STEAM BOILERS, POWER-PLANT FUELS, BURNER UNITS, AND BOILER AUXILIARY EQUIPMENT

Numerically Simulating the Parameters of Submicron Particles Generated in Coals Burning

N. M. Kortsenshteyn[a], * and L. V. Petrov[a, b]

[a]*Krzhizhanovskii Power Engineering Institute, Moscow, 119071 Russia*
[b]*National Research University Moscow Power Engineering Institute, Moscow, 111250 Russia*
*e-mail: naumkor@yandex.ru

Abstract—Bulk condensation of substance vapors releasing from the mineral part of coals in burning them is regarded to be the possible mechanism through which environmentally dangerous submicron particles are generated. The possibility of certain toxic microelements contained in coals to condense on the surface of particles is an additional negative factor associated with the generation of particles during coal combustion. To set up a particle trapping process that would make it possible to decrease the emission of submicron particles into the atmosphere in burning coals, information on the parameters of condensation aerosols generated during the combustion is necessary. The required data, in particular about the concentration of particles and their distribution by sizes, can be obtained through numerically simulating the bulk condensation process. A condensation model describing the generation of submicron particles of potassium and sodium sulfate in burning coals is proposed. The proposed model is based on applying a combined approach (involving the use of thermodynamic and kinetic analysis) to describing the bulk condensation process in the coal combustion products. It is assumed that the generation of potassium and sodium aluminosilicates in the volume of a burning coal particles "freezes" after the particle burning process terminates and the particle temperature decreases; part of potassium and sodium in the composition of aluminosilicates is removed from the combustion products with slag and fly ash, and the other part that was not included in the aluminosilicates remains in the gaseous phase and forms sulfate condensation aerosol as the temperature decreases. The proposed model implemented by means of software was used to numerically simulate the bulk condensation of potassium sulfate vapors in the coal combustion products as they are cooled in the process path. Data on the concentration of the generated particles and on their distribution by sizes are obtained. The calculated and experimental data on the fractional composition of particles are compared with each other.

Keywords: coal combustion, combustion products, bulk condensation, submicron particles, numerical simulation

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Combustion of coals in the furnaces of boilers entails, among other processes, bulk condensation of vapors of different substances released from the mineral part of coals, as a result of which submicron particles are generated, which is known as the solid–vapor–particulate pathway [1, 2]. The existing limitations (including those specified by the regulations in the United States) on the concentration of submicron particles in the air medium stem from their hazard to the environment, as is evident from the data of [3]. In view of this circumstance, the United States national standard on the surrounding air quality [4] stipulates limitations on the concentration of class $PM_{2.5}$ particles in the air, i.e., particles smaller than 2.5 μm in size. Since 2015, the content of class $PM_{2.5}$ particles suspended in the surrounding air is also subject to monitoring in Russia [5]. The fact that certain toxic microelements contained in coals can condense on the surface of particles generated during coal combustion is an additional negative feature associated with the generation of these particles [6–9].

To decrease the emissions of submicron particles into the atmosphere by trapping them, it is necessary to know the parameters of condensation aerosols generated during coal combustion. Information about the concentration of particles and their distribution by sizes can be obtained through numerically simulating the bulk condensation process. As far as the coal combustion products are concerned, which constitute a multicomponent reacting system, it is worthwhile to use a comprehensive thermodynamic and kinetic approach in modeling such a system [10]. At the first stage, equilibrium compositions of the gaseous and condensed phases and the sequence in which different substances condense as the temperature of combustion products decreases along the process flow path

Table 1. Temperatures (K) at which potassium and sodium compounds contained in the combustion products of the considered coals transfer into the condensed phase without (w/o) and with (w) taking into account potassium and sodium aluminosilicates without the "freezing" phenomenon [11]

