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## Mathematical model of coal self-heating in a stack

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### ABSTRACT

The article presents a mathematical model of coal self-heating in the stack in which the heat exchange and gas exchange processes are described by a system of two non-linear differential equations of the second order with respect to the temperature  $t$  of coal self-heating and the volume fraction  $C$  of oxygen in the voids of the stack with boundary and initial conditions. The differential equations took into account that self-heating of coal in the stack and appearance of spontaneous combustion are observed in a relatively small layer adjacent to the surface of its contact with the air and called the zone of oxygen influence. In the mathematical model, the influence on the process of coal self-heating of parameter  $F$ - specific heat release power was taken into account, which in addition characterises the stability of coal during storage. When compiling the differential equations, such physical parameters as thermal conductivity, diffusion coefficient, specific heat capacity of coal in the stack, bulk density, thermal effect of oxidation, stack voidness, temperature coefficient of exponential growth of heat release power were also used. For numerical implementation of the mathematical model, dimensionless variables and criteria were introduced, which allowed us to apply the net method. Analysis of the obtained results allowed to get: change in the stack temperature profiles with time; change in the stack oxygen concentration profiles with time; influence on the stack temperature profile of the specific heat release power; influence on the stack temperature profile of the parameter characterizing exponential growth of heat release intensity with temperature increase. It has been determined that the dynamics of coal self-heating in the stack is mostly influenced by the Lykov criterion, proportional to the diffusion coefficient, and the Nusselt criterion related to the effective thermal conductivity and to the effective thermal diffusivity of coal. The obtained results suggest that self-heating in the stack is due on the one hand to intensive penetration of air oxygen and on the other hand to a weakened heat transfer. Self-heating and the transition of self-heating into ignition are associated with the occurrence of turbulent diffusion in the stack, arising from increased thermal blowing, whose impact can be enhanced by directing it perpendicular to the surface of the stack.

**Keywords:** self-ignition, stack, self-heating in the stack, heat and gas exchange processes, coal self-heating.

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### Introduction

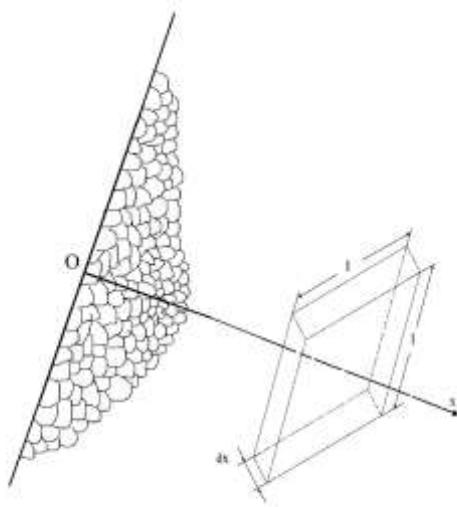
The theory of heat and mass transfer considers a number of mathematical models in the form of ordinary differential equations and equations of mathematical physics derived from the laws of

chemical kinetics, diffusion, filtration, convective motion, thermal conductivity, moisture exchange. These equations together with initial and boundary conditions, determining uniqueness of their solution, to a greater or lesser extent reflect those real physical conditions, under which the process

under study proceeds. This measure, obviously, depends on the number of considered factors and details in description of geometry and boundaries of the environment, in which the process is considered. The number of considered factors must be sufficient for the corresponding mathematical model to reflect essential regularities and features of the process; on the other hand, the number of considered factors must not be burdensome for the solution of the arising problem and visibility of the results of its solution. This last circumstance is associated with the so-called simplifying assumptions, which are accepted in the compilation of mathematical models and consist in neglecting some factors and circumstances, the influence of which on the studied process is either negligible or is such that it does not change the regularities of the process in principle.

### Experimental part

Development of recommendations for preventing self-heating of coal in stacks requires the study of heat and gas exchange processes arising from the chemical reaction of coal oxidation, heat transfer, diffusion of oxygen and oxidation products.



