Mechanism and Mathematical Modeling of Coal-Water Slurry Combustion in Swirl Adiabatic Combustion Chamber

Sergey Pavlovich Mochalov, Inna Anatolievna Rybenko and Ludmila Aleksandrovna Ermakova

Siberian State Industrial University, st. Kirova 42,
Kemerovo region, 654007, Novokuznetsk, Russia

Abstract: This paper presents the mechanism describing the process of burning of suspension water-coal fuel droplets. To solve the problems of modeling and optimization of static modes, method and system for calculating have been developed. The method is based on thermodynamic modeling, material and thermal balance calculation and solutions for optimization task. Using the method and system for calculating, a dynamic mathematical model of physico-chemical process in swirl burner for burning water-coal fuel was implemented.

Key words: Swirl adiabatic combustion chamber · Suspension coal-water fuel · Mathematical model · Combustion of fuels

INTRODUCTION

Currently coal enrichment as well as coal mining is rapidly developing that results in accumulation of fine waste which get in the dump and pollute the environment. One on the ways of waste coal utilization is to burn them in furnaces of various designs in the form of coal- water slurry (CWS) [1-3]. In this case the whole amount of coal is used for its intended purpose and the ash forming in the process of combustion is a good building material.

To develop the technology of CWS combustion in swirl adiabatic combustion chamber it is necessary to study the mechanism of coal-water slurry drops combustion and to develop the method and system for calculating CWS combustion using thermodynamic and mathematical modeling.

Mechanism of Coal-water Fuel Combustion: When studying coal-water fuel combustion, in a number of works [4-9] they revealed the differences in inflammation and combustion processes of slurry drops caused by powdered solid fuel combustion that should be taken into account while describing CWS combustion. To describe the process of CWS drops combustion the following physico-chemical model consisting of several independent parallel-serial stages can be suggested (Picture1)

- *On the drop surface* - instant heat and moisture evaporation from the surface, low-temperature activation of reaction surface of the fuel before the combustion, coal micro particle combustion on the surface of the drop;

- *Inside the drop* - gradual heat of the drop, moisture evaporation from the interior of the drop, devolatilization and combustion of volatiles near the CWS drop, coal micro particles transfer to the drop surface with formation of hollow sphere, coal micro particles combustion in chemical reaction with air oxygen and water vapor;

When a CWS drop gets in a hot combustion chamber there is immediate warm-up of the drop surface and water evaporation from the drop surface. Inside the drop there is gradual warming and as the temperature is increasing the moisture evaporates from the interior of the drop. The process of water evaporation can be described by the following equation:
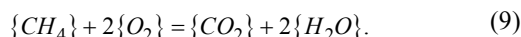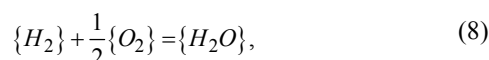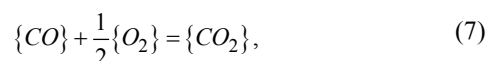
$$H_2O = \{H_2O\}. \tag{1}$$

With the temperature increasing there is the process of thermal destruction (pyrolysis) of organic matter on the surface of CWS drop, accompanied by release of volatile substances. As the thermal front penetrates deep into the

Corresponding Author: Sergey Pavlovich Mochalov, Siberian State Industrial University,
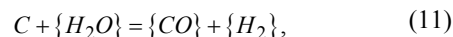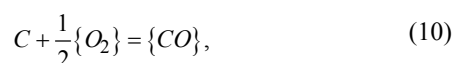st. Kirova 42, Kemerovo region, 654007, Novokuznetsk, Russia.

drop the release of volatile substances from the interior of the drop begins. These are the following equations describing the release of volatile substances:

$$CO = \{CO\}, \tag{2}$$
$$CO_2 = \{CO_2\}, \tag{3}$$
$$CH_4 = \{CH_4\} \tag{4}$$
$$H_2 = \{H_2\} \tag{5}$$
$$N_2 = \{N_2\} \tag{6}$$