No.	Coal	Potassium		Sodium	
		w	w/o	w	w/o
1	Krasnoyarskugol', Berezovo open-pit mine, RF)	1250	1250	1300	1050
2	Kuznetsk coal basin, CC2CCPOKI, RF	2650	1400	1850	1150
3	Kuznetsk coal basin, Mokhovo open-pit mine, RF	1850	1350	1600	1100
4	Kuznetsk coal basin, Mokhovo open-pit mine, RF	1600	1250	1650	1100
5	Pechora coal basin, Vorkuta mine, RF	2800	1400	1950	1150
6	Moscow coal region basin, Novomoskovsk mine, RF	2600	1350	1700	1050
7	Khabarovsk krai, Urgal coal field, RF	2700	1300	2000	1100
8	Chukotka, Bukhta Ugol'naya coal field, RF	2550	1350	1850	1150
9	Republic of Sakha, Neryungri coal field, RF	2550	1300	1800	1100
10	Donetsk coal field, SSh anthracite culm, Ukraine	2800	1500	1950	1350
11	Ekibastuz coal field, Kazakhstan	2800	1400	1850	1100
12	Yanzhou, PRC	1300	1300	1300	1050
13	YZLS, PRC	2050	1350	1600	1050
14	Baotou, PRC	1800	1300	1550	1050
15	Wangfg, PRC	2400	1300	1700	1050

are determined using chemical thermodynamics methods. At the second stage, the sought condensation aerosol parameters are determined by solving the bulk condensation kinetic equation taking into account the thermodynamic analysis results. In so doing, conservation of thermodynamic equilibrium in the gaseous phase is adopted as an assumption.

In [11], the results from the first (thermodynamic) stage of a study carried out for 15 kinds of power-generating coals from different fields in Russia, Ukraine, and the People's Republic of China (PRC) are presented. In studying the mechanism through which a highly dispersed fly ash is generated, it is of interest to investigate the behavior of substances that evaporate at furnace temperatures during coal combustion and that can subsequently transform into submicron fly ash particles in the course of bulk condensation as they cool down. Potassium and sodium are the most volatile ash forming coal elements. Therefore, it is particularly these elements that were chosen to carry out the thermodynamic analysis aimed at studying how the vapors of these elements and their compounds are generated and condensed during the combustion of coals. It should be pointed out that the considered coals are characterized by a wide range of composition. In particular, the contents of ash, sulfur, potassium, and sodium vary in the ranges 5.75–48%, 0.3–6.5%, 0.4–3.5%, and 0.2–1.9%, respectively.

It has been found from the thermodynamic analysis results [11] summarized in Table 1 that, with taking aluminosilicates into account, the gaseous phase may contain a noticeable quantity of potassium and sodium compounds only at temperatures above those typically existing in furnaces. Hence, their bulk condensation from the combustion products is impossible (except with coal nos. 1 and 12).

In view of the obtained results, the second (kinetic) stage of the analysis aimed at determining the parameters of condensation aerosols in the coal combustion products was carried out in [10] under the assumption that potassium and sodium aluminosilicates are not generated. At the same time, the experimental data obtained in [2] for part of coals considered in [10] show that the particles generated during coal combustion are characterized by a bimodal distribution of their sizes: the fraction 0.06 μm in diameter (of the condensation origin) is represented by alkali metal sulfates, and the fraction 1 μm in size (of an origin other than condensation) is represented by aluminosilicates. Thus, a model more realistic than that used in [10] must take into account the generation of aluminosilicates.

THERMODYNAMIC PRINCIPLES OF THE MODEL DESCRIBING GENERATION OF HIGHLY DISPERSED PARTICLES

The basic assumption adopted in the new model is that the interaction of potassium and sodium with silicon and aluminum to produce aluminosilicates in the volume of a burning coal particle "freezes" after the particle burning process is over and the particle temperature decreases. The potassium and sodium that have produced aluminosilicates are removed from the

combustion products with slag and fly ash. The potassium and sodium evaporated during the particle burning process, which have not produced aluminosilicates, remain in the gaseous phase of combustion products and condense in the form of sulfates as the temperature decreases. Hence, the equilibrium composition of combustion products at a temperature below the "freezing" temperature (denoted as T_{fr}) must be calculated at a decreased (as compared with that in the initial coal) content of potassium, sodium, silicon, and aluminum. The value by which their content must be decreased is equal to the calculated content of potassium and sodium in the aluminosilicates of the condensed phase of initial coal combustion products at the temperature equal to T_{fr}. To estimate the effect that the uncertainty in selecting the T_{fr} value has on the calculation results, two values of temperature equal to 1700 and 1900 K were used. This temperature range belongs to the temperature variation region 1350−1700°C of a truly liquid state of slag from coal nos. 1−11 presented in Table 1 [12]. Similar data for coal nos. 12−15 were not known to us.

