage the surrounding soil.

This natural hazard of underground coal seam fire has been recognized as a worldwide problem. Thus, research area on underground coal fire is of growing interest due to the need to exterminate greenhouse gases emission associated with the coal fire and accordingly protect the world from global warming threat [1].

In particular, the fire extinction researches on underground coal fire are tremendously useful for identifying underground coal fire problems in our investigating area in North China. In this area the fire has been spreading over 62 coal mines in the area of 720 km². This, in turn, has dramatically burned 20 millions tones of coals and destroyed more than 100 millions tones annually and caused the economic loss of $125-250 millions [2].

In this work, we investigate hydrodynamic and heat-mass transfer phenomena of underground coal fire. The investigating underground coal fire to be modeled is depicted in Figure 1.

The geological setting was created referring to the situation in Wuda coal fire zone in China according to Gielisch and Kus [3]. The coal seam is located approximately at a depth of 20 m underground. It lies 200 m distance from one edge to another.

The model will be validated with experiments and the results will be devoted to strategic development of underground coal fire extinction technology within the framework of Sino-German coal fire research initiative phase B.

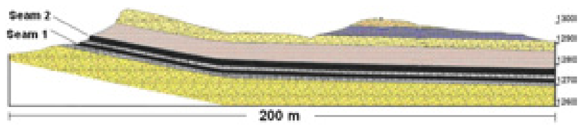


Figure 1. Geological structure of the investigated coal seam. Numeration on the hand side denotes altitude [m].

2. Governing Equations

2.1. Reaction kinetics

It is generally acknowledged from previous considerable literatures (for instance Wang, Dlugogorski and Kenedy [5] and Krause Schmidt and Lohrer [4]) that the chemical reaction taking place in underground coal fire is a complicated phenomenon. In general, the reaction mechanism involves the transport of reactive gases in coal pores, gas adsorption as well as the generation of gaseous and solid products.

Wang, Dlugogorski and Kennedy [5] have overviewed investigations on various chemical reactions occurring during low temperature oxidation of coal and proposed reaction mechanism of coal oxidation to indicate the characteristics of oxygen consumption, solid-oxygenated formation, thermal decomposition and generation of gaseous products.

However, whereas low oxidation of coal has emphasized the kinetic models applicable for predicting self ignition of coal stock pile in low temperature regime, Krause, Schmidt and Lohrer [4],[6] presented reaction kinetic as well as refined numerical models in relatively higher temperature regime. The model is aimed at simulating describe smoldering coal fire and its application in underground coal fire.

In addition, the model consists of a set of partial differential equations for heat and mass transfer phenomena and then described the field scale application of self ignition and fire propagation of coal seam fire in China. The model considered moisture effect through adsorption, evaporation and condensation processes on self ignition leading to coal seam fire propagation.

Following the model of Krause et.al, each component is converted at its specific reaction rate during respective reaction steps. Coal is decomposed according to equation (1) and exhibit an Arrhenius reaction rate as follows:

$$\frac{\mathrm{d}C_\mathrm{f}}{\mathrm{d}t} = -C_\mathrm{f} k_0 \exp\left(-\frac{E}{RT}\right) \tag{1}$$

where k_0 is the pre-exponential factor (s^{-1}), E is the apparent activation energy ($J.mol^{-1}$), and R is the ideal gas constant ($J\ mol^{-1}\ K^{-1}$) and T temperature (K). The reaction rate is a first order reaction. The index *f* refers to fuel, which in this case is coal.

For the rate of the generated products, following equation is applied:

$$\frac{\mathrm{d}C_i}{\mathrm{d}t} = \frac{v_i}{v_c}\frac{M_i}{M_\mathrm{C}}\frac{\mathrm{d}C_\mathrm{C}}{\mathrm{d}t} \tag{2}$$

where the index i stands for the components, v_i the stoichiometric coefficients and M_i the molecular weight.

