Modelling of CWS combustion process

I A Rybenko and L A Ermakova
Siberian State Industrial University, 42 Kirova Street, Novokuznetsk, Russia, 654007
E-mail: ermakova@sibsiu.ru

Abstract. The paper considers the combustion process of coal water slurry (CWS) drops. The physico-chemical process scheme consisting of several independent parallel-sequential stages is offered. This scheme of drops combustion process is proved by the particle size distribution test and research stereomicroscopic analysis of combustion products. The results of mathematical modelling and optimization of stationary regimes of CWS combustion are provided. During modeling the problem of defining possible equilibrium composition of products, which can be obtained as a result of CWS combustion processes at different temperatures, is solved.

1. Introduction
In recent years, requirements to the quality of the energy supplies used in industry and in the housing and utilities infrastructure have significantly increased, which in turn led to the development of coal processing technology. As a result of the processing the fine wastes (fine particles of coal and mineral inclusions) are formed, which are placed into the piles polluting the environment.

An effective method of disposing waste coal is its combustion in the vortex adiabatic chamber in the form of CWS [1-3]. This approach to utilization allows the mined coal to be used for generation of heat and energy, and the ash produced is a good building material.

To develop CWS combustion technology in the vortex adiabatic chamber it is necessary to study the process of CWS drops combustion, as well as to solve the problem of modelling and optimization of static combustion modes of CWS in the vortex chamber.

2. Physico-chemical scheme of CWS drops combustion
Describing the process of CWS combustion it is necessary to consider the main differences between the process of ignition and burning of a slurry drop from the combustion of pulverized solid fuel. As the laboratory studies presented in [4-9] showed CWS drops combustion occurs simultaneously with the evaporation of moisture from its inner part, and evaporation of moisture does not slow down the carbon combustion process. The released vapor jets from the inner part of the drop activate the combustion on the drop surface, as a result of the simultaneous flow of these two processes, the suspension drop turns into a highly porous body [4]. To describe the combustion process of CWS drops the following physico-chemical process scheme consisting of several independent parallel-sequential stages can be offered:

- on the drop surface – instant heating and surface evaporation, low temperature activation of the fuel reaction surface prior to its ignition, combustion of coal microparticles on the drop surface;
- inside the drop – gradual drop heating, evaporation of moisture from the inner part of the drop, volatile yield and combustion of volatiles near CWS drop, transfer of coal microparticles to the drop
surface with the formation of a porous cenospheres (hollow spheres), combustion of coal microparticles as a result of chemical reaction with oxygen and vapour.

When the CWS drop gets into the hot combustion chamber its surface almost instantaneous gets heated and the moisture evaporation heating of the surface of the drops and the moisture evaporation from the drop surface. It is followed by the moisture evaporation from the inner part of the drop. The process of evaporation is described by the equation:

$$H_2O = \{H_2O\}. \quad (1)$$

As the temperature of the drop surface rises the pyrolysis of organic matter on the CWS drop surface begins, accompanied by the yield of volatile substances. With the temperature front advancing inside the drop the process of volatiles yield from the inner part of the drop starts. The basic equations describing the volatile yield are as follows:

$$CO_2 = \{CO_2\},$$

$$H_2 = \{H_2\},$$

$$CH_4 = \{CH_4\},$$

$$CO = \{CO\}. \quad (2)$$

The emitted flammable gaseous components react with oxygen [4]:

$$2[H_2] + [O_2] = 2[H_2O],$$

$$[CH_4] + 2[O_2] = [CO_2] + 2[H_2O],$$

$$2[CO] + [O_2] = 2[CO_2]. \quad (3)$$

Due to the water vapour, formed during the moisture evaporation from the surface, the low temperature activation of coal microparticles on the CWF drop surface occurs leading to their ignition, which results in a significant reduction in the CWS ignition temperature. In the process of volatiles combustion the heating of drops takes place and the coke residual of coal microparticles on its surface ignites. On the surface the combustion reactions take place due to the interaction of carbon with oxygen, water vapour and CO$_2$, obtained because of the volatiles yield, combustion of volatiles and coke base of fuel. Combustion reactions occur in accordance with the following reactions [4]:

$$C + [O_2] = [CO_2],$$

$$2C + [O_2] = 2[CO],$$

$$C + [CO_2] = 2[CO],$$

$$C + [H_2O] = [CO] + [H_2]. \quad (4)$$

The combustion process on the surface of CWS drop takes place in parallel with the processes of evaporation and volatiles yield from the depth of the drop. During the process of moisture evaporation and volatiles yield the coal microparticles move from the inner part of the drop to its surface [4], at the same time, water evaporation zone expands to the inner layers of a drop, thus, causing an increased pressure and enlargement of the drop size [4]. On the drop surface the carbon particles burn out, and the mineral part cokes forming a porous hollow sphere. Graphic scheme of the combustion stages of CWS drops is given in [10].

