Mathematical modeling of burn-out of the coal particle coke residue

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Abstract. Combustion of solid fuels in general includes a number of stages: heating, drying, devolatilization, ignition, and burn-out of coke. The stage of coke residue burn-out is the leading one. In this paper, analytical solutions for the burn-out of the coke part of an anthracite particle were developed using the asymptotic procedures, and combustion of anthracite particles with the size of 100 µm and less (presented size for the flare process) and 12 mm or more (characteristic size for burning in a fluidized bed) was calculated. In the first case, combustion occurs in the kinetic regime, and in the second, it occurs in the diffusion regime. The models of the “hard” ash frame, as well as the model “with segregating” ash, have been implemented.

1. Introduction
The Novosibirsk Region has unique reserves of high-quality anthracite (Ultra High Grade) of the Listvyansko-Gorlovsky deposit with a total geological resource of ~7 billion tons. There are only three such anthracite deposits in the world. Coal, mined by JSC “Sibantratsit”, is consumed as follows: ~20% is used for technological needs, and ~80% is presented by low-reaction screenings of up to 13 mm in size [1]. The most effective use of anthracite screenings is energy production. The Institute of Thermophysics of the Siberian Branch of the Russian Academy of Sciences in cooperation with the Central Boiler-Turbine Institute has developed and used the technology of burning anthracite screenings in a fluidized stationary bed as the most simple that allowed reconstruction and modernization of physically obsolete steam and hot water boilers [2]. The cost of modernization amounted ~10% of the cost of new boiler construction. Using these developments, JSC “Sibantratsit” has reconstructed the boilers of its own boiler house, where anthracite screenings have been used for a number of years.

Further improvement of the technology of such combustion with consideration of the tightened requirements for ecology, energy efficiency, economics, safety, and other conditions is almost impossible without detailing the processes of thermal preparation and combustion of anthracite particles.

It is known [3, 4] that combustion of solid fuels generally involves a number of stages: heating, drying, devolatilization, ignition, and coke burn-out. The stage of coke residue burn-out is the leading one. In this paper, analytical solutions for the burn-out of the coke part of an anthracite particle were
developed using the asymptotic procedures, and combustion of anthracite particles with the size of 100 µm and less (presented size for the flare process) and 12 mm or more (characteristic size for burning in a fluidized bed) was calculated.

As D. Spalding [4] notes, “the purpose of combustion analysis is derivation of formulas for the time of carbon particle burning in an atmosphere containing oxygen. Such dependencies can help the designer of furnaces, who, even without knowing exactly how long each particle remains in the combustion chamber (due to the complexity of the flow structure), can at least set a real lower limit of this time”.

2. Statement of the problem of burn-out of a coal particle coke residue

The following assumptions are accepted: the particle has spherical symmetry; thermophysical properties of coal and ash are considered conditionally constant; heat is fed to the particle from the flame by radiation and convection simultaneously; the temperature of gas medium $T_g$ is taken constant; a heterogeneous exothermic first-order oxidation reaction takes place on the carbon surface; under the heat flux influence temperature of coke ignition $T_{ig}$ is reached at the initial moment of time $t_{in}$ on the surface of particle; in future, the supplied heat is spent on heating and burn-out of the coke residue, as well as ash frame overheating above $T_{ig}$ temperature.

The kinetic or diffusion regime of coal particle combustion can be determined by the following estimates [3]. If the diffusion exchange coefficient $\alpha_d$ (m/s) is much larger than the kinetic constant of burning rate $K$ (m/s), then combustion occurs in the kinetic region. Vice versa, combustion takes place in the diffusion region. The value of $\alpha_d$ is determined from expression

$$\alpha_d = \frac{Nu_D D}{d_0},$$

where $Nu_D$ is diffusion Nusselt number; $d_0$ is outer diameter of particle, m; $D$ is coefficient of oxygen diffusion in gas, m²/s, determined from [5].

$$D = 0.18 \cdot 10^{-4} \left( \frac{T_g}{273} \right)^{0.9};$$

$K$ is determined from the Arrhenius law

$$K = K_0 \exp\left(-\frac{E}{RT}\right),$$

where $E$ is activation energy, J/mole; $K_0$ is pre-exponent, m/s; $R$ is molar gas constant equal to 8.31 J/(mole-K).