Since underground coal fire progressed in a high temperature regime, therefore the reaction mechanism is referred to the burn off reaction sequence which is suggested to be similar to the combustion of solid fuel. Hence, this present work considered only the oxidation of carbonaceous solid material which constitutes into following reaction mechanism:

$$C + O_2 \rightarrow CO2 + \text{Ash/solid products} \tag{3}$$

Thus, the chemical reaction above was formulated from four chemical components, namely two solids (coal and solid products) and two gases (oxygen and gaseous combustion products).

In order to derive stoichiometric data the elemental composition analysis of the coal, the solid products as well as the analysis of the gaseous products compositions have been performed. The results of stoichiometric data along with the reaction kinetics data have been previously presented by Krause, Schmidt and Lohrer [4] and used in this present model.

2.2. Fluid dynamics

Taken into consideration underground coal seam as a porous medium, Darcy law is expected to be valid to model the existence of hydrodynamic phenomena in underground coal fire. The law states that the velocity vector is determined by the pressure gradient, the fluid viscosity and the structure of the porous media:

$$\mathrm{u} = -\frac{\kappa}{\eta}\nabla \mathrm{p} \tag{4}$$

If it is assumed that no external force affected to the flow (e.g. Boussinesq approximation from Buoyancy force is not considered), the continuity equation can be applied as follow:

$$\frac{\partial(\rho\varepsilon)}{\partial \mathrm{t}} + \nabla\cdot\rho\mathrm{u} = 0 \tag{5}$$

Including u from equation (4) into equation (5):

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \nabla\cdot\left(\rho\left(\frac{-\kappa}{\eta\nabla p}\right)\right) = 0 \tag{6}$$

where κ denotes the permeability of the coal (m^2), η the viscosity of gas phase ($kg.\ m^{-1}.s^{-1}$), p the pressure (Pa.s), ε the volume fraction of the coal, ρ the density ($kg.m^{-3}$) and u the velocity vector ($m.s^{-1}$).

Pressure dependence of gas density for an ideal gas is described by the ideal gas law:

$$\rho = \frac{\mathrm{pM}}{\mathrm{RT}} \tag{7}$$

Darcy’s law in combination with the continuity equation and the ideal gas law gives the following equation:

$$\nabla\cdot\left(-\frac{\kappa M}{\eta RT}p\nabla p\right) = 0 \tag{8}$$

where M denotes the molar mass ($kg.mol^{-1}$).

For a given pressure of p_0, a boundary condition is defined as:

$$\mathrm{p} = \mathrm{p}_0 \tag{9}$$

And for symmetric boundary condition:

$$-\frac{\kappa}{\eta}\nabla \mathrm{p} = 0 \tag{10}$$

whereas, for a specific inflow or outflow perpendicular to the boundary, the boundary conditions is:

$$\frac{\kappa}{\eta}\nabla \mathrm{p} = u_0 \tag{11}$$

The default boundary condition on an interior boundary is continuity:

$$(\rho_1 u_1 - \rho_2 u_2) = 0 \tag{12}$$

The model in this work considered a constant dynamic viscosity and not considered temperature dependence. To allow pressure difference and hence Darcy model is applicable, the right hand edge has been set to have lower pressure than another edge. The model does not consider the Buoyancy force model in the calculation. Dynamic viscosity in this model is constant and not considered temperature dependence.

2.3. Heat transfer

The transfer of heat consisting solid and moving fluid in underground coal fire is influenced by physical, chemical and hydromechanics mechanism. Thus, heat can be transferred by both conduction and convection.

The heat transfer through conduction in coal seam can be represented by combining Fourier's law and energy conservation law:

$$\rho C_p \frac{\partial T}{\partial t} - \nabla \cdot (\lambda \nabla T) = Q \tag{13}$$

Gas flow on the other hand, can transfer the heat through convection. Therefore, a convective flux term must be coupled with momentum balance by introducing convective heat transfer term:

$$q = \rho C_p T u \tag{14}$$

Rearranging equation (13) and (14), coupled convective and conductive can be formulated as follow:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-\lambda \nabla T) = Q - \rho C_p u \cdot \nabla T \tag{15}$$

where Q denotes the heat source ($W.m^{-3}$), λ thermal conductivity ($W.m^{-1}.K^{-1}$) and C_p heat capacity ($J.kg^{-1}.K^{-1}$).