The compositions of coal combustion products as a function of temperature were calculated using the TETRAN-PRO computer program developed at Krzhizhanovskii Power Engineering Institute (ENIN) (computer program state registration certificate no. 2016663354). The necessary data on the thermodynamic properties of individual substances were obtained from [13−15]. In all, 194 substances formed from 14 atoms were considered in the calculations. The calculations were carried out with due regard to the information presented in [16] for a four-phase system containing one gaseous phase and three condensed phases. The condensed phases included an ideal solution of substances containing potassium, an ideal solution of substances containing sodium, and an ideal solution of substances not containing potassium or sodium.

The concentrations of potassium and sodium sulfates in the gaseous phase of Kuznetsk coal combustion products (no. 2 in Table 1) calculated according to the new model taking into account the generation of aluminosilicates and "freezing" are shown in Fig. 1 (the calculation results obtained for all coals considered in the study are similar in nature). For comparison purposes, these figures show similar data from [11], in which the "freezing" was not taken into account. It can be seen that the results obtained in [11] indicate the minimal and maximal values—with and without taking into account the generation of aluminosilicates, respectively—of condensing component concentrations in the gaseous phase.

The "freezing" considered in this study facilitates an increase in the content of potassium and sodium sulfates in the gaseous phase by four to five orders of magnitude as compared with the data obtained taking aluminum silicates into account but without "freez-
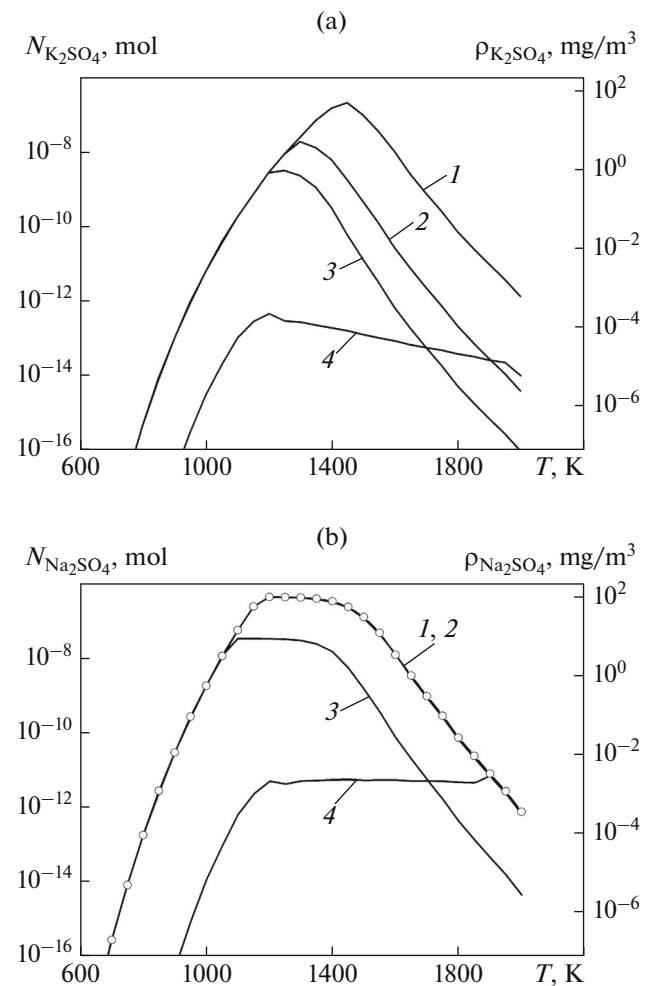

Fig. 1. Concentration of (a) potassium sulfate and (b) sodium sulfate in the products from combustion of coal no. 2: *1*—Without taking into account aluminosilicates [11]; *2* (points)—with taking into account the generation of aluminosilicates and "freezing" at T_{fr} = 1900 K; *3*—with taking into account the generation of aluminosilicates and "freezing" at T_{fr} = 1700 K; and *4*—with taking into account the generation of aluminosilicates but without "freezing" [11].

ing." It should be pointed out that a growth of T_{fr} results in higher concentrations of condensing substances in the gaseous phase. In particular, sodium is not bound in aluminum silicates for some of the considered coals at T_{fr} = 1900 K (including coal no. 2); this is why curves *1* and *2* coincide with each other (see Fig. 1b). Nonetheless, the increased values of potassium sulfate concentrations remain an order or two lower than the values obtained without taking into account aluminosilicates at all. On the whole, the data of [10] obtained without taking the generation of aluminosilicates can be regarded as an assessment of the maximal content of condensing aerosols in the coal combustion products.