According to [6], for anthracite, $K_0 = 8700$ m/s, $E = 118$ kJ/mole. Based on the theory of combustion, in the diffusion regime, the burning time is determined by the time of oxidizing agent delivery to carbon, and in the kinetic regime, it is characterized by the time of reaction with the oxidizing agent. Using the above estimates, we come to the following conclusions. Combustion of anthracite particles of 100 µm or less proceeds in the kinetic regime, and it is reasonable to adapt the model of “segregating ash.” In this case, during combustion, the ash layer is almost instantly carried away from the surface of a carbon particle, and it changes its size during combustion. For the particles with a size of 12 mm or more (in the case of its continuity), combustion takes place in the diffusion regime, and in this case “the hard ash frame” model is implemented, that is, the outer diameter of a particle remains almost the same, and only the diameter of carbon surface changes. When solving a more complex second model, it is assumed that all heat inside the carbon sphere is transferred due to thermal conductivity through “the ash skeleton”, and the temperature of the ash frame and gas filtered through it do not differ from each other at any point of the porous structure. We should note that the solution by the first model can be represented as a particular case of the solution by the second more complex model with almost complete ash entrainment.
Let us denote by index 1 the parameters related to the ash layer, and by index 2, the parameters of coke residue. The system of equations that defines a common problem, that is, burn-out by to “the hard ash frame” model, has the following form:
- the energy equation for the ash frame
  \[
  \frac{\partial T_1(r,t)}{\partial t} = a_{ef} \left[ \frac{\partial^2 T_1(r,t)}{\partial r^2} + \frac{2}{r} \frac{\partial T_1(r,t)}{\partial r} \right]
  \]  \hspace{1cm} (3)

\( r(t) < r < r_0, \) \( T_1 > T_{ig}, \) \( t > t_{in}. \) \( a_{ef} = \frac{\lambda_{ef}}{c_{ef} \rho_{ef}} \) is effective coefficient of thermal diffusivity, \( m^2/s, \)

\( \lambda_{ef} = \lambda(1-\rho) \) is effective coefficient of heat conductivity, \( W/mK; \) \( \rho \) is porosity; \( c_{ef} = c(1-\rho) \) is effective heat capacity, \( J/kg-K; \) \( \rho_{ef} = \rho(1-\rho) \) is effective density, \( kg/m^3; \)

\( r(t) \) is radius of moving “ash-carbon” boundary for the model with ash layer entrainment, \( m; \) \( T_{ig} \) is temperature of coke residue ignition, \( K; \) \( t_{in} \) is time of coke ignition;

– the energy equation for coke residue
  \[
  \frac{\partial T_2(r,t)}{\partial t} = a_2 \left[ \frac{\partial^2 T_2(r,t)}{\partial r^2} + \frac{2}{r} \frac{\partial T_2(r,t)}{\partial r} \right]
  \]  \hspace{1cm} (4)

\( 0 < r < r(t), \) \( T_0 < T_2 < T_{ig}. \)

According to [7], the initial condition is written as

\[
T_2(r, t_n) = T_{ig} + T_g \left[ \frac{(r/r_n)^2 - 1}{2} \right] \left[ \frac{\alpha_{ef} r_n}{\lambda_2} \left( 1 - \frac{T_g}{T_{ig}} \right) \right],
\]  \hspace{1cm} (5)

where \( \alpha_2 \) is total coefficient of heat transfer through convection and heat radiation from flue gases to a particle, \( W/m^2K; \) \( T_{co} \) is temperature of carbon combustion.

The boundary condition is

\[
\lambda_e \frac{\partial T_1(r_n, t)}{\partial r} = \alpha_2 (T_{ig} - T_{in})
\]  \hspace{1cm} (6)

where \( T_{in} \) is temperature on the outer surface of a particle.