**Figure 1** - Calculation diagram for the heat transfer equation

It is known [1, 2, 3], that self-heating of coal in the stack and occurrence of self-ignition is observed in a relatively small layer adjacent to the surface of its contact with the air, called the zone of oxygen influence. Based on the observed values of coal temperatures in the stack at great depths obtained in practice, it can be assumed that at a considerable distance from the surface of the stack the coal temperature is constant. It gives a reason to consider the fields of temperature and oxygen

concentration in the stack as one-dimensional, depending only on the distance  $x$  from the surface of the stack, considered flat (Fig. 1). If we neglect the influence on the temperature and oxygen concentration in the zone of oxygen influence of the values of these values at sufficiently distant points, we will consider the stack to be unlimitedly extended in the direction perpendicular to the bounding surface under the above and some other natural simplifying assumptions.

The dynamics of the changes in the self-heating temperature  $t$  of the coal and the volume fraction  $C$  of oxygen in the stack cavities are described by a system of differential equations:

$$\frac{\partial t}{\partial \tau} = a \frac{\partial^2 t}{\partial x^2} + C_y^{-1} \cdot \frac{C}{C_0} \Phi_0 \exp[\delta(t - t_0)], \quad (1)$$

$$\frac{\partial C}{\partial \tau} = D \frac{\partial^2 C}{\partial x^2} - \frac{1}{\Pi q} \rho \frac{C}{C_0} \Phi_0 \exp[\delta(t - t_0)],$$

Here  $a$ ,  $D$  are effective thermal diffusivity, diffusion coefficient respectively,  $m^2/c$ ;  $C_y$  is specific heat capacity of the coal in the stack,  $J/(kg \cdot K)$ ;  $\rho$  - bulk density of coal in the stack,  $kg/m^3$ ;  $q$  - thermal effect of oxidation,  $J/m^2$ ;  $\Pi$  - stack voidness;  $\Phi_0$  - the specific heat release power corresponding to the initial temperature  $t_0$  and oxygen concentration  $C_0$ ,  $W/kg$ ;  $\delta$  is temperature coefficient of exponential growth of heat release power,  $K^{-1}$ . It is common to characterise the stability of coals during storage by value  $\Phi$ , measured at temperature  $70^\circ C$  [2, 10]. This value is related to the oxygen sorption rate constant, known in the theory of self-ignition of industrial materials, by the simple combination of  $= C \cdot u q$ .

Assuming that at the initial moment  $\tau=0$  the temperature at all points in the stack is the same and equals  $t_0$ , we get the initial condition for the temperature

$$t|_{\tau=0} = t_0 \quad (2)$$

The boundary condition for temperature is naturally assumed to correspond to the free heat transfer between the stack surface and the environment:

$$\lambda \frac{\partial t}{\partial x} - \alpha(t - t_b)|_{x=0} = 0, \quad (3)$$

where  $\lambda$  is effective thermal conductivity of coal in the stack,  $W / (m \cdot K)$ ,  $\alpha$  is external heat transfer coefficient,  $W/(m^2 \cdot K)$ .

The second boundary condition is:

$$t|_{x \rightarrow \infty} = t_0 \quad (4)$$

If the volume fraction of oxygen in the ambient air is  $C_0$ , the boundary condition for it is

$$C|_{x=0} = C_0 \quad (5)$$

As for the initial condition for the oxygen concentration, it would be obviously unnatural to suggest that it is the same at all distances from the surface of the stack at the initial moment of time. As the initial values of the oxygen volume fraction, we should obviously take those values that are established in the voids, at the initial temperature  $t=t_0$ . Such a stationary distribution is described, under the assumptions made earlier, by the differential equation derived from the second equation (1), if there will be assumed  $t=t_0$ ,  $\frac{\partial c}{\partial \tau} = 0$ ;

$$\frac{\partial^2 c}{\partial x^2} - \rho \Pi^{-1} \cdot \Delta^{-1} \cdot q^{-1} C \cdot C_0^{-1} \Phi_0 = 0$$

A bounded solution of the equation satisfying condition (5) is the function:

$$C(x) = C_0 \exp[-(\rho \Phi_0 \Pi^{-1} \cdot \Delta^{-1} \cdot q^{-1} \cdot C_0^{-1})^{1/2} x].$$

Thus, we obtain the initial condition for the oxygen volume fraction:

$$C/\tau = 0 = C_0 \exp[-(\rho \Phi_0 \Pi^{-1} \cdot \Delta^{-1} \cdot q^{-1} \cdot C_0^{-1})^{1/2} x]. \quad (6)$$

System (1) under conditions (2) - (6) is solved by the numerical net method.