The temperatures at which potassium and sodium sulfates transfer into the gaseous phase obtained for

Table 2. Temperatures (K) at which potassium and sodium compounds contained in the combustion products of the considered coals transfer into the condensed phase evaluated taking into account the generation of potassium and sodium aluminosilicates and the "freezing" phenomenon at two values of T_{fr}

Coal	Potassium at T_{fr}, K		Sodium at T_{fr}, K	
	1700	1900	1700	1900
1	1250	1250	1050	1050
2	1200	1250	1050	1150
3	1250	1350	1100	1050
4	1250	1300	1100	1100
5	1100	1250	1050	1100
6	1200	1300	1050	1050
7	1100	1200	1000	1050
8	1150	1250	1050	1050
9	1200	1250	1050	1100
10	1150	1250	1050	1100
11	1150	1250	1000	1100
12	1250	1300	1050	1050
13	1200	1300	1050	1050
14	1200	1300	1050	1050
15	1200	1250	1050	1100

two values of T_{fr} according to the algorithm described above are given in Table 2. It can be seen that the transition temperatures are noticeably lower than the temperature of combustion products in the combustion zone. Hence, potassium and sodium compounds may
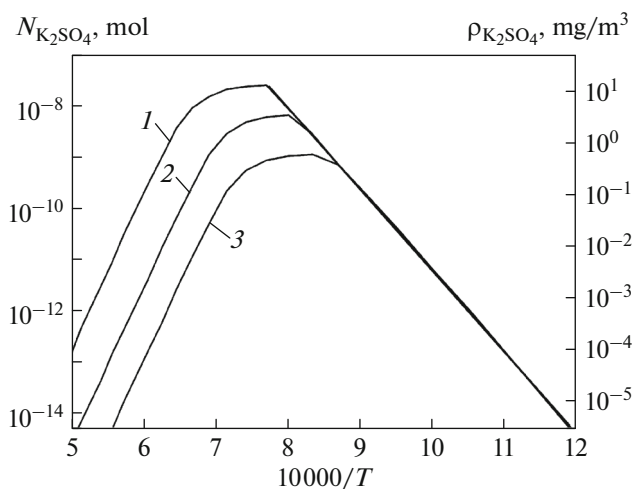

Fig. 2. Temperature dependence of the number of moles and mass concentration of potassium sulfate in the gaseous phase of the products from combusting the considered coals. Coals: *1*—no. 12; *2*—no. 6; *3*—no. 10.

undergo bulk condensation. It is also seen that the transition temperature for potassium sulfate is higher than it is for sodium sulfate. It can be supposed—similar to the way it is done in [10]—that, during the cooling of the combustion products, condensation nuclei will emerge from potassium sulfate, on which sodium sulfate will subsequently condense.

An excess of partial pressure of the condensing component over the equilibrium value at a given temperature, which is characterized by the supersaturation ratio, is the condensation motive force. In application to the considered case, the expression for supersaturation ratio can be written as follows:

$$s = N_{K_2SO_4} \big/ N_{K_2SO_4}^s . \qquad (1)$$

In formula (1), $N_{K_2SO_4}$ is the current number of potassium sulfate moles in the gaseous phase corresponding to one-phase thermodynamic equilibrium (with "frozen" condensation) in the gaseous phase (an analog of partial steam pressure), and $N_{K_2SO_4}^s$ is the number of potassium sulfate moles in the gaseous phase corresponding to two-phase thermodynamic equilibrium in the system (an analog of saturated vapor pressure). It should be pointed out that expressions (1)−(5) (see below) written for potassium sulfate also hold for sodium sulfate.

