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Research article

# Analytical prediction of coal spontaneous combustion tendency: Velocity range with high possibility of self-ignition

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ABSTRACT

Coal spontaneous combustion is an inherent problem in coal mines throughout the world. The analysis of stationary-states, including stable point and critical point, is an effective method to judge its ignition tendency. A lower critical point temperature means that it is more likely to cause fire. In the past, due to the limitation of mathematical methods, the consumption and distribution of oxygen concentration are usually neglected. In order to accurately analyze coal ignition tendency, this paper takes coal bulk as a porous system and develops an improved model by a combination of oxygen species and energy equation. The model is solved for stationary-states of the system. Qualitative analysis of the stationary-states gives a mechanism explanation for the reason why coal spontaneous ignition is hard to be extinguished and indicates that the temperature of initial endpoint and that of internal site can be uniquely determined from each other. It further points out a trend that the location of critical point moves inward as the inlet air velocity increases, which correlates well with simulation results of the existing literatures. Then, for stationary-states, calculation results of Killoch 6015 coal are obtained. Quantitative analysis of them finds a trend that the temperature of critical point rises rapidly after its slow increase. At last, a velocity range, in which the possibility of fire is extremely high, is presented by simulation computation, e.g., the range of Killoch 6015 coal is determined as $8 \times 10^{-5}$–$3 \times 10^{-3}$ m/s when the critical ignition temperature is set as 150 °C.

## 1. Introduction

Spontaneous combustion occurs worldwide in all manner of substances (e.g., coal, wool, grain, hay) when they are stockpiled or stored for long periods, or transported in bulk. Among them, self-heating of stored coal leads to the loss of precious coal resources and the emission of greenhouse gas, which is a serious problem for both coal producers and users. Approximately 20% in USA [1] and 90% in China [2] of coal mine fires were caused by spontaneous combustion and the number expected to increase because of greater consumption, deeper coal mining and utilization of lower rank coals.

A powerful way to explore the process of coal spontaneous combustion is mathematical modeling. Spontaneous combustion of coal bulk is mainly studied with respect to recognizing basic variables affecting the process of self-heating [3–6]. For example, air entering a stockpile was found to play a complex role [7–11]. In recent decades, some research groups [12–15] have developed models for simulating coal spontaneous combustion, which are based on active site theory, two parallel sequences consuming oxygen and two thermal decomposition pathways producing carbon oxides. Though numerical simulations [16–20] have successfully revealed some natures of coal spontaneous combustion, they spend lots of computer resources and time. Instead, analytical solutions give an insight into the character of the solutions, and will allow answers to be obtained quickly and easily. But it is difficult to obtain due to limitations of mathematical methods except simple cases [21]. In practical engineering, forecast of coal spontaneous combustion is used by the statistical method [22], the analogy method [23] and the test method [24,25]. But these methods have inherent defects because they are based on the existing data with experience errors.

Coal oxidation takes place while coal contacts with oxygen. Physical adsorption and chemical adsorption during coal oxidation are the cause of heat evolution, and the adsorption reaction forms solid oxygenated complexes. The temperature of coal increases as the reaction proceeds, which accelerates coal oxidation reaction. When the temperature reaches the threshold for thermal decomposition, the coal oxidation and the thermal decomposition of oxidized coal contribute to the emission of carbon oxides and the release of heat, which are called two parallel reaction sequences [26]. The thermal decomposition of solid oxygenated complexes regenerates active sites for oxygen adsorption, and thus promoting the coal oxidation reaction [27]. Then, the temperature increases rapidly and coal

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**Nomenclature**

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|---|---|
| $A$ | pre-exponential factor in the Arrhenius expression |
| $A_{\mathrm{coal}}$ | pre-exponential factor for coal |
| $A_{\mathrm{ad}}$ | ash of coal |
| $\tilde{a}$ | intrinsic average (or local) concentration of oxygen |
| $a$ | phase average (or global) concentration of oxygen ($a = \varepsilon\tilde{a}$) |
| $a_0$ | ambient oxygen concentration |
| $C$ | integration constant |
| $c_{\mathrm{P}}$ | heat capacity at constant pressure |
| $D_{\mathrm{m}}$ | diffusion coefficient of oxygen in porous medium |
| $E$ | activation energy |
| $F(x)$ | medium function ($F(x) = \int[-\exp(-x)\sum_{k=1}^{n}(k-1)!\delta^k x^{k-1}]dx$) |
| $F_{\mathrm{k}}(x)$ | the $k$th term of function $F(x)$ |
| $G(x)$ | medium function |
| $k$ | reaction rate constant when the temperature is $T$ |
| $k_0$ | reaction rate constant when the temperature is $T_0$ |
| $L(\theta)$ | heat loss rate |
| $MW_{\mathrm{coal}}$ | molar weight of coal |
| $MW_{\mathrm{O2}}$ | molar weight of oxygen |
| $N$ | medium parameter ($N = \frac{E}{RT_0{}^2}\frac{Qa_0}{(\rho c_{\mathrm{p}})_{\mathrm{f}}}$) |
| $Q$ | exothermicity of oxygen |
| $Q_{\mathrm{coal}}$ | exothermicity of coal |
| $R$ | gas constant |
| $R(\theta)$ | heat release rate |
| $T$ | phase average temperature |
| $T_0$ | ambient temperature |
| $t_{\mathrm{c}}$ | characteristic time ($t_{\mathrm{c}} = 1/k_0$) |
| $\tilde{u}$ | intrinsic average (or local) velocity |
| $u$ | phase average (or global) velocity ($u = \varepsilon\tilde{u}$) |
| $V_{\mathrm{daf}}$ | volatile matter of coal |
| $z$ | distance from inlet of the coal bulk |
| $\tau$ | time |
| $\lambda$ | conductivity coefficient |
| $\varepsilon$ | porosity of the coal bulk |
| $\rho$ | density |
| $\theta$ | dimensionless excess temperature ($\theta = \frac{T-T_0}{RT_0{}^2/E}$) |
| $\gamma$ | fractional conversion of reactant |
| $\delta$ | medium parameter ($\delta = RT_0/E$) |

