Kinetic model of ignition and combustion of finely-disperse coal-water fuel

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Abstract. The article proposes a model of the process of ignition and combustion of fine water-coal fuel (FWCF) in a cyclone primary furnace. The model is intended to form an engineering approach to calculating the composition and quantity of combustion products of the FWCF and the definition of the structural and layout characteristics of the actual cyclone primary furnace. Approximation of process modeling is determined by the following assumptions: the quasistationarity of the processes; the constancy of heat capacities and heat transfer coefficients at an average process temperature; isothermal fuel particles; representation of fuel particles in the form of a water-coal drop of a given size; inertness of ash components; record keeping of the determining chemical reactions of interaction with the oxidizing agent; one-dimensional flow. This approach allows to carry out an analytical analysis of the process and to obtain final expressions suitable for engineering calculations.

1. Introduction
Considering the movement of fuel in the form of a fine water-coal slurry inside a cyclone pre-furnace, similar to that considered in [1, 2].

The wall temperature is $T_{wall}$. The initial fuel is characterized by a fine droplet which size is $\delta = 30 \div 100$ micron with initial temperature of $T_{fuel}$. Fuel is supplied to the extended furnace along the generatrix of the cyclone with air and twists in the form of a spiral. When advancing through the gas suspension extended furnace, as the temperature rises, moisture evaporates, volatiles are released, and combustion products are formed. In this section, the temperature of the gas suspension is characterized by the mixture temperature $T_{mix}$ and the particle temperature $T_{c}$. The zone of active combustion can be located both in the extended furnace and in the furnace space of the boiler (figure 1).

2. A model of the process of ignition and combustion of fine water-coal fuel
Assuming that the fuel moves inside a certain channel, which, in turn, twists into a vortex flow along the generatrix of the cyclone, the temperature change over time can be represented as [3, 4]:

$$\frac{dT_{gas}}{d\tau} = -A_{gas} T_{gas} + F_{gas}$$

(1)
In this equation

\[ A_{\text{gas}} = \psi_c \frac{1}{V_{\text{mix},c_{\text{mix}}}} \left( Nu \lambda d + \alpha_r \right) = 3\text{BiFo} \tau^{-1} \frac{c_c}{V_{\text{mix},c_{\text{mix}}}} \left( 1 + \frac{\alpha_r \psi_c}{3\text{BiFo} \tau^{-1}} \right) \]  

(2)

\[ F_{\text{gas}} = \psi_c \frac{1}{V_{\text{mix},c_{\text{mix}}}} \left( \frac{Nu \lambda}{d} T_c + \alpha_r T_{\text{wall}} \right) = 3\text{BiFo} \tau^{-1} \frac{c_c}{V_{\text{mix},c_{\text{mix}}}} \frac{T_{\text{wall}}}{T_{\text{wall}}} + \frac{\alpha_r \psi_c}{3\text{BiFo} \tau^{-1}} \]  

(3)

where \( T_{\text{wall}}, T_c \) are the temperature of the wall and fuel particles; \( \alpha_r \) is radiation heat transfer coefficient \([6, 10, 11]\); \( \psi_c = \frac{6}{\delta \rho_c} \) is particle surface per 1 kg of fuel; \( d \) is channel diameter; \( \rho_c \) is density of coal particles.

After integration (using the Laplace transform) we get:

\[ T_{\text{gas}} = T_{\text{fuel}} \exp \left( -A_{\text{gas}} \tau \right) + \frac{F_{\text{gas}}}{A_{\text{gas}}} \left[ 1 - \exp \left( -A_{\text{gas}} \tau \right) \right] = T_{\text{fuel}} \exp \left[ -3\text{BiFo} \tau^{-1} \frac{c_c}{V_{\text{mix},c_{\text{mix}}}} \left( 1 + \frac{\alpha_r \psi_c}{3\text{BiFo} \tau^{-1}} \right) \right] + \]

\[ + T_{\text{wall}} \left( \frac{T_{\text{wall}}}{T_{\text{wall}}} + \frac{\alpha_r \psi_c}{3\text{BiFo} \tau^{-1}} \right) \left[ 1 - \exp \left( -3\text{BiFo} \tau^{-1} \frac{c_c}{V_{\text{mix},c_{\text{mix}}}} \left( 1 + \frac{\alpha_r \psi_c}{3\text{BiFo} \tau^{-1}} \right) \right) \right] \]  