3. Particle size analysis of CWS and its combustion products

To conduct the study a laser analyzer of particle sizes Mastersiser 2000 (Malvern, UK) was used. Table 1 shows the results of experimental study on particle size distribution of CWS produced from
the waste coal at processing plant of mine “Antonovskaya” and two dust samples taken in the
vortex dust collector in the course of the experiment on CWS combustion in the vortex adiabatic
chamber.

**Table 1.** Particle size distributions of CWS and ash.

| Range of sizes, mm | CWS  | Ash (sample No.1) | Ash (sample No.2) |
|-------------------|------|-------------------|-------------------|
| 0.0000-0.0002     | 0    | 0                 | 0                 |
| 0.0002-0.0007     | 5    | 2.25              | 2.25              |
| 0.0007-0.0020     | 1    | 7.36              | 7.36              |
| 0.0020-0.0056     | 0    | 20.35             | 20.35             |
| 0.0056-0.0158     | 0.04478 | 33.65             | 33.65             |
| 0.0158-0.04478    | 0.12619 | 29.16             | 29.16             |
| 0.04478-0.3556    | 0.3566 | 6.47              | 6.47              |
| 0.3556-2.000      | 0    | 0                 | 0                 |

The estimate of the density distribution \( f(d) \) of particle by sizes on the basis of experimental data is performed in the class of regular distributions in the range \((d_{\text{min}}, d_{\text{max}})\) in the form of a lognormal distribution taking into account the minimum and maximum particle diameters \(d_{\text{min}}\) and \(d_{\text{max}}\):

\[
f(d) = \frac{\lambda (d_{\text{max}} - d_{\text{min}})}{(d_{\text{max}} - d)(d - d_{\text{min}})\sigma \sqrt{2\pi}} e^{-\frac{\left(\ln\left(\frac{d_{\text{max}}}{d_{\text{max}} - d}\right) - \ln a\right)^2}{2\sigma^2}},
\]

where \(\lambda, a\) – distribution parameters.

The specific form \(\hat{f}_m(d)\) is determined by the values of parameters \(\lambda^*, a^*\) and \(\sigma^*\), which minimize the functional:

\[
\Phi(\lambda^*, a^*, \sigma^*) = \min_{\lambda, a, \sigma} \sum_{i=1}^{N_f} \left( f(d_i) - S_i \right)^2,
\]

where \(N_f\) – number of fractions of the corresponding substance;

\(d_i\) – particle size in the i-th fraction, mm;

\(S_i\) – share of the i-th fraction%.

The obtained values of particle density distribution by sizes for CWS and products of its combustion are given in Table 2.

**Table 2.** Values of particle density distribution by sizes for CWS and ash.

| Material             | \(d_{\text{min}}\) mm | \(d_{\text{max}}\) mm | \(\lambda\) | \(a^*\)  | \(\sigma^*\) |
|---------------------|------------------------|------------------------|------------|----------|-------------|
| CWS                 | 0.00028                | 0.31698                | 0.611      | 2.555    | 1.177       |
| Ash (sample No. 1)  | 0.00448                | 0.63246                | 0.703      | 7.668    | 0.846       |
| Ash (sample No. 2)  | 0.00317                | 2.00000                | 1.701      | 8.194    | 1.011       |

Figure 1 shows the experimental data in the form of histograms of CWS and ash particles distribution by sizes and the resulting graph of density distribution in the form of equation (5). The particle sizes are arranged on a logarithmic scale.
Figure 1. Histograms of CWS and ash particles distribution by sizes: a – CWS; b – ash (sample No. 1); c – ash (sample No. 2).

Research of CWS combustion products. The chemical composition of ash, sampled in the vortex dust collector in the course of the experiment on the CWS combustion in the vortex adiabatic chamber, was defined by X-ray fluorescent analysis. For X-ray fluorescent analysis the scanning (single-channel) spectrometer XRF-1800 (Shimadzu, Japan) was used with the X-ray tube with Rhodium anode, voltage – 40 kV and current strength – 95 mA, calculating time for all elements – 552 seconds, the calculation method – method of fundamental parameters. Table 3 shows the component composition of ash.