When calculating the temperature and oxygen concentration fields in the stack using the developed programme, the following parameter values were recorded:

- initial temperature of coal in the stack  $t_0 = 10^0 C$ ;
- thermal conductivity of coal in the stack  $\lambda = 0,3 \frac{BT}{(m \cdot K)}$ ;
- thermal diffusivity of coal in the stack  $a = 1,7 \cdot 10^{-7} \frac{m^2}{c}$ ;
- stack voidness  $\Pi = 0,2$ ;
- stack density of coal  $\rho_y = 1200 kg/m^3$ ;
- specific heat capacity  $C_y = 1400 J/(kg \cdot K)$ ;
- thermal effect of oxidation  $q = 12,6 \cdot 10^6 \frac{J}{m^3}$ ;
- (oxygen volume fraction) in the ambient air  $C_0 = 0,2$ .

The variables whose influence was studied varied in the following intervals:

- ambient air temperature  $t_B = 15 \div 35^0 C$ ;
- specific heat release rate  $\Phi_0 = 0,02 \div 0,10 W/kg$ ;
- exponential rate  $\delta = 0,04 \div 0,09 K^{-1}$ ;
- diffusion coefficient  $D = 0,18 \cdot 10^{-4} \div 0,90 \cdot 10^{-4} m^2/c$ ;
- external heat transfer coefficient  $\alpha = 2,5 \div 250 W/(m^2 \cdot K)$ .

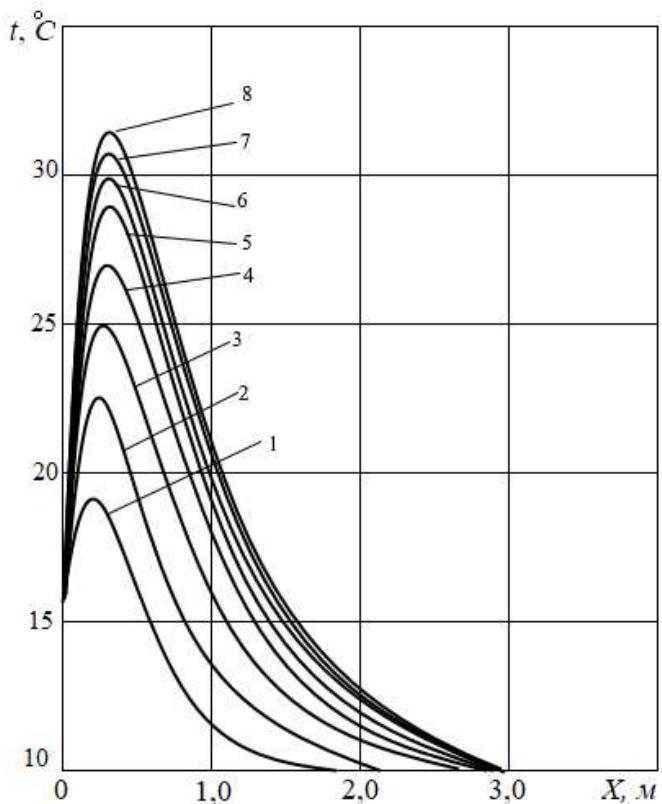


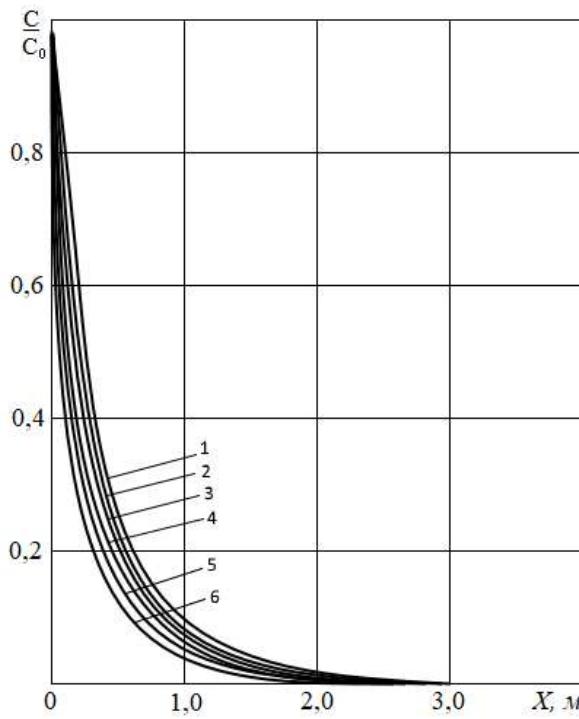
Figure 2.a - Changes in stack temperature profiles over time

Figure 2.a. shows changing in stack temperature profiles over time: 1,2,3,4,5,6,7,8 -  $\tau = 5, 10, 15, 20, 25, 30, 40, 50$  day.