Escaping combustible gaseous components react with air oxygen:

$$\{CO\} + \frac{1}{2}\{O_2\} = \{CO_2\}, \tag{7}$$

$$\{H_2\} + \frac{1}{2}\{O_2\} = \{H_2O\}, \tag{8}$$

$$\{CH_4\} + 2\{O_2\} = \{CO_2\} + 2\{H_2O\}. \tag{9}$$

Because of water vapor generating as the result of water evaporation from the surface there is low-temperature activation of coal micro particles on the surface of CWS drop before its combustion that leads to substantial temperature drop of CWS combustion. In the process of volatiles combustions the surface of the drop gets warm and carbon residue of coal micro particles combusts on the drop surface. On the surface there are combustion reactions due to the interaction of carbon with air oxygen, water vapor and CO_2 obtained from volatiles release and partial volatiles and coke base combustion. Combustion can be described by following reactions:

$$C + \frac{1}{2}\{O_2\} = \{CO\}, \tag{10}$$

$$C + \{H_2O\} = \{CO\} + \{H_2\}, \tag{11}$$

$$C + \{O_2\} = \{CO_2\}, \tag{12}$$

$$C + \{CO_2\} = 2\{CO\}. \tag{13}$$

The process of combustion the surface of CWS drop takes place in parallel with the processes of water evaporation and release of volatile substances from the interior of the drop. In the processes of water evaporation and release of volatile substances coal micro particles transfer from drop interior to its surface resulting in CWS drop transformation into hollow sphere.

The suggested process model is proved by results of study of the ash taken from swirl combustion chamber after CWS combustion. Stereomicroscopis study showed that the ash corresponds to hollow spherical particles or fragments of spherical particles that fully corresponds to the mechanism described above. The given physicochemical scheme of combustion of coal-water slurry (CWS) drops is used at process modelling of suspension coal fuel combustion in the swirl combustion chamber.

Modelling and Optimization of Static Modes of Coal-Water Slurry (CWS) Combustion: It presupposes the development of the method and system for calculating, based on thermodynamic modelling, calculations of material and thermal balances and the solution of the problem of optimization.

Methods of thermodynamic modelling are applied for an assessment of process course conditions, ranges of variation and structure of phases of output streams. The calculations realized with use of a program complex «TERRA», developed in Moscow State Technical University n.a. N.E. Bauman [10], allowed to estimate maximum equilibrium concentration of components of a gas phase for adjustment of factors and parameters of the process at material and thermal balances calculation of coal-water fuel combustion.

The mathematical formulation of parameter correlation of streams and process is received as a result of a finding of the basic parities of material and thermal balances.

The solution to the problem of optimization consists in the determination of materials compulsion at the set criterion of optimization and restrictions.

Comparison of modelling results of each stage to laboratory findings of experiments is provided.

The equations of material balance were built on the basis of mass conservation law concerning components of heterogeneous system [2].

By model definition combustion chamber and combustion were considered in following approximation:

- Two input streams inflow into the combustion chamber;
- Coal fuel slurry, consisting of inorganic matter, ashes, moisture and effluent gases, inflows with the first input stream;
- Air inflows with the second input stream;
- The heterogeneous mixture in combustion space consists of two phases: condensed and gas one;

- All the components of an inorganic matter of fuel do not participate in the combustion and make up an oxide phase; the output of ashes will be defined by mass of all oxide of the cindery part, inflowing into the combustion chamber in unit of time;
- The effluent gases composition is calculated according to the conditions of reaction course of organic carbon oxidation, devolatilization, coal-volatile matter combustion and moisture evaporations.

By the derivation of an equation of thermal balance it is accepted, that the basic defining processes for a thermal condition are: moisture evaporation (1); reactions of allocation and combustion of volatile components (2-9); chemical reactions of organic carbon combustion (10, 12); reactions of interaction of carbon with CO_2 and H_2O, consumption of ashes and gas heating and heat exchange with an environment. The equations of thermal balance are built on the basis of the law of conservation of energy $Q_{in} = Q_{out}$.