For stereomicroscopic study of dust sampled in the vortex dust collector in the course of the experiment on CWS combustion in the vortex adiabatic chamber, the sample was dissolved in water and divided in it into 2 fractions. The heavy fraction 80-85% is located at the bottom of the assay cup, the light one floats to the surface of water. These fractions were separately investigated under the stereomicroscope with magnification from 20 to 300 times. All particles are well visible, of spherical type, or, more often, their fragments (Figure 2).

Table 3. Component composition of the ash, %.

| Sample No.          | C  | SiO₂ | Al₂O₃ | Fe₂O₃ | S  | CaO | K₂O | Na₂O | MgO | TiO₂ | P  |
|---------------------|----|------|-------|-------|----|-----|-----|------|-----|------|----|
| Ash (sample No. 1)  | 8.05 | 51   | 17.23 | 6.18  | 0.68 | 4.61 | 2.75 | 2.47 | 1.99 | 1.01 | 0.14 |
| Ash (sample No. 2)  | 5.47 | 53.7 | 18.38 | 5.23  | 0.62 | 4.59 | 2.85 | 2.47 | 2.25 | 0.94 | 0.18 |
The light part is composed of graphite particles and other mineral particles. The graphite particles form either whole hermetically closed micro spherulites or segmental fragments of these spherulites. Graphite is recrystallized, but the crystals are very small, except for spherical and hemispherical particles there are linearly stretched graphite particles. They represent an aggregate of plate micaceous crystals. The spherical shape of particles creates an impression about their significant predominance over other particles. The spherical graphite particles are shiny, black, have a proper shape of a sphere or elongated ovaloid, the spheres sizes are different from 2-3 micrometers to 100 micrometers.

The brownish-yellow particles are presented by silicate glass, colored by iron oxides. Large particles are agglomerate of glassy microsphaerolites. Medium and small isometric particles are larger microsphaerolite; they are more often represented by segment fragments. The silicate glass content in the ash reaches 48%, in the cyclone dust ranges from 3.5 to 35%.

The crystalline silica is represented mainly by crystobalite, more seldom α- and β-quartz; their total content ranges from 0.5 to 8.5%. The carbides and nitrides of silicon, aluminum and alkaline earth metals have a greenish-gray color and are about 1%. Especially there is much hollow graphite microsphaerolites in the dust. By volume, they represent in different samples from 5 to 35%, by weight from 2 to 18%. There are particles of an emerald-green color; and in the beginning they could not be seen, they appeared with the course of time. It was found that it is iron-copper sulfate (chalcanthite) due to the presence of calcium, iron and copper sulfides in a sufficient amount in the ash (about 2%).

These results agree well with the data [4] obtained while investigating the ash particles produced by combustion of dry dust and coal-water slurry from the same coal: during the slurry combustion the number of ash particles reduces, their sizes increases (from 0.01-0.05 to 0.5-1.5 mm) and the surface structure changes.

4. Mathematical modelling of stationary regimes of waste coal combustion in the adiabatic chamber
To solve the problems of modelling and optimization of static modes of CWS combustion in the vortex chamber a methodology and calculation system, based on the thermodynamic modeling, calculations of material and heat balances and solving optimization problems, was developed.

Thermodynamic modelling allows various tasks to be solved with the help of software “Terra” [10], which implements the principle of maximum entropy and thermodynamic analysis of co-occurrence in the system of possible chemical reactions on the basis of the calculation of changes in Gibbs energy and equilibrium constants.

At the stage of the calculation of the material and heat balances a flexible choice of a input and output parameters of the system is foreseen, taking into account the results obtained at the stage of thermodynamic modeling for the chosen type of process and the range of parameters; and it makes possible to obtain a mathematical description of the relationship of flows and process parameters, which are the basis for solving the optimization problem concerning the determination of the costs of materials at a selected optimization criteria and constraints.

In the thermodynamic modelling the process of CWS combustion in the vortex chamber was regarded as a complex thermodynamic system, which receives condensed (water coal fuel) and
gaseous (air) incoming flows; the final products are ash and gas. With the flows the following substances get into the reactor: condensed phase – C, O, H, N, P, As, HCl, SiO₂, Al₂O₃, Fe₂O₃, CaO, MgO, MnO, TiO₂, P₂O₅, S, K₂O, Na₂O, H₂O; gas phase – O₂, N₂. The elements constituting these compounds are: Fe, C, O, As, HCl, Mn, Si, S, P, Al, Ca, Mg, Na, K, H, Ti, N.