## Results and discussion

An analysis of the solutions obtained with the parameter values typical for brown and bituminous coals has shown that, in the presence of only molecular diffusion ( $D \approx 0,2 \cdot 10^{-1} m^2/s$ ) the self-heating intensity fades with time, after 30-40 days a stationary temperature field is established which remains practically unchanged over time. On fig.1a shows how the temperature profile in the stack changes every 5 days ( $\Phi_0=0,06 W/kg$ ,  $\delta=0,06 K^{-1}$ ,  $t_B = 15^0 C$ ).

While at the beginning of the process the maximum daily increase is 2K, after 15 days it is only 0.4K and on the 30th day it is less than 0.1K. During the last 30 days, the maximum temperature increases by no more than 2K. The temperature at other points in the stack changes even less. The maximum temperature is set at a distance of 0.4-0.5 m. As the heat release specific power  $\Phi_0$  and the temperature coefficient increases  $\delta$  the stationary maximum temperature rises and shifts slightly towards the surface of the stack.

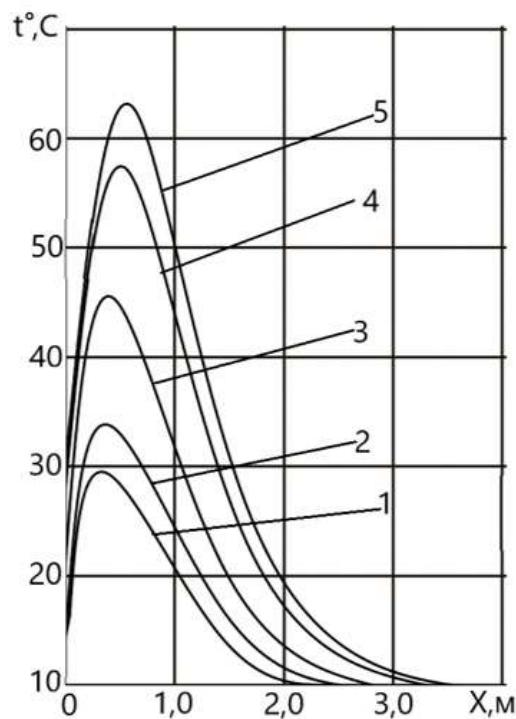


**Figure 2.b** - Change in stack oxygen concentration profiles

Figure 2.b. shows a change in stack oxygen concentration profiles over time: 1,2,3,4,5,6;  $\tau = 5; 10; 15; 20; 25; 30$  day.

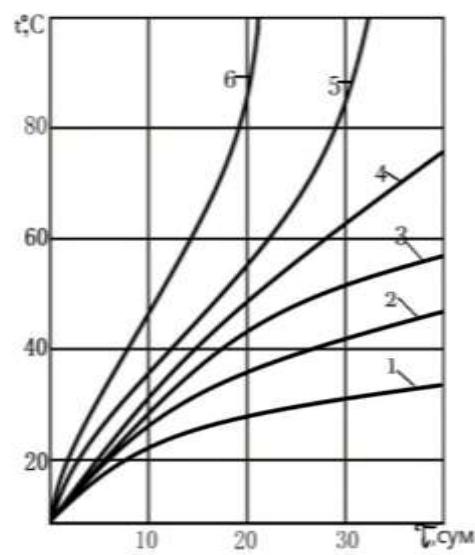
Similarly, a steady-state profile of oxygen concentration is established, characterised by a monotonic decrease with distance from the surface of the cluster (Fig. 2), where the profiles are shown for ease of comparison  $\frac{C}{C_0}$ . The boundary of the oxygen-affected zone is quite clear from the given profiles. From the given profiles the boundary of the oxygen influence zone is clearly visible, which in this case is located at a distance of 0.8 m from the surface (beyond this boundary the oxygen fraction does not exceed 1%).