The Stefan condition on the moving “ash-carbon” boundary is

\[
\lambda_1 \frac{\partial T_1(r, t)}{\partial r} \bigg|_{r(t)+0} - \lambda_2 \frac{\partial T_2(r, t)}{\partial r} \bigg|_{r(t)-0} = \rho_2 Q_e \frac{dr(t)}{dt}
\]  \hspace{1cm} (7)

where \( \rho_2 \) is coke residue density (for anthracite \( \rho_2 = 1440 \) kg/m\(^3\)), \( Q_e \) is heat released at combustion of 1 kg of coke residue (for anthracite \( Q_e = 3\times10^7 \) J/kg)

\[
T_1(r_0, t) = T_2(r_0, t) = T_{co}.
\]  \hspace{1cm} (8)

Symmetry condition

\[
\frac{\partial T_2(0, t)}{\partial r} = 0
\]  \hspace{1cm} (9)

To generalize the study, we turn the system of equations (3)–(9) into dimensionless form:

\[
K_a \frac{\partial \theta_1(X, Fo)}{\partial Fo} = \frac{\partial^2 \theta_1(X, Fo)}{\partial X^2} + \frac{2}{X} \frac{\partial \theta_1(X, Fo)}{\partial X}
\]  \hspace{1cm} (10)

\( R(Fo) < X < \) \( \theta_1(X, Fo) > 1; \) \( Fo > Fo_{in}, \)

where \( R(Fo) = r(t)/r_0, \) \( K_a = \alpha_{ef}/\alpha_1, \) \( \theta_1(X, Fo) = T_1(x, t)/T_{ig} \)

\[
\frac{\partial \theta_2(X, Fo)}{\partial Fo} = \frac{\partial^2 \theta_2(X, Fo)}{\partial X^2} + \frac{2}{X} \frac{\partial \theta_2(X, Fo)}{\partial X}
\]  \hspace{1cm} (11)

\( 0 < X < R(Fo), \) \( \theta_0 < \theta_2(X, Fo) < 1, \)
where $\Theta_2(X, Fo) = \frac{T_2(x, t)}{T_{ig}}$, $\Theta_0 = \frac{T_0}{T_{ig}}$

$$\frac{\partial \Theta_2(0, Fo)}{\partial X} = 0,$$

$$\Theta(X, Fo) = \frac{3}{X^2} \int_0^X X^2 \Theta_0(X, Fo) dX,$$  \hspace{1cm} \text{(13)}

where $K = \frac{c_0}{\lambda}$, $M = \frac{Q_0}{c_0 T_{ig}}$, $i=1,2$, $Fo = \frac{a_t}{r_0}$.

$\theta_2(X, Fo_{in}) = \theta_c + B_i \sum \frac{X^2-1}{2}[\theta_c-1]\hspace{1cm} \text{(14)}$

where $Bi$ is Biot number for coal particle, $\theta_c = \frac{T_s}{T_{co}}$.

Boundary condition

$$\frac{\partial \theta}{\partial X} \bigg|_{W} = Bi_{ef} (\theta_c - \theta_{1w}) = Ki(Fo)$$  \hspace{1cm} \text{(15)}

Stefan condition

$$\frac{\partial \Theta_1(R, Fo)}{\partial \chi} - K_h \frac{\partial \Theta_2(R, Fo)}{\partial \chi} = -M \frac{dR}{dFo},$$

$$\theta_1(R, Fo) - \theta_2(R, Fo) = 1.$$  \hspace{1cm} \text{(16)}

Then, caloric condition (16) was used in form

$$Q_1(Fo) - K_i Q_2(Fo) = V(Fo).$$  \hspace{1cm} \text{(17)}

Separating asymptotics with consideration of two terms of expansion [7] in the temperature field, described by the system of equations (10) - (16) with known $\Theta_2(X, Fo_{in})$ and $Fo_{in}$, we obtain solution for the “ash” frame and for coke residue

$$Q_2(Fo) = Q_2(\theta_c) R^4 \exp \left[ -15 \int_{\theta_c}^{R} \frac{dFo}{R^4(\theta_c)} \right],$$  \hspace{1cm} \text{(18)}

where $Q_2(\theta_c) = Q_2(Fo_{in}) = Bi_{2}(\theta_c - 1)$

The correlation for finding $R(Fo)$ is as follows:

$$\tilde{m}Fo = I_1(R) + I_2(R) + I_3(R) + P_1(Q_2, R) + P_2(Q_2, R) + P_3(Q_2, R),$$

$$\text{where } \tilde{m} = \frac{\theta_c - 1}{M}, \quad \Phi(R) = \frac{\alpha_2(R)}{A(R)} \left[ \beta_2(R) - \alpha_2(R) B(R) \right] V(R).$$  \hspace{1cm} \text{(19)}

In expression (19), the first term of $I_1(R)$ is a solution with neglecting the heat capacity of the “ash” frame and coke residue; from the physical point of view, sum $\sum_{i=1}^{3} I_i(R)$ takes into account “ash” frame overheating, and $\sum_{j=1}^{3} P_j(Q_2, R)$ takes into account coke residue heating.