The mass balance equations were developed on the basis of the law of mass conservation with respect to the components of a heterogeneous system. The main feature of the calculation is the examination of the process in the form of a balanced system on three levels: flows, substances and elements:

\[
\sum_{k=1}^{K^f} G_k^f + \sum_{k=1}^{K^g} G_k^g = \sum_{l=1}^{L^f} G_l^f + G^g
\]

\[
\sum_{k=1}^{K^f} \sum_{l=1}^{N_k^f} \left( G_k^f / M_{E_k} \right) / 100 + \sum_{k=1}^{K^g} \sum_{l=1}^{N_k^g} \left( G_k^g / M_{E_k} \right) / 100 = \sum_{l=1}^{L^f} \sum_{n=1}^{N_l^f} \left( G_l^f / M_{E_l} \right) / 100 + \sum_{l=1}^{L^g} \sum_{n=1}^{N_l^g} \left( G_l^g / M_{E_l} \right) / 100 - x_m M_{E_l} + \sum_{n=1}^{N_l^g} G_l^g \{ E_m \} / M_{E_m}
\]

(7)

where 
\( K^f, K^g \) – number of condensed and gaseous flows;
\( G_k^f, G_k^g \) – mass consumption of condensed and gaseous flows, kg/s;
\( L^f \) – number of condensed output flows;
\( G_l^f, G_l^g \) – mass yield of the \( l \) condensed and gaseous flows, kg/s;
\( N_k^f, N_k^g \) – amount of substances in the \( k \) flow;
\( R_m, \{ R_m \} \) – substance content \( R_m \) in the \( k \) condensed and gaseous input flow, %.

\( l \) \( E_{i\alpha} \) \( E_{\beta} \) \( k \) \( E_{i\alpha} \) \( E_{\beta} \) \( E_{i\alpha} \) \( E_{\beta} \) – concentration of \( m \) substance containing element \( E_i \) in the condensed \( k \) input gaseous flow, %;

\( l \) \( E_{i\alpha} \) \( E_{\beta} \) \( l \) \( E_{i\alpha} \) \( E_{\beta} \) \( E_{i\alpha} \) \( E_{\beta} \) – concentration of \( n \) substance containing element \( E_i \) in \( l \) condensed or gaseous output flow, %;

\( N_k^f, N_k^g \) – amount of substances containing the element \( E_i \) in \( k \) condensed gaseous input flow, respectively;

\( N_l^f, N_l^g \) – amount of substances containing the element \( E_i \) in \( l \) condensed gaseous output flow; 

\( x_m, y_m, \alpha_m, \gamma_m \) – stoichiometric coefficients of \( m \) and \( n \) element compound \( E_i \);

\( M_{E_m}, M_{E_l} \) – molar mass of element \( E_i \) and its compound, kg/mol.

\[
\sum_{k=1}^{K^f} G_k^f \{ R_m \} / 100 \cdot \sum_{k=1}^{K^g} G_k^g \{ R_m \} / 100 = \sum_{l=1}^{L^f} G_l^f \{ R_m \} + G^g \Delta H^f + \sum_{l=1}^{L^g} \sum_{n=1}^{N_l^g} \left( G_l^g \{ E_m \} / 100 - \sum_{k=1}^{K^g} G_k^g \{ E_m \} / 100 \right) + Q_{in}
\]

(8)

The heat balance equations are constructed on the basis of energy conservation law. The main defining processes for the thermal state are the inflow and outflow of heat through the input and output
material flows; the heat exchange with the environment and chemical reactions with the appropriate thermal effects:

\[ \sum_{k=1}^{K} G_k^i \Delta H_k^i + \sum_{k=1}^{K} G_k^g \Delta H_k^g = \sum_{i=1}^{I} G_i^f \Delta H_i^f + G^g \Delta H^g + \sum \Delta H_{c.r.} + Q_{los}, \]  

(9)

where \( \Delta H_k^i \), \( \Delta H_k^g \) – enthalpy of a unit mass of \( k \) condensed or gaseous input flows with respect to the temperature 298 K, kJ/kg;

\( \Delta H_i^f \), \( \Delta H^g \) – enthalpy of a unit mass of \( l \)-ro condensed or gaseous output flows with respect to the temperature 298 K, kJ/kg;

\( Q_{los} \) – heat losses into to the environment, kJ;

\( \sum \Delta H_{c.r.} \) – total heat effect of chemical reactions, kJ.

Using the developed methodology and calculation system the calculations and studies of the CWS combustion process in the vortex chamber were performed.