(4)

When evaluating \( T_{\text{fuel}} \) as a first approximation, we can take:

\[ T_{\text{gas}} = T_{\text{mix},c_{\text{mix}}} + T_{\text{wall}} \left[ 1 - \exp \left( -3\text{BiFo} \tau^{-1} \frac{c_c}{V_{\text{mix},c_{\text{mix}}}} \right) \right] \]  

(5)

where \( c_c, c_{\text{mix}} \) are heat capacity of fuel particles and gas suspension.

The process of evaporation of moisture from a drop of fuel is presented as:

\[ \frac{dm_w}{dT_w} = \frac{d}{dT_w} \left( \frac{\pi \delta^3}{6} \rho_w \frac{w}{1-w} \right) \frac{\pi \delta^3}{6} \rho_w \frac{w}{1-w} \frac{dw}{d\tau_w} = -\pi \delta \frac{T_{\text{fuel}} - T_{\text{fuel}}}{r} \]  

(6)

where \( \delta = \sqrt{\frac{\delta^3 \rho_w}{\rho_w (1-w)}} = 1.25 \delta \left( \frac{w}{1-w} \right)^{0.33} \)
It follows that:
\[
\frac{dm_w}{d\tau_w} = -1.25 \frac{W}{r} \alpha \left(T_{mix} - T_{fuel}\right)(1-w)^{1.67} w^{0.33}
\]
where \(\alpha\) is the heat transfer coefficient; \(r\) is heat of evaporation; \(\tau_w\) is the time of moisture evaporation.
It is important to determine the end time of the evaporation process for the entire amount of completely evaporated moisture from the fuel, since practically only after this the heating of the particles begin.

Using the Euler method, we obtain an approximate solution in the form:
\[
w = 1.25 \frac{W}{r} \lambda Nu \left(T_{mix} - T_{fuel}\right)(1-w_0)^{1.67} w^{0.33}\tau_w
\]
where \(w_0\) is the initial value of the relative moisture content in the fuel.

Thus, the total time of thermochemical transformations of fuel will be determined by the sum \(\tau = \tau + \tau_w\).

In thermochemical reactions, the yield equation for the components (CH\(_4\), CO\(_2\), CO, H\(_2\), H\(_2\)O) can be represented as
\[
\frac{dC_j}{d\tau} = (C^0_j - C_j) a_j = f_i
\]
where \(a_j = K_j \exp\left(-E_j R^{-1} T^{-1}\right), K_j, E_j\) are the preexponential factor, the rate constant of the output of the components and the corresponding activation energy of the \(j\)-th thermochemical reaction; \(R\) is universal gas constant; \(C^0_j\) is the initial concentration of the components.

From this expression we find:
\[
C_j = C^0_j \left(1 - e^{-a_j \tau}\right).
\]

A chemically reactive vapor-gas mixture is moving inside the channel.
Heat transfer coefficient for gas suspension:
\[
\lambda = \lambda_{gas} + \lambda_{n,T} + \lambda_{tc}
\]
where \(\lambda_{gas}, \lambda_{n,T}, \lambda_{tc}\) are thermal conductivity, apparent thermal conductivity, turbulent thermal conductivity.

The coefficient of turbulent thermal conductivity:
\[
\lambda_{tc} = 0.9 I^2 D_i \sqrt{\frac{\xi}{273}} \frac{c_{mix}}{W_w} \frac{\sigma_{wall}P_{wall}W_w}{0.5d Pr_w} \left(1 - 0.5 \eta\right)
\]
In this formula \(y = 0.25d; c_{mix} = 2.3 \left(\frac{T_{gas}}{273}\right)^{0.1}; l = 0.08d \left(\frac{2y}{d}\right)^{0.8}\) are length of the mixing path;
\(D_i = \left[\exp\left(-\frac{\eta}{26}\right)\right]^2\) is a damping factor; \(\eta = y \sqrt{\sigma_{wall}P_{wall} \frac{1}{\nu_{wall}}}\) is dimensionless coordinate (calculated when \(T_{wall}\)); \(\sigma_{wall} = 0.125 \xi \rho_{wall} \xi \) is a shear stress; \(\xi = (1.828 \lg \text{Re} - 1.64)^2\);
Pr$_s$ = $1.2 - 0.45 \exp(-1.5 \cdot 10^{-3} \text{Re})$ is a Prandtl number; $w_s = w \left(1 - 0.845 \frac{\lg \text{Re}}{10} \right)$ is the speed on the axis of the channel.