The model is default in COMSOL and assumes incompressible fluid ($\nabla \cdot u=0$).

For underground coal fire, coal combustion process is taken into consideration as a source of heat generation in the coal seam and computed as follows:

$$S_T = \frac{1}{\rho c}\sum_{i=1}^{4} \Delta H_{R,i} \frac{dC_i}{dt} \tag{16}$$

where S_T denotes heat generation rate ($J.m^{-3}.s^{-1}$), H_R heat of reaction ($J.kg^{-1}$), C mass concentration ($kg.m^{-3}$) and the subscript i the component, respectively.

At the surface, the heat flux may be calculated as follows:

$$q = \alpha (T_s - T_a) \tag{17}$$

where q denotes the heat flux ($w.m^{-2}$), α convective heat transfer coefficient ($W.m^{-3}.K^{-1}$), the subscripts s and a denote the ambient and surface conditions, respectively.

In this present model, the right hand edge was modeled as an adiabatic wall while the left hand edge was assumed having an initial temperature of 293 K, while another edge was assumed as free convection at the boundary condition.

2.4. Mass transfer

The mass balance for underground coal seam is described by:

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i + c_i u) = r_i \tag{18}$$

where r denotes reaction term ($mol.m^{-3}.s^{-1}$), D_i the diffusion coefficient of component i ($m^2.s^{-1}$). The expression within the brackets represents flux vector, where the first term describes the transport by diffusion and the second represents the convective mass flux.

The mass flux of an individual component i into the coal seam can be computed using an analogous following equation:

$$j_i = \beta (C_i - C_{ia}) \tag{19}$$

where j_i denotes mass flux of component i ($kg.m^{-2}.s^{-1}$), β_i the mass transfer coefficient of component i ($m.s^{-1}$), C_i the concentration of component i at the surface (mol), C_{ia} the concentration of species i at the ambient atmosphere (mol).

3. Simulation results

Figure 2 presents simulation result showing temperature evolution in coal seam fire. It shows that fire propagation progressed starting from the initial coal seam and propagated into another end. After two and half years the coal seam has burned out generating high temperature and the combustion centers have spread along the seam in horizontal direction. Accelerating fire shows high temperature (>800°C).

Table 1 Input parameters and variables

Physical quantity	Value
Density of air, kg/m^3	1.205
Density of rock, kg/m³	2700
Acceleration due to gravity, m/s²	9.81
Initial temperature, K	293
Molecular weight of air, kg/kmol	29
Universal gas constant (R), J/(kmol·K)	8314
Initial pressure, Pa	1.01 x 10^5
Convective heat transfer coefficient, W/(m³·K)	8
Pre-exponential factor, s^{-1}	1.5 x 10^{-5}
E_A/R , K	10000
Diffusion coefficient of oxygen, m²/s	2.10^{-5}
Reaction enthalpy, J/mol	2.2 x 10^7
Initial concentration of solid fuel, kg/m³	560
Initial concentration of, O_2 mol/m³	0.252
Heat capacity of coal, J/(kg·K)	1000
Thermal conductivity of rock, W/(m·K)	4
Thermal conductivity of coal, W/(m·K)	0.1
Thermal conductivity air, W/(m·K)	0.025
Permeability, m²	1 x 10^{-12}