Calculation of material and thermal balances is realized in EXCEL Environment by the use of built-in optimizer for evaluation of air consumption spent on combustion and calculation of the derived temperature.
The dynamic mathematical model of physical-chemical processes in the swirl combustion chamber during the coal-water combustion is developed with use of the method and system for calculating stationary modes of coal-water slurry combustion (CWS).

Physical-chemical processes, proceeding during suspension coal fuel combustion can de presented in the form of reactions (1-13).

By the formation of the differential equations of dynamics of structure variation of a gas phase in the combustion chamber it is accepted, that variation of volume concentration of i substance inside combustion space is defined by rate of delivery of the given substance into the unit, variation of concentration inside of volume as a result of course of chemical reactions and rate of substance abstraction with effluent gases from the combustion chamber.

$$\frac{dn^{vol}_i}{d\tau} = \dot{n}^{in}_i / V - \sum W_i - \upsilon_{gas} \cdot \dot{n}^{vol}_i \qquad (14)$$

Where n^{vol}_i - volume concentration of *i* substance inside of combustion chamber, mole/m³•s;

$\dot{n}^{in}_i$ = Income of *i* substance with input stream, mole/s;

V = Volume of combustion chamber, m³;

ΣW_i = Total rate of all chemical transformations of *i* substance in unit of volume, mole/m³•s;

υ_{gas} = Rate of gas output stream, m³/s.

Variation of concentration of substances in volume of combustion chamber in unit time as a result of chemical transformations is defined by a difference of rates of formation and consumption of these substances as a result of course of all chemical reactions (1-13):

$$\frac{dn_{\{CO_2\}}}{d\tau} = W_3 + W_7 + W_9 + W_{12} - W_{13}; \qquad \frac{dn_{\{H_2\}}}{d\tau} = W_5 - W_8 + W_{11};$$

$$\frac{dn_{\{CO\}}}{d\tau} = W_2 + W_{10} - W_7 + W_{11} + 2W_{13}; \qquad \frac{dn_{\{H_2O\}}}{d\tau} = W_1 + W_8 + 2W_9 - W_{11};$$

$$\frac{dn_C}{d\tau} = -W_{10} - W_{11} - W_{12} - W_{13}; \qquad \frac{dn_{\{CH_4\}}}{d\tau} = W_4 - W_9;$$

$$\frac{dn_{\{O_2\}}}{d\tau} = -0.5W_7 - 0.5W_8 - 2W_9 - 0.5W_{10} - W_{12}; \qquad \frac{dn_{\{N_2\}}}{d\tau} = W_6;$$

$$\frac{dn_{H_2O}}{d\tau} = -W_1, \qquad\qquad (15)$$

where W_1-W_{13} - rates of chemical reactions (1-13).

Subject to the equations (14) and (15) we get differential equation system of structure variation of a gas phase during the time inside the combustion chamber as a result of suspension coal-water fuel combustion.

The thermal balance equation of suspension coal-water fuel combustion action is:

$$\frac{dQ}{d\tau} = -\sum_{i=1}^{13} \Delta H^0_i k_i n^{vol}_i - \dot{Q}_{loss} - \dot{Q}_{gas} \qquad (16)$$

Where

ΔH^0_i = Thermal effect of *i* chemical reaction (1-13), Kilojoule/mole;

k_i = Rate constant of *i* chemical reaction (1-13);

$\dot{Q}_{loss}$ = Heat loss in an environment, Kilojoule/s;

$\dot{Q}_{gas}$ = Heat content of output stream, Kilojoule/s.

$$\dot{Q}_{gas} = \upsilon_{gas} \rho_{gas} C_{P gas}(t - t_0) \qquad (17)$$

Where

ρ_{gas} = Density of effluent gas, kg/m³;