The apparent coefficient of thermal conductivity, which characterizes the convective transfer of heat by particles of fuel:

$$\lambda_{a,t} = \left(\frac{\xi_{a,t}}{\xi_0}\right) \left(\frac{c_n \varphi_{wall} \nu}{\varphi_{a}}\right)$$

(12)

where $\xi_{a,t}/\xi_0$ is relative hydraulic resistance of gas suspension,

$$\xi_{a,t}/\xi_0 = 0.28 \left(\frac{d}{\delta}\right)^{0.4} K \left(\frac{w/\delta}{w^0/\delta^0}\right) \exp\left[-2 \frac{w}{\delta} \left(\frac{d}{\delta}\right)^{0.8}\right]$$

(13)

In this expression:

$$c_n = 1.09 \left(\frac{T}{273}\right)^{0.054} = 2.73 \left(\frac{d}{\delta}\right)^{0.53} \rho_{wall} = \rho_0 \left(\frac{273}{T_{wall}}\right)$$

(14)

Here $w$ is a gas velocity; $\dot{\gamma}_s^0$ is the speed of soaring fuel particles; $K$ is the consumable mass concentration of particles; $\varphi_{a}$ is a speed slip factor.

The value $\xi_0$ is determined by the Blasius law:

$$\xi_0 = 0.1364 \text{Re}^{-0.25}$$

(15)

Speed slip factor:

$$\varphi_{a} = 0.09 \left(\frac{w}{\dot{\gamma}_s^0}\right)^n \left(\frac{d}{\delta}\right)^m K^c$$

(16)

where $n = 0.0937 + 1.1 \left(\frac{d}{\delta}\right)^{0.5} + 0.333 \exp\left[-0.48 \frac{w}{\dot{\gamma}_s^0}\right] ; m = 0.467 \left(\frac{d}{\delta}\right)^{-0.1}$;

$$c = 0.0234 \left(\frac{\dot{\gamma}_s^0}{g\delta}\right)^{0.26} \exp(-3.5 \cdot 10^{-5} \text{Re}) ; \text{Re} = \frac{wd}{\nu} \text{ are Reynolds criterion; } \nu = 24.6 \cdot 10^{-6} \left(\frac{T_{gas}}{273}\right)^{1.73}$$

is a gas viscosity; $\lambda_{gas} = 7.49 \cdot 10^{-5} \left(\frac{T_{gas}}{273}\right)^{0.86}$ is a thermal conductivity of gas.

Convective heat transfer in the extended furnace is described by the equation:

$$Nu = 0.48(1 + 0.3K) \left(\frac{d}{L}\right)^{0.86} \text{Re}^{0.52c(\frac{d}{L})^{-0.481}}$$

(17)

where $L$ is a fuel conversion channel length.

Dependencies are valid for parameters: $\text{Re} \leq 20 \cdot 10^3$; $K \leq 8$; $\delta = 0.0001 \ldots 0.0012$ м, the parameters are determined by the arithmetic mean flow rates of the phases and the composition of the gas.
It should be noted that obtaining universal, generalizing kinetic dependences of the pyrolysis and combustion of different types of fuels, including coal-based FWCF, is difficult and true only for specific response conditions. This is due to the large variety of properties and the complexity of the structure of fuels.

The yield of pyrolysis products and the composition of combustion products determine a number of basic reactions, which are presented below.