*Subscripts*

| | |
|---|---|
| eff | effective parameter ($(\cdot)_{\mathrm{eff}} = \varepsilon(\cdot)_{\mathrm{f}} + (1-\varepsilon)(\cdot)_{\mathrm{s}}$) |
| f | fluid (air) |
| s | solid (coal) |
| 0 | the ambient or inlet |

spontaneous combustion would occur before long. In these processes, governing equations of heat transfer are enough to develop the mathematical modeling. Owing to the presence and form of the nonlinear term, i.e. the source item of the energy equation, an analytical solution of the energy equation in closed form is not possible. To simplify mathematical model, Semenov [28,29] developed the thermal explosion which further development by Frank-Kamenetskii [30]. Gray and Harper [31] had set out two approximations employed (exponential and quadratic) to simplify the source term, and then Gray et al. [32] gave an infinitesimal approximation which could replace exponential approximation. Based on above theory, some researchers [23,32–36] theoretically analyzed the self-heating system under different simplifications or conditions. But none of them consider the oxygen consumption in coal bulk, which plays an important role especially under the high temperature. Though Griffiths and Scott [21] introduced oxygen concentration into the energy equation in CSTR (continuous-flow, stirred-tank reactor), their model was not suitable for coal spontaneous combustion.

As part of a comprehensive study of coal self-heating, a simple mathematical model to give insight into the nature of self-heating phenomenon needs to be developed. The model should include all the important physical processes occurring in coal self-heating system, while remaining simple enough to be solved without excessive computation. In order that the model be simple enough to solve with analytical solutions, the coal bulk may be considered to be a perfectly insulated tube with no radial gradients [37], thus allowing the equations to be formulated for one space dimension. The similar one-dimensional approximate model has been used before [38,39]. In order to more accurately analyze coal spontaneous combustion potential, a mathematical model of coal bulk is presented by combining oxygen species equation and energy equation. Based on the stabilities theory of exothermic reactions, stationary states of the system are derived by integrating and deducing. Then multiplicities of stationary states are analyzed by qualitative and quantitative analysis, respectively.

## 2. The stability of exothermic reaction for coal self-heating

Though the principal features of stability for simple reactions have extensive studies [35,40] on Chemical Engineering, there is no enough attention to the domain of porous medium, such as coal oxidation at low temperatures.

In our study, it is assumed that the coal self-heating system resembles a porous medium, with the pores being the voids between the coal lumps. The influent airflow is forced into the system from one end, and flows through the inside of it. Air stream provides oxygen for the reaction inside the coal self-heating system, while it would take away the heat generated by reaction when the influent air is colder than that of the interior of the system.

### 2.1. Assumptions

Some assumptions utilized in the following derivation are introduced here for simplicity:

a) The rate of reaction obeying an Arrhenius temperature dependence [34].
b) There is no volume change due to reactions or heating [16] and the porosity is constant [41].
c) Air is forced into coal bulk from one end, and flows through it with a constant rate [7,8,42]. The diffusions of heat and mass inside the system are ignored.
d) Partial thermal equilibrium assumption was used. That is to say that there is no temperature difference between solid and gas.

### 2.2. Two kinds of stationary-states on stability

In this section, it is intended to explore a general analytical method for locating the critical conditions. Under "stationary-states" conditions, heat generation balances heat loss by the mechanisms of conductive, convective, and radiative heat transfer. Self-heating occurs when this balance is lost, that is, when heat generation outstrips heat loss [43]. It means that the spontaneous combustion tendency could be studied by analyzing the stationary state.

In early stages, thermal explosion theory [28,29] is a well-known theory of spontaneous combustion, which commonly used for premixed gas. Then Gugan [44] and Bowes [45] intended to express applications of thermal explosion model on coal self-heating. They indicated that the "thermal explosion" phenomenon in porous self-heating solids was represented for the condition of convective rather than conductive heat losses. However, it is important to note that the thermal explosion theory shown in Fig. 1 could not be applied to coal bulk because it assumes a spatially uniform internal temperature with a step at the boundary which coal self-heating system would never have. In this paper, the model considers the distributions of oxygen concentration