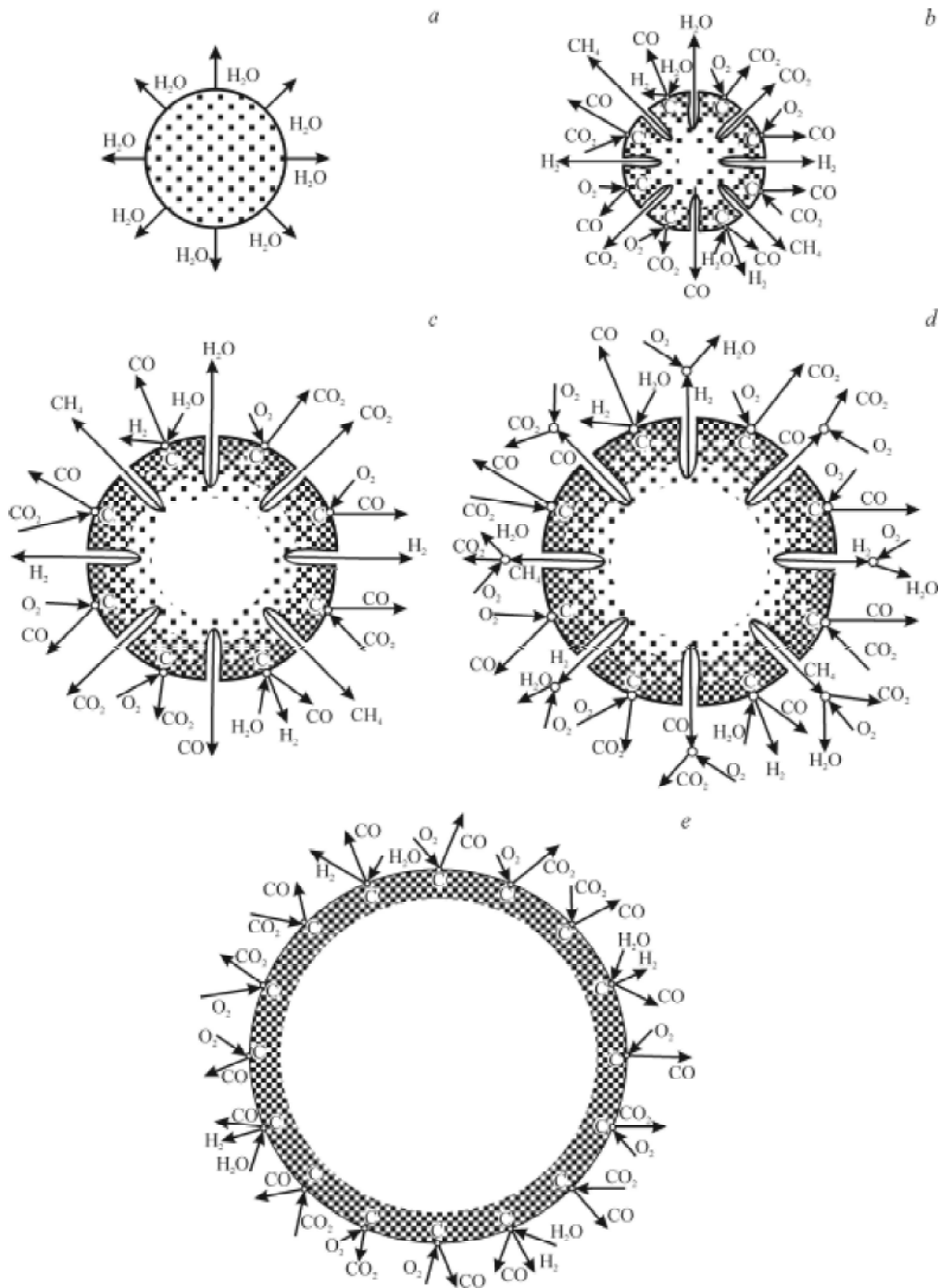$C_{p\,gas}$ = Heat capacity of effluent gas, Kilojoule/mole •degree;