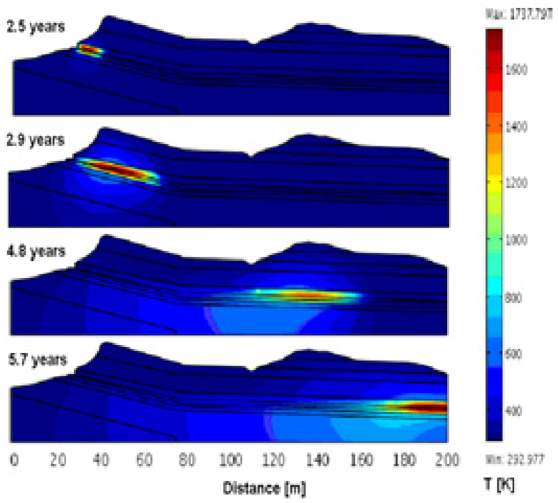


Figure 2. Temperature evolution during fire propagation in underground coal seam

Figure 3 presents simulation result of vertical profile of temperature from overburden zone (upper layer of adjacent rock above coal seam) until underlying zone (lower layer of adjacent rock below coal seam) showing temperature evolution in vertical direction. It shows a distinct temperature profile of coal seam and its adjacent rocks which indicate existing fire propagation. Temperature of the adjacent rocks increased gradually since the underground fires heat up the rocks above. This phenomenon is recognized as a nature of surface anomaly characteristics which have been detected previously by in situ investigations.

For example, the investigation conducted by BGR (Federal Institute for Geosciences and Natural Resources) [7] and DLR (German Aerospace Center) [8] showed that a thermal anomaly indicates important signs of progressing underground coal fire. For further scientific observation, present results will be further used as the basic model for the mapping of demarcated underground coal fire areas and its relation on exhaust gases released.

Furthermore, the results of this model shall present the significant parameters affecting fire propagation velocity. Two relevant parameters for this study are convective effect of gas transfer and permeability of reacting gases components.

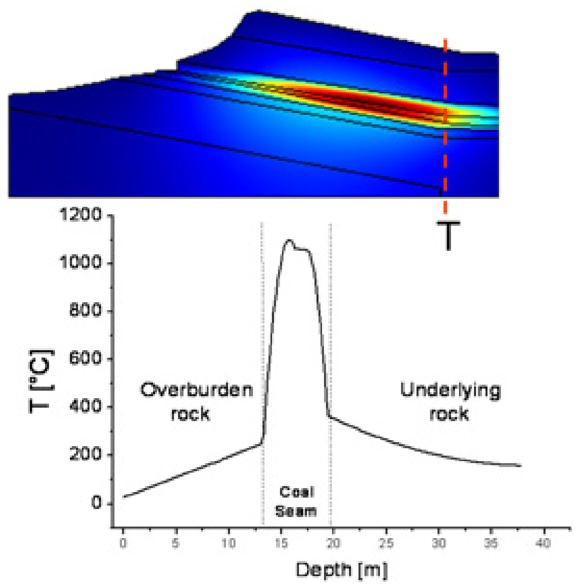


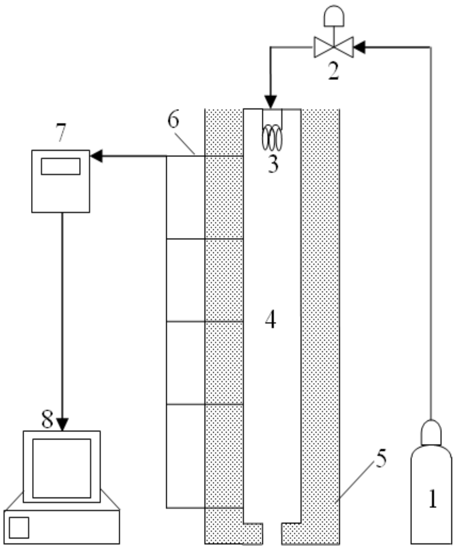
Figure 3. Cross sectional temperature profile of the above selected coal seam.

4. Experiment

4.1. Set up

Two types of experimental set-up have been designed to validate the simulation, namely vertical reaction furnace and quasi adiabatic furnace.