The temperature profile in the stack is most strongly influenced by variations in the diffusion coefficient  $D$ , which is usually related to wind influence. Wind blowing on the stack surface leads to filtration flows, the influence of which on mass transfer can be accounted for by introducing the concept of turbulent diffusion. It is known [4, 8] that turbulent diffusion coefficient can exceed the molecular diffusion coefficient by tens and even hundreds times. When considering mass transfer in porous media it is reasonable to introduce an effective diffusion coefficient  $D_\alpha$ , determining the cumulative effect of molecular and turbulent diffusion.



**Figure 3** - Steady-state self-heating temperature profiles

Figure 3 is a steady-state self-heating temperature profiles at different diffusion coefficients: 1-5D – 1,8; 3,6; 5,4; 7,2; ; 9 ·  $10^{-4} \text{m}^2/\text{s}$ . It shows the steady-state temperature profiles at different values of the diffusion coefficient. In calculating the curves, it is taken into account that wind blowing on the stack surface simultaneously with an increase in the diffusion coefficient leads to an increase in the  $\alpha$  external heat transfer.



**Figure 4** - Diagram of maximum self-heating temperature variation

Therefore, with an increase of diffusion coefficient by a factor of 2, 3, 4, 5 the external heat transfer coefficient (based on known empirical data [5, 7] increases by a factor of 5, 15, 40, 100 respectively. Despite such sharp increase of heat transfer, maximum temperature, as seen from figure, strongly increases with increase of diffusion coefficient.

$$\begin{aligned} 1, 2, 3, 5 - D &= 1,8; 5,4; 7,2; 9 \cdot 10^{-4} \text{ m}^2/\text{s}, \text{ at } \alpha = 2,5; 25; 125; 2,5 (\text{W/m}^2 \cdot \text{K}), \\ 4 - D &= 5,4 \cdot \frac{10^{-4} \text{ m}^2}{\text{c}}; \alpha = 1,5 \text{ W/m}^2 \cdot \text{K}, \\ 6 - D &= 1,5 \cdot \frac{10^{-4} \text{ m}^2}{\text{s}}; \alpha = 2,5 \text{ W/m}^2 \cdot \text{K}. \end{aligned}$$

When the stack surface is exposed to wind, it is also possible that an increase in the effective diffusion coefficient occurs without a corresponding change in the external heat transfer coefficient. Some of the resulting graphs of the change in

maximum self-heating temperature are shown in Figure 4. The figure shows that at  $\alpha < 2,5 \frac{\text{W}}{\text{m}^2 \cdot \text{K}}$  and  $D_e > 5,4 \cdot 10^{-4} (\text{m}^2/\text{c})$  there is a progressive increase in temperature, which is known to be associated with the transition [6, 9] from self-heating to combustion.

## Conclusions

The given results testify to the decisive influence of wind impact on self-ignition of coal in stacks and to the effectiveness of fire prevention measures based on preventing the penetration of air oxygen into the stack and enhancing heat transfer from its surface. This explains the measure known from practice consisting in orienting the long side of the stack along the heating of the prevailing wind.

**Conflict of interests.** On behalf of all authors, the correspondent author declares that there is no conflict of interests.

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## Штабельдегі көмірді өздігінен қыздырудың математикалық моделі