The yield of volatile methane is determined by the interaction of the carbon of the coal with the hydrogen released by the heating of the coal:

\[ C + 2H_2 \rightarrow CH_4 + 6.2 \text{ mJ/kg}. \]

The yield of volatile carbon dioxide is determined by the combustion of carbon when interacting with the released oxygen of the coal:

\[ C + O_2 \rightarrow CO_2 + 33.8 \text{ mJ/kg} \]

and in the further process, the cost of CO2 for the partial carbon dioxide gasification of carbon with the formation of CO:

\[ C + CO_2 \rightarrow 2CO - 14.4 \text{ mJ/kg}. \]

In addition, the yield of volatile carbon monoxide is determined by the oxidation of carbon in coal by oxygen, taking into account the previous cost of oxygen for the combustion reaction:

\[ C + CO_2 \rightarrow 2CO + 9.4 \text{ mJ/kg} \]

Also, evaporation of moisture and, in this connection, partial steam gasification of semi-coke carbon should be taken into account:

\[ C + H_2O \rightarrow CO + H_2 - 10.3 \text{ mJ/kg}. \]

Combustion of carbon and formed CO, H₂ и CH₄ are due to the presence of oxygen in the primary and secondary (if necessary) air and passes through the reactions:

\[ C + O_2 \rightarrow CO_2 + 12.3 \text{ mJ/kg} \]
\[ H_2 + O_2 \rightarrow 2H_2O + 17.8 \text{ mJ/kg} \]
\[ CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O + 27.8 \text{ mJ/kg} \]
\[ CO + 0.5 O_2 \rightarrow CO_2 + 8.9 \text{ mJ/kg} \]

Kinematic parameters of the reaction are presented in table 1.

| Reactions | \(k_0 \text{ (c}^{-1}\)) | \(E, \text{ (kJ/kmol)}\) |
|-----------|--------------------------|--------------------------|
| Moisture out of the fuel | \(H_2O^{FUEL} \rightarrow H_2O\) | \(8 \cdot 10^{15}\) | 215 \cdot 10^3 |
| Fuel output CO | \(CO^{FUEL} \rightarrow CO\) | \(2 \cdot 10^{12}\) | 186 \cdot 10^3 |
| Fuel output CO₂ | \(CO_2^{FUEL} \rightarrow CO_2\) | \(2 \cdot 10^{11}\) | 137 \cdot 10^3 |
| Methane output from fuel | \(CH_4^{FUEL} \rightarrow CH_4\) | \(1.6 \cdot 10^{14}\) | 216 \cdot 10^3 |
| Steam char gasification | \(C+H_2O \rightarrow CO+ H_2\) | \(2 \cdot 10^{11}\) | 115 \cdot 10^3 |
| Carbon dioxide char gasification | \(C+CO_2 \rightarrow 2CO\) | \(1.6 \cdot 10^{13}\) | 112 \cdot 10^3 |
| Coal burning | | | 84 \cdot 10^3 |
| Burning CH₄ | | | 125 \cdot 10^3 |

3. Calculation results

Using the presented provisions, calculations of combustion of fine water-coal fuel based on Kuznetsk coal OS grade with the ratio of solid and liquid phases by mass 0.6/0.4 when spraying it in an air flow.
with a drop size $\delta = 30$ mm with a stoichiometric ratio of combustion products and oxygen. The composition and characteristics of FWCF in terms of operating mass are presented in Table 2.

**Table 2.** Physico-chemical characteristics of FWCF.

| $Q'/\text{MJ/kg}$ | $W'$ | $C'$ | $H'$ | $O'$ | $N'$ | $A'$ |
|-------------------|------|------|------|------|------|------|
| 13.8              | 0.4  | 0.378| 0.019| 0.007| 0.012| 0.18 |

The combustion process of FWCF with $T_{gas} = T_{wall} = T_{mix} = 1670$ K causes the release of 1.48 kg of CO$_2$ per kilogram of initial fuel (figure 2). It can be seen that the material balance of the initial fuel and combustion products converge with an accuracy of 0.5%.

The time of evaporation of moisture from a drop of fuel is about 0.5 s. This, in turn, means that the evaporation section (figure 1) with a linear velocity along the axis of the extended furnace of 1-2 m/s is 0.5-1 m. Such a result means that the developed kinetic model of combustion of the FWCF can be used in engineering calculations when creating boiler equipment with the use of FWCF.

**Figure 2.** The material balance of combustion FWCF with the stoichiometric ratio of combustion products and oxygen.

4. **Findings**
1. A kinetic model of ignition and combustion of FWCF has been developed.
2. The efficiency of the model and its applicability for engineering calculations is shown.

5. **References**
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