The former one, depicted in Figure 4, consists of a vertical tube filled with coal, thermocouples, an ignition source, and a data logger. The tube is 1.2 m in length and 0.07 m in diameter. Five thermocouples are placed at the edge of the tube to measure the existing combustion temperature. A transformer of 7V/7A was used to heat up a wire and thus acted as an ignition source. The tube is isolated by vermiculite to minimize the heat loss into surrounding.



1-Compressed air; 2-Air flow controller; 3-Ignition source; 4-Reaction tube; 5-Insulator filled with vermiculite; 6-Thermocouple, numbered from top to down; 7-Data logger; 8-Computer.

Figure 4. Vertical reaction tube

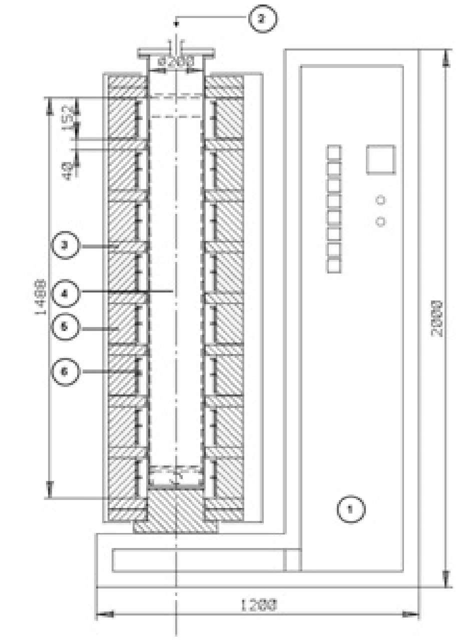
The propagation velocity of each experiment was determined as follows:

$$\dot{v} = \frac{L}{t} \qquad (20)$$

where $\dot{v}$, L and t represent respectively the propagation velocity ($m.s^{-1}$), the distance between the first and the last temperature measurements (m) and the required time to achieve maximum temperatures on both measuring points (s).

The later one, depicted in Figure 5, is cylindrical and vertically oriented furnace, 0.2 m in diameter and 1.5 m in length. This furnace has eight heating zones and is insulated with highly compressed magnesium oxide to avoid thermal dissipation from the reaction tube to the surrounding. The inner temperature was measured using thermocouple located in the middle of the tube.

The system was developed in a compact way to enable controlling an adiabatic condition, e.g. the outer side temperature of reaction furnace equals to its inner side temperature. In contrast, particular temperature difference between the inner side and the outer side of the furnace can be set-up to withdraw some extent of heat.



1-Oven casing, consists of temperature controller, flow meter controller, display and data logger; 2-location for air input; 3-thermocouple; 4-reaction tube; 5-insulator; 6-heating coils.

Figure 5. Quasi adiabatic furnace

4.2. Results

Figure 6 shows temperature profile of fire propagation experiment for three different volumetric air flows of 300, 450 and 600 l/h respectively. At those volumetric air flows, the reaction front reached the last measuring points 2800 min, 1800 min and 100 min after ignition, respectively. As stated in experimental section in this paper, coal fire propagation occurred as forward reaction.

Figure 6 shows that the evolution of combustion temperatures moved upward to downward, or in other words, it moved in the same direction as air flow.

In accordance to Figure 6, Table 1 was created presenting the results of propagation velocities from different volumetric air flows as well as their associated maximum temperature. The times presented in Table 1 are equal to fire propagation velocities of 175.2, 280.3 and 467.2 m/year, respectively. Note that the calculation of fire propagation velocity considered the velocity amongst the temperature peaks. It shows from Table 1 that the faster air flows, the faster fire propagation occurred. Table 1 also shows the fact that the maximum temperature achievement was also higher as the volumetric air flow increased.