The initial data for calculation were as follows: the calculation is made for the CWS consumption 1 tonne/h, moisture – 37%, ash content – 37.5%. The fuel combustion is carried out with the use of air. The chemical composition of the organic part of the sludge and are ash shown in Table 1.

| Organic part, % | C   | H   | N   | O   | P   | As  | Cl  |
|----------------|-----|-----|-----|-----|-----|-----|-----|
|                | 82.588 | 5.50 | 2.50 | 9.30 | 0.041 | 0.004 | 0.068 |

| Ash, % | SiO₂ | Al₂O₃ | Fe₂O₃ | CaO | MgO | TiO₂ | MnO | P₂O₅ | S   | Na₂O | K₂O |
|--------|------|-------|-------|-----|-----|------|-----|------|-----|------|------|
|        | 60.455 | 19.00 | 4.20  | 7.25 | 2.00 | 0.725 | 0.02 | 1.05  | 2.75 | 0.55  | 2.0  |

Tables 2 and 3 contain the calculated heat and material balances for CWS consumption 75 l/h (90 kg/h). The flue gas temperature at the given parameters is 1345 °C.

| Input flows | Consumption, kg/h | Output flows | Yield, kg/h |
|-------------|-------------------|--------------|-------------|
| CWS         | 90.000            | Gas          | 476.187     |
| Air         | 406.927           | Ash          | 20.740      |
| Total:      | 496.927           | Total:       | 496.927     |

| Input reactions | kg/h | MJ/kg | MJ/h | Consumption | kg/h | MJ/kg | MJ/h |
|-----------------|------|-------|------|-------------|------|-------|------|
| Exothermic      |      |       |      | Products enthalpy | | 827.3 | |
| \( C+1/2O₂=CO \) | 2.92 | 9.6   | 28.0 | Ash         | 20.7 | 1.6   | 33.1 |
| \( C+O₂=CO₂ \) | 26.3 | 33.1  | 873.6| Gas         | 476  | 1.7   | 794.2|
| \( H₂+1/2O₂=H₂O \) | 1.75 | 125.9 | 220.8| Endothermic reactions | | 182.9 | |
| Moisture evaporation | 33.3 | 5.5   | 182.9| Heat losses | 112.0 | |
| Residual error | 0.00% |       |      |             |      |       |      |
| TOTAL INPUT    | 1122.4 | TOTAL CONSUMPTION | 1122.4 | | | | |

Using the developed methods the combustion modes of CWS, produced from waste coal, were studied at various moisture values, ash content (Figure 3), CWS and air consumption rates.
5. Conclusions

Thus, the conducted particle size distribution analysis and stereomicroscopic study confirm that as a result of CWS combustion hollow spherical particles of larger sizes than the initial CWS are formed, which corresponds to the proposed CWS combustion process description above.

The mathematical modelling of stationary regimes of CWS combustion in the vortex chamber is carried out. The method of calculation of stationary CWS combustion regimes in the vortex chamber is developed, which is based on calculations of material and heat balances and solution of the optimization problem. With the use of the developed method and calculation system the the stationary modes of CWS combustion in the vortex chamber are calculated, the combustion process parameters are defined for various CWS characteristics (moisture, ash content). The mathematical modelling of CWS combustion at different consumption rates of CWS and air is performed.

References

[1] Sarychev V D, Kuksov I A et al 2012 Steel in Translation B 42 (8) 620–623
[2] Kuksov I A, Mochalov S P, Sarychev V D 2012 World Applied Sciences Journal B 19 (1) 100–105
[3] Mochalov S P, Rybenko I A et al 2012 Steel in Translation B 42 (8) 611–613
[4] Kantorovich B V and Delyagin G N 1962 Heat Mass Transfer 5 11
[5] Kobayashi H, Howard J B and Sarofim A F 1976 Proc. of the 18th Symp. on Combustion (Pittsburgh: Combustion Institute) p 411
[6] Smoot D J and Smith P J 1985 Coal Combustion and Gasification. The Plenum Chemical Engineering series, New York

[7] Kijo-Kleczkowska A 2011 Archives of Thermodynamics 32 (1) 45–75

[8] Dunn-Rankin D, Hoornstra J, Gruelich F A and Holve J 1987 Fuel 66 (8) 1139–45

[9] Murdoch P L, Pourkashanian M and William A 1985 Proc. of Symp. on Combustion 20 (1) 1409–18

[10] Mochalov S P, Rybenko I A and Ermakova L A 2012 World Applied Sciences Journal B 19 (1) 20–25

[11] Sinyarev G V et al 1982 Computer Application of Thermodynamic Calculations of Metallurgical Processes (M.: Nauka) p 263