Time of total burn-out of coke $Fo$ is found from (19) at $R(Fo) = 0$

$$\tilde{m}Fo_k = I_1(0) + \sum_{i=1}^{2} I_i(0) + \sum_{j=1}^{3} P_j(0)$$
Let us estimate parameter \( \tilde{m} \):

\[
\tilde{m} = \frac{c_i T_g}{Q_e} \left( \frac{T_g}{T_{ig}} - 1 \right)
\]

For anthracite, \( T_{ig} = 973 K; c_2 = 950 J/kg \cdot K; \)
At \( T_g = 1600 K \) (for particles of 100 \( \mu m \)), \( \tilde{m} = 0.02 \); 
At \( T_g = 1273 K \) (for particles of 12 mm), \( \tilde{m} = 0.01 \).

Thus, in the range of real values of the parameters of anthracite particle combustion, the complex \( \tilde{m} \) has very small values. This makes it possible to simplify significantly the general solution (19).

1. In the case of implementation of “the hard ash frame” model, the solution is

\[
\tilde{m} F_O = \frac{1 - R^3(F_O)}{3} \left[ \frac{1}{B_{i_1}} + A_2(R) \right],
\]

Calculations by simplified dependencies (20) were carried out for the following thermal-physical properties of anthracite ash taken from [9] \( \lambda = 0.13 \) W/m\( \cdot \)K; \( c_1 = 750 J/kg \cdot K; \rho = 780 \) kg/m\(^3\); \( a_1 = 0.22 \times 10^{-6} \) m\(^2\)/s.

2. In the case of implementation of “segregating” ash model \( \sum I_i = 0 \), expression (19) is transformed under the condition of \( R(F_O) \rightarrow 1 \), and this is typical of the initial stage of burn-out

\[
F_O \approx \frac{M}{3 B_{i_1} (\theta_c - 1)} \left[ 1 - R^3(F_O) \right] + \frac{1}{15}
\]

At the end of coke burn-out under the conditions of \( R(F_O) \rightarrow 0 \), \( R(F_O) \) can be determined by formula

\[
R(F_O) \approx \sqrt[2]{\frac{\chi - \sqrt{\chi^2 - \xi}}{2}} + \sqrt{\chi - \sqrt{\chi^2 - \xi}}
\]

where \( \chi = 1 + \frac{1}{B_{i_1}} \), \( \xi = 3 - 2\tilde{m} F_O \).

We should note that the total time of anthracite particle burn-out can be obtained by summing the time of heating up to particle ignition from [7] and time of coke residue burn-out to a certain value of mechanical underburning \( R(F_O) \). These diagrams are shown in Figures 1 and 2.

**Figure 1.** Total time of combustion of an anthracite particle with the size of 100 \( \mu m \) at gas temperature \( T_g = 1600 K \)

**Figure 2.** Total time of combustion of an anthracite particle with the size of 12 mm at gas temperature \( T_g = 1273 K \)
It should be noted that the results obtained for the total time of burn-out of anthracite particles with the size of 100 µm have very good convergence with the experimental data obtained by Babiy V.I. and given in [9]. The error does not exceed 3%. The same comparison for the 12-mm particles has a slightly larger error, but it does not exceed 7%.

Let us also estimate the relative portion of heating in the total time of complete combustion of particle (R = 0). For anthracite particles with the size of 100 µm at gas medium temperature $T_g = 1600$ K, it will be 0.016, and for particles of 12-mm size it will be 0.001 at gas temperature $T_g = 1273$ K. These results confirm the statement that the time of coke residue burn-out is the longest and takes up most of the time required for complete combustion of an anthracite particle.

3. Conclusion

1. The problem of burn-out of coal particle coke residue was stated with a set of reasonable assumptions for two models of ash layer behavior: 1) “hard ash frame” model and 2) model of “segregating” ash.
2. An original method of approximate analytical solution of this complex nonlinear system, based on asymptotic procedures, is developed.
3. The performed calculations confirm that the stage of coke residue burn-out is the limiting one in the overall balance of time of anthracite particle burning.
4. In general, a motivated conclusion that this approach can be effectively applied to approximate analytical studies of the burn-out of single coal particles within the framework of mathematical modeling was made.

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