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### ТҮЙІНДЕМЕ

Бұл мақалада шекаралық және бастапқы жағдайларда штабельдің құыстарындағы оттегінің С көлемдік үлесі мен көмірдің өздігінен қызыуының температурасына қатысты жылу және газ алмасу процестері екінші ретті сыйықты емес екі дифференциалдық теңдеулер жүйесімен сипатталып көмірдің өздігінен қызыуының математикалық моделі келтірілген. Дифференциалдық теңдеулерді құрастыру кезінде штабельдегі көмірдің өздігінен қызыу және өздігінен жанудың пайда болуы, оның ауамен жанасу бетіне жақын орналасқан және оттегінің әсер ету аймағы деп аталағын қатардың мөлшерімен салыстырғанда салыстырмалы түрде аз қабатта байқалатындығы ескеріледі. Бұл математикалық модельде құрастыру кезінде көмірдің орнықтылығын сипаттайтын  $\Phi$  - жылу шығарудың мешікті құтты параметрінің, көмірдің өзіндік қыздыру процесіне әсері ескерілді. Дифференциалдық теңдеулерді құрастыру кезінде температура мен өткізгіштік, диффузия коэффициенті, штабельдегі көмірдің мешікті жылу сыйымдылығы, сусындалы тығыздық, тотығудың жылу әсері, қатардың бос болуы, жылу шығару құттының экспоненциалды өсуінің температуралық коэффициенті сияқты физикалық параметрлер қолданылды. Осы математикалық модельді іске ассыру үшін өлшемсіз айнымалылар енгізілді, бұл тор әдісін қолдануға мүмкіндік береді. Алынған нәтижелерді талдау келесі нәтижелерді алуға мүмкіндік береді: үақыт өте келе температура профильдерінің өзгеруі; қатардағы оттегі концентрациясының профильдерінің үақыт өте келе өзгеруі; жылу шығарудың мешікті құттының қатарындағы температура профиліне әсері, температураның жоғарылауымен жылу шығару қарқындылығының экспоненциялдық өсуін сипаттайтын параметрдің температура профиліне әсері. Лыковтың диффузия коэффициентіне пропорционалды критерийлері және Нуссельттің тиімді жылу өткізгіштігімен және көмірдің тиімді температуралық өткізгіштігімен байланысты критерийлері көмірдің өздігінен қызыуының динамикасына ең көп әсер ететін анықталды. Алынған нәтижелер қатардың өзіндік қызыу бір жағынан аяу оттегісінің қарқынды енүімен, ал екінші жағынан әлсіреген жылу қабылдағышқа байланысты деп айтуга мүмкіндік береді. Өзіндік қыздыру және өзіндік қыздырудың отқа ауысы

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жылу соққысының күшөінде пайда болатын турбулентті диффузияның пайда болуымен байланысты, оның әсері штабельдің бетіне перпендикуляр бағытта күшейуі мүмкін.

**Түйін сездер:** өздігінен тұтану, штабель, штабельдегі өздігінен қызу, жылу алмасу және газ алмасу процестері, көмірдің өздігінен қызыу.

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## Математическая модель самонагревания угля в штабеле

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**АННОТАЦИЯ**

В данной статье приводится математическая модель самонагревания угля в штабеле, в которой теплообменные и газообменные процессы описаны системой двух нелинейных дифференциальных уравнений второго порядка относительно температуры  $t$  самонагревания угля и объемной доли  $C$  кислорода в пустотах штабеля с граничными и начальными условиями. При составлении дифференциальных уравнений учитывалось, что самонагревание угля в штабеле и возникновение очагов самовозгорания наблюдается в сравнительно небольшом по сравнению с размерами штабеля слое, примыкающем к поверхности его соприкосновения с воздухом и называемом зоной кислородного влияния. В данной математической модели учитывалось влияние на процесс самонагревания угля параметра Ф-удельной мощности тепловыделения, которая к тому же характеризует устойчивость угля при хранении. При составлении дифференциальных уравнений использовались также такие физические параметры как температуро-проводность, коэффициент диффузии, удельная теплопемкость угля в штабеле, насыпная плотность, тепловой эффект окисления, пустотность штабеля, температурный коэффициент экспоненциального роста мощности тепловыделения. Для численной реализации данной математической модели были введены безразмерные переменные и критерии, что позволило применить метод сеток. Анализ полученных результатов позволил получить: изменение профилей температуры в штабеле со временем; изменение профилей концентрации кислорода в штабеле со временем; влияние на профиль температуры в штабеле удельной мощности тепловыделения; влияние на профиль температуры в штабеле параметра, характеризующего экспоненциальный рост интенсивности тепловыделения с ростом температуры. Установлено, что наибольшее влияние на динамику самонагревания угля в штабеле оказывают критерий Лыкова, пропорциональный коэффициенту диффузии, и критерий Нуссельта, связанный с эффективной теплопроводностью и с эффективной температуропроводностью угля. Полученные результаты позволяют утверждать, что самонагревание в штабеле связано с одной стороны интенсивным проникновением кислорода воздуха, а с другой стороны – ослабленным теплоотводом. Самонагревание и переход самонагревания в возгорание связано с возникновением в штабеле турбулентной диффузии, возникающей при усилении теплового обдува, влияние которого может быть усилено при направленности перпендикулярно к поверхности штабеля.

**Ключевые слова:** самовозгорания, штабель, самонагревание в штабеле, теплообменные и газообменные процессы, самонагревания угля.

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