The calculated data on potassium sulfate concentration in the gaseous phase of products from combustion of some coals (nos. 6, 10, 12) are shown in Fig. 2. The calculation results obtained for other coals are similar in nature: in the two-phase equilibrium region, they lie on a common curve typical for the saturated vapor pressure temperature dependence.

Temperature approximations of the following form were obtained for the denominator of (1) based on the abovementioned data

$$\log N^s = A^s - B^s \big/ T . \qquad (2)$$

In formula (2), N^s is the number of potassium sulfate moles in the combustion product's gaseous phase in the state of two-phase equilibrium; A^s (dimensionless) and B^s, K are the approximation coefficients; and T is temperature, K.

For determining the numerator of (1), we wrote a system of two equations (for the mass action law and the material balance) for the main potassium containing components in the gaseous phase (KOH and K_2SO_4) with the "frozen" condensation in the temperature region of interest:

$$\left.\begin{array}{r} N_{K_2SO_4} \big/ N_{KOH}^2 = K_{eq}; \\ 2N_{K_2SO_4} + N_{KOH} = \Sigma_K, \end{array}\right\} \qquad (3)$$

where

$$\Sigma_K = N_K^0 - \Delta N_K.$$

The analytic solution of equation system (3) is given by

$$N_{K_2SO_4} = \left(\sqrt{1 + 8\Sigma_K} - 1\right)^2 \Big/ \left(16K_{eq}\right). \qquad (4)$$

In expression (4), N_K^0 is the concentration of potassium in coal, ΔN_K is the loss of potassium from the gaseous phase due to condensation, which is determined at each step in the course of numerically solving the bulk condensation kinetic equation (see below), and K_{eq} is the equilibrium constant for the potassium sulfate generation reaction in the gaseous phase of combustion products, mol^{-1}.

The equilibrium constant temperature dependence for all considered coals was approximated, based on the calculated data, by two-term polynomials of the form

$$\log K_{eq} = A + B/T, \qquad (5)$$

where A (dimensionless) and B, K are the approximation coefficients, which have different values for each coal.

The results obtained in the form of correlations (2), (4), and (5) form the thermodynamic basis for the model describing the generation of highly dispersed particles of a condensing origin during coal combustion, which takes into account the generation of aluminum silicates when there is "freezing."

KINETIC ANALYSIS

In accordance with the approach widely encountered in the literature, we used the following kinetic equation for the droplet (particle) size distribution function in modeling the volume condensation of potassium sulfate from the coal combustion products [17]:

$$u\frac{\partial f}{\partial x} + \frac{\partial(\dot{r}f)}{\partial r} = \frac{I}{\rho_\Sigma}\delta(r - r_{cr}), \qquad (6)$$

where f is the mass function of droplet size distribution normalized for the number of droplets per unit mass of vapor–gas–droplet mixture, m^{-1} kg^{-1}; u is the flow velocity, m/s; x is the coordinate along the flow axis, m; r is the droplet radius, m; $\dot{r}$ is the droplet size growth rate, m/s; I is the nucleation rate, m^{-3} s^{-1}; ρ_Σ is the vapor–gas–droplet mixture density, kg/m^3; δ is the Dirac delta function; and r_{cr} is the droplet critical radius determining the minimal size of viable droplets generated during nucleation, m.

Subject to the condition that the size of generated droplets is much smaller than the mean three path of gas molecules, equation (6) can successfully be solved using the method of moments, the application of which makes it possible to obtain the system of moment equations equivalent to (6) for the first four moments of the distribution function [17]:

$$\frac{d\Omega_n}{dx} = n\frac{\dot{r}}{u}\Omega_{n-1} + \frac{I}{u\rho_\Sigma}r_{cr}^n, \quad n = 0,...,4. \qquad (7)$$

The distribution function moments Ω_n, m^n/kg, are determined as follows:

$$\Omega_n = \int_{r_{cr}}^{\infty} r^n f dr, \quad n = 0,...,3. \qquad (8)$$

The condensation aerosol parameters are expressed in terms of the distribution function moments:

$$n_p = \rho_\Sigma \Omega_0; \qquad (9)$$

$$r_p = \Omega_1/\Omega_0; \qquad (10)$$

$$\rho_p = 4\pi\rho_l\rho_\Sigma \Omega_3/3, \qquad (11)$$

where n_p is the countable concentration of particles, m^{-3}; r_p is the average size (radius) of particles, m; ρ_p is the mass concentration of particles, kg/m^3, and ρ_l is the density of particle substance, kg/m^3.