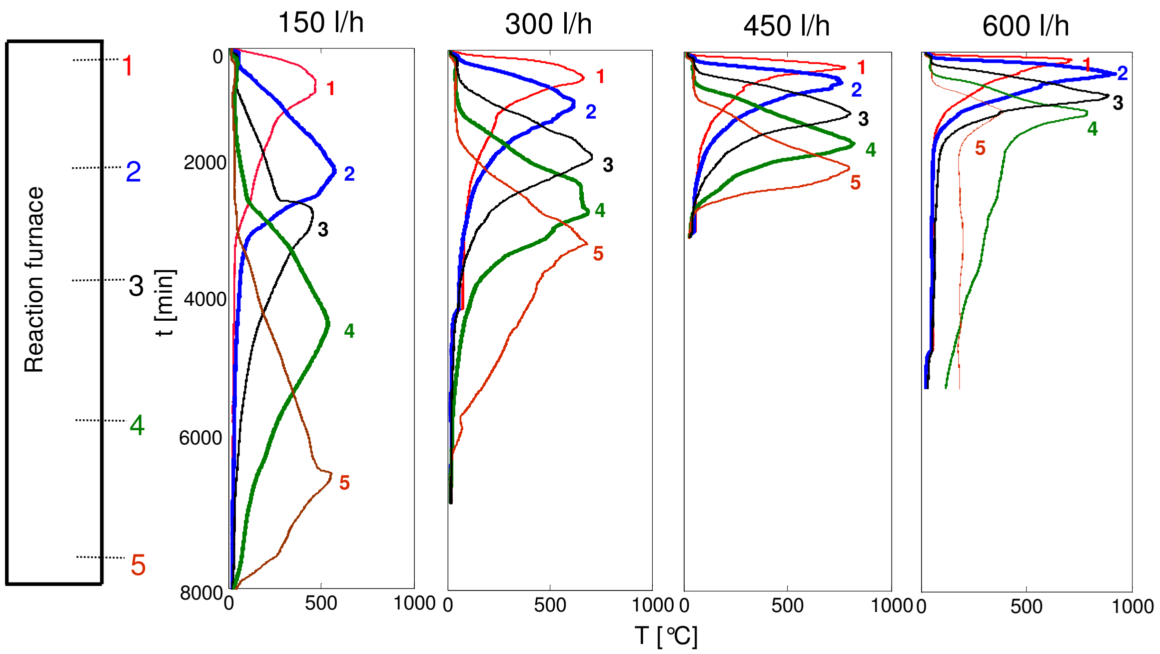


Figure 6. Effect of volumetric air flow on fire propagation velocity. Temperature profiles for each consecutive zone are distinguished by dotted and solid lines respectively. The numbering system (1 – 5) refers to the zones in the reaction furnace.

Table 1. Fire propagation velocity and associated maximum temperature for different volumetric air flows

$\dot{Q}$ [liter/hour]	υ [m/a]	T_{max} [°C]
600	467.2	919
450	280.3	815
300	175.2	705
150	32	575
75	No fire propagation	196

The results from this experiment revealed that the fire propagation at definite air flow leads to a characteristic temperature and propagation velocity of the reaction front. As shown in Table 1 of the reaction front and the maximum combustion temperature increase as the air flow rate increased. It is obvious that higher air velocity constitutes to a more oxygen transport to the coal deposit and thus provides better combustion process.

Figure 7 presents a typical result of temperature evolution of quasi adiabatic furnace. This particular result was achieved from the experiment where the first zone of the furnace was set at 800°C and volumetric air velocity was set at 300 l/h. The temperature profile showed in this typical figure consisted of both wall and inner temperatures for all zones (denoted from the numeration of 1,2,…,8).

As shown in Figure 7, after the furnace turned on, wall temperature of the first zone raised rapidly until reached a set point temperature of 800 °C and heated up its inner temperature and eventually reached a constant temperature of 800°C. The next zones (zone 2 – 8) showed a fact regarding adiabatic behavior of the furnace, which was indicated by the relatively equal temperature profiles of the wall and inner temperatures.