Fig. 1: Physicochemical model of coal-water slurry combustion:
  a. moisture evaporation from the surface of the coal-water slurry drop;
  b. coal micro particle combustion on the surface of the coal-water slurry drop, moisture evaporation from the interior of the drop;
  d. coal micro particle combustion on the surface of the coal-water slurry drop, devolatilization from the interior of the drop;
  d. coal micro particle combustion on the surface of the coal-water slurry drop, coal-volatile matter combustion;
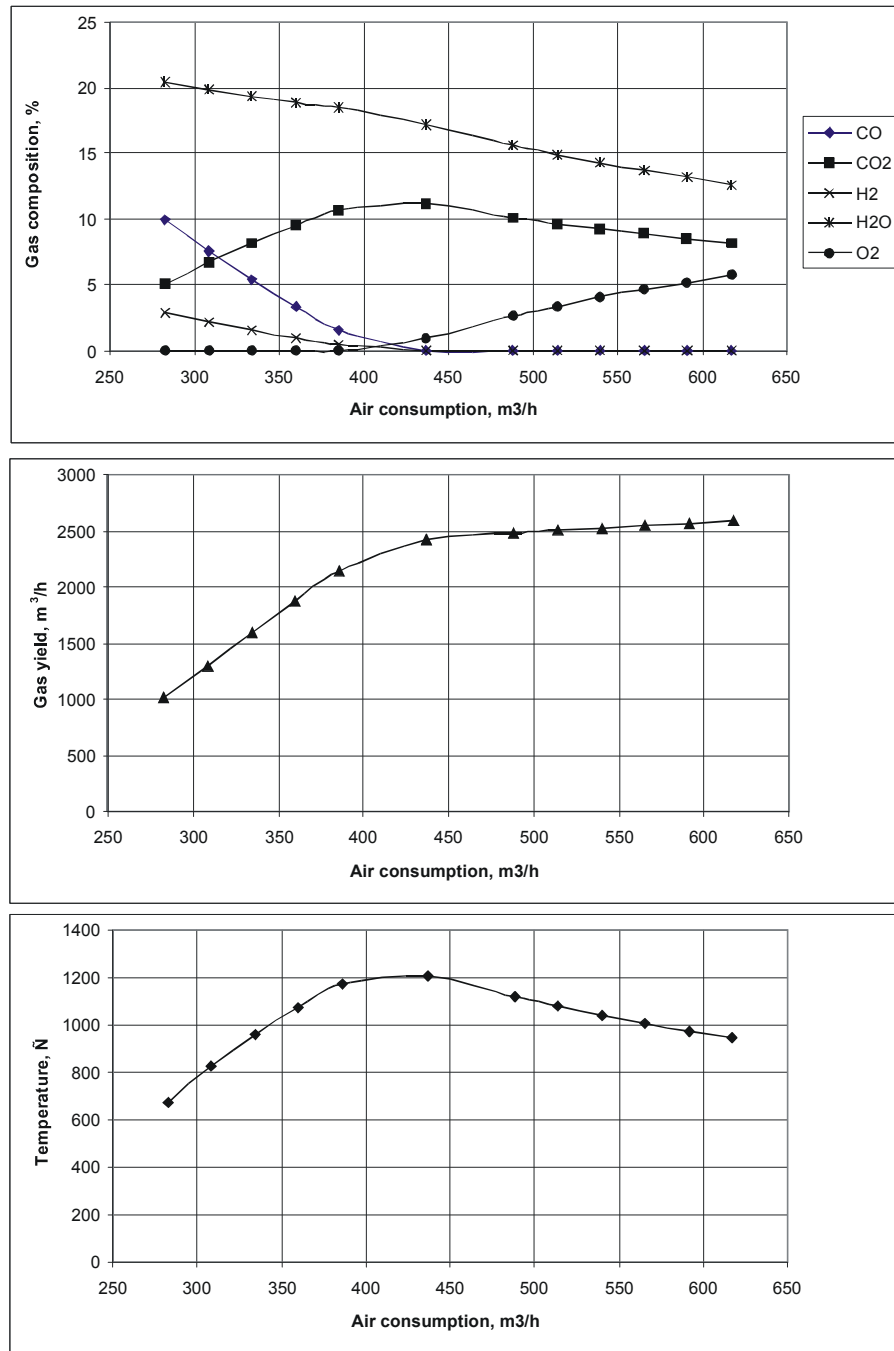   e - coal micro particle combustion