The distribution function itself is restored proceeding from the solution results based on the procedure described in [17].

The generation of condensing aerosol that takes place in cooling the coal combustion products was modeled by numerically integrating the system of equations (7) and the obtained thermodynamic correlations (2), (4), and (5). The nucleation rate was calculated using the classical theory of Folmer–Frenkel–Seldovich [18], and the droplet growth size was determined using the Hertz–Knudsen formula [19]. Numerical integration was carried out using the COND-KINET-1 computer program developed at ENIN (computer program state registration certificate no. 2017664075). The simulation results are shown in Figs. 3–6.

It follows from Figs. 3 and 4 that the parameters of condensation aerosol contained in the coal combustion products estimated taking into account the "freezing" phenomenon in the generation of aluminosilicates vary in a two-fold manner. On the one hand (see Fig. 3), the mass concentration of appearing particles decreases, which is consistent with the thermodynamic calculation data (see Fig. 1). On the other hand (see Fig. 4), a decrease in the content of potassium sulfate in the gaseous phase entails a growing number of generated submicron particles [the area under the curve $f_v(r_p)$; $f_v = f/\rho_\Sigma$] with a simultaneous decrease of their size. This circumstance must be taken into account in providing dust trapping arrangements for removing the generated particles from the coal combustion products.

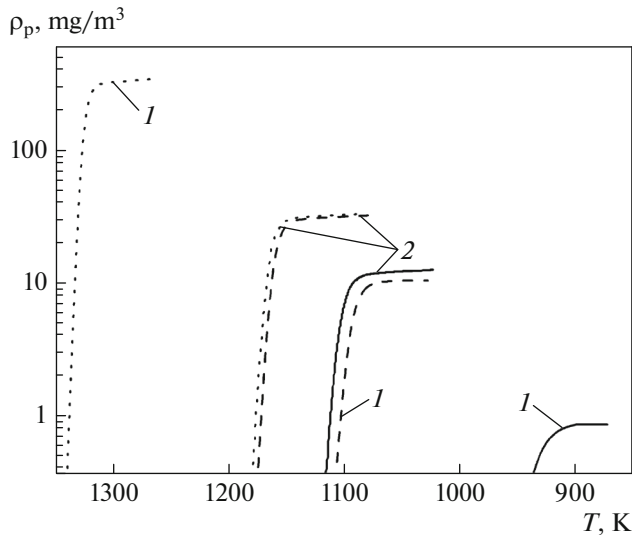A similar effect, i.e., growth in the countable concentration of particles generated in firing coals with a

ρ_p, mg/m^3

Fig. 3. Change in the mass concentration of particles generated during bulk condensation of vapors in the coal combustion products. *1*—Coal no. 5 (with the highest loss of potassium during the generation of aluminosilicates); *2*—coal no. 12 (with the smallest loss of potassium during the generation of aluminosilicates). Dotted curves represent the assessments obtained without taking into account the generation of aluminosiilicates; dashed curves represent the assessments obtained with taking into account the generation of aluminosiilicates and "freezing" at T_{fr} = 1900 K, and solid curves represent the assessments obtained taking into account the generation of aluminosiilicates and "freezing" at T_{fr} = 1700 K.
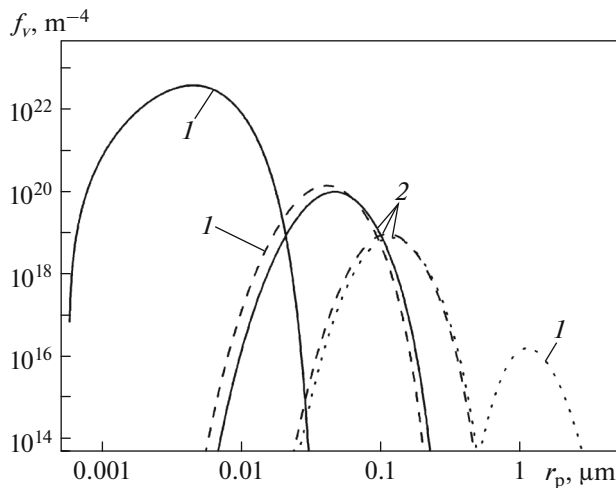
f_v, m^{-4}

Fig. 4. Size distribution function for particles generated during volume condensation of vapors in the coal combustion products. The data are normalized for the number of particles per unit volume (countable concentration). The notation is the same as in Fig. 3.