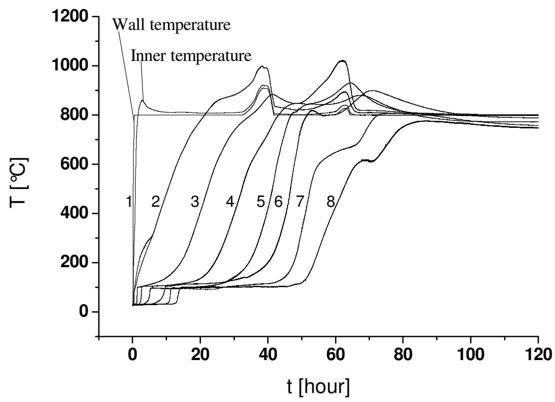


Figure 7. Typical temperature evolution of quasi adiabatic furnace experiment.

Based on these presented results, our further investigation will simulate a strategy for heat extraction since the "generic recipe" of fire extinction told that the phenomena of coal fire propagation can be precluded through particular continuous heat withdrawal. The experimental work for validation is achievable through applying particular temperature difference between inner and outside temperature in our adiabatic furnace experiment.

6. Conclusions

In this paper, we explore the utilization of coupled models available in COMSOL for simulating underground coal fire. The simulation results provided a clear illustration regarding the effects of heat and mass transfer on coal fire propagation process. Heat and mass transfer during underground coal fire is of eminent scientific interest for the fundamental investigation of coal fire dynamic and subsequent extinction scenario.

In addition, simulation results rendered possibilities for extinction strategies of underground coal fire which can be validated by laboratory experiment as well as in situ observation.

We observed that since computation results largely depend on the accuracy and validity of utilized input parameters, hence the availability of reliable experiment is important aspect for further research in this area.

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References

[1] ERSEC: Ecological Book Series – 4, Spontaneous Coal Seam Fires: Mitigating a Global Disaster. Springer – Tsinghua University Press, 2008.

[2] Kuenzer C, Zhang J, Tetzlaff A, et al., Uncontrolled coal fires and their environmental impacts: Investigating two arid mining regions in north-central China. *Applied Geography*, 27,42–62, 2007.

[3] Gielisch H and Kus J., 2005. An anomalous coalification distribution in the Northern Helan Shan – A possible key into the geological history of the Helan Shan area. *Proceeding of International Conference on Coal Fire Research – ERSEC Conference on Understanding, Extinction and Prevention of Spontaneous Coal Seam Fires*. Beijing, China, 2005.

[4] Krause U, Schmidt M, Lohrer C., A numerical model to simulate smoldering fires in bulk materials and dust deposits. *Journal of Loss Prevention in the Process Industries*,19,218 – 226, 2006.

[5] Wang H., Dlugogorski B.Z., Kenned E.M., 2003. Coal oxidation at low temperatures: oxygen consumption, oxidation products, reaction mechanism and kinetic modeling. *Progress in Energy Combustion and Science*, 29, 487-513.

[6] Krause U, Schmidt M, Lohrer C. Refined Numerical Model to simulate Coal Fire Generation and Propagation, *in*: *Ecological Book Series – 4, Spontaneous Coal Seam Fires: Mitigating a Global Disaster.* Springer – Tsinghua University Press, 2008.

[7] Schloemer, Stefan, Manfred Teschner, Jürgen Poggenburg and Christian Seeger, 2007. *Gas and Temperature Monitoring of a Spontaneous Coal Fire in Wuda Coal Mining Area.* Report of coal fire project phase A part B: Innovative Technologies for Exploration, Extinction and Monitoring of Coal Fires in North China.

[8] Voigt S., Tetzlaff A., Zhang J., Künzer C., Zhukov B., Strunz G., Oertel D., Roth A., Dijk P., Mehl H., 2007. *Integrating satellite remote sensing techniques for detection and analysis of uncontrolled coal seam fires in North China.* Report of coal fire project phase A part B: Innovative Technologies for Exploration, Extinction and Monitoring of Coal Fires in North China.