Fig. 2 - Dependences of parameters of suspension coal fuel combustion action on air consumption

The left part of the thermal balance equation represents the heat assimilation speed in swirl adiabatic combustion chamber, the right part includes total heat absorption (evolution) at the course of all chemical reactions connected with substances transformation, speed of heat loss in an environment and speed of heat ablation with effluent gases.

The developed mathematical model can be used in combustion modes development and creation of control systems of the automated energy-generating complexes.

The purpose of researching and optimization of the modes of coal-water slurry (CWS) combustion

The parameters of suspension coal fuel combustion have been calculated with the application of the method and system for calculating stationary modes at various air consumption for base coal-water slurry (CWS) consumption of 90 kg/h (75 l/h) at ash content of 32,3% and humidity of 39,2%. Air consumption was changed within the limits from 283 up to 617 m^3/h. The results of calculations are presented in picture 2. With the increase of air consumption from 283 up to 437 m^3/h *CO* remains in a gas phase. The temperature increases from 676 up to 1205 °C, the further increase of air consumption leads to full *CO* afterburning, in a gas phase oxygen starts to appear, the temperature of effluent gases drops to 947 °C.

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REFERENCES

1. Miller, S.F., 1996. The effect of cojiring coal-water slurry firel formulated from waste coal fines with pulverized coal on NO, emissions / S.F. Miller, J.L. Morrison, A.W. Scaroni // In 21st International Technical Conference on Coal Utilization & Fuel Systems. Clearwater, FL: Coal Water Slurry Association, Washington, D.C.

2. Development of scientific and technical bases for the formation of technology of preparation and combustion of suspension coal fuel prepared on the basis of waste coal and the pilot sample of the automated energy-generating complex. Research record, Stage 3. SibSIU, Novokuznetsk. 2011.

3. Murko, V.I., 2011. The development of heat-generators for combustion of coal-water slurry from waste coal / V.I. Murco, V.I. Fedyaev, V.I. Karpenuk // Clean Coal Technology, 17(6): 111-113.

4. Kantorovich, B.V., 1962. Heat and Mass Transifer in the Process of Fuel Combustion in Air Stream / B.V Kantorovich. G.N. Delyagin. - Int. J/ Heat Mass. Transfer, pp: 5-11.

5. Kobayashi, H., 1976. Coal Devolatilization at High Temperatures / H. Kobayashi, J.B. Howard, A.F. Sarofim // 18th Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, PA, pp: 411.

6. Smoot, D.J., 1985. Coal Combustion and Gasification / D.J. Smoot, P.J. Smith // The Plenum Chemical Engineering series, New York.

7. Kijo-Kleczkowska, A., 2011. Analysis of cyclic combustion of the coal-water suspension / A. Kijo-Kleczkowska // Archives of Thermodynamics, 32(1): 45-75.

8. Dunn-Rankin, D., J. Hoornstra, F.A. Gruelich and J. Holve, 1987. Combustion of coal-water slurries. Evolution of particle size distribution for coals of different rank. Fuel, 66: 1139-1145.

9. Patricia, L., M. Murdoch, Pourkashanian and Alan William, 1985. The mechanism of combustion of coal-water slurries Original Research Article Symposium (International) on Combustion, 20(1): 1409-1418 .

10. Sinyarev, G.V., N.A. Vatolin, B.G. Trusov and G.K. Moiseev, 1982. Computer application for thermodynamic calculation of metallurgical processing. M.: Nauka: pp: 263.