Fig. 5. Fractional composition of particles generated in burning coal no. 12. (a) Solid curves represent the results of calculations carried out taking into account the generation of aluminosilicates and the "freezing" at T_{fr} = 1700 K for two values of the condensation coefficient: β = 1 (*1*) and β = 0.3 (*2*), and dashed curve *3* represents the experimental data of [2]. (b) Solid curves represent the results of calculations carried out taking into account the generation of aluminosilicates and the "freezing" at T_{fr} = 1900 K for two values of the condensation coefficient: β = 0.3 (*4*) and β = 0.1 (*5*), and dashed curve *6* represents the experimental data of [2].

lower content of potassium, was pointed out in [10]. In all likelihood, this is due to a decrease in the growth rate of generated particles with decreasing the concentration of the condensing compound (potassium sulfate) in the gaseous pha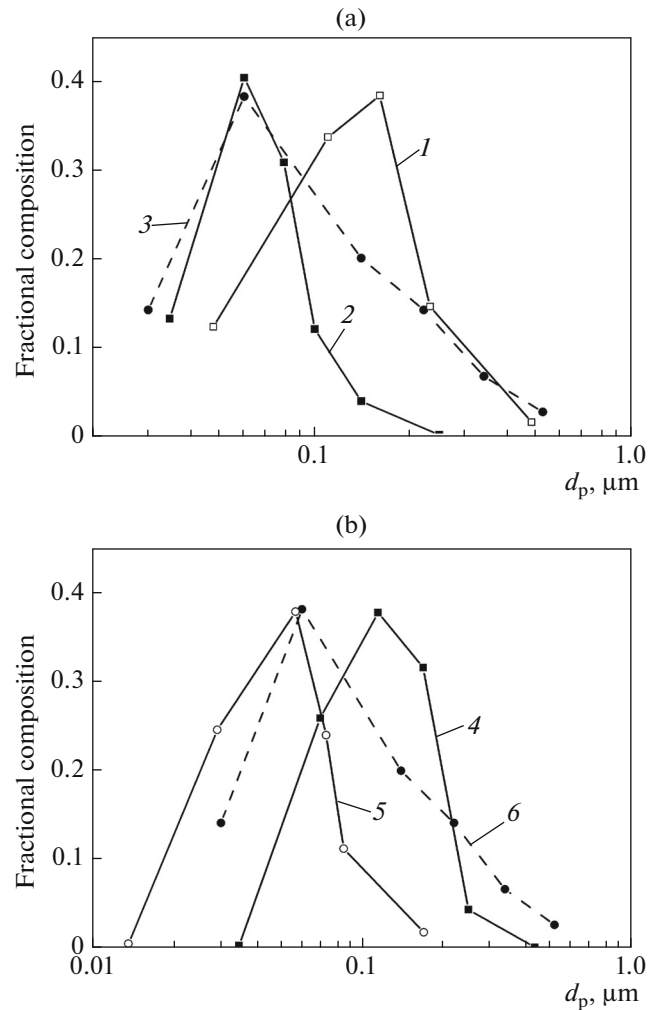se. As a consequence, the supersaturated state vanishes rather slowly with cooling the combustion products, and a high nucleation rate is retained.

It can be seen from Figs. 3 and 4 that, although the obtained results are quite similar in a qualitative respect, they differ essentially in a quantitative respect for two selected coals (with the highest and lowest loss of potassium sulfate in the gaseous phase due to the generation of aluminosilicates). According to [10], it can be supposed that the calcium-to-silicon ratio equal to 0.06 and 1.4 for selected coal nos. 5 and 12, respectively, behaves as the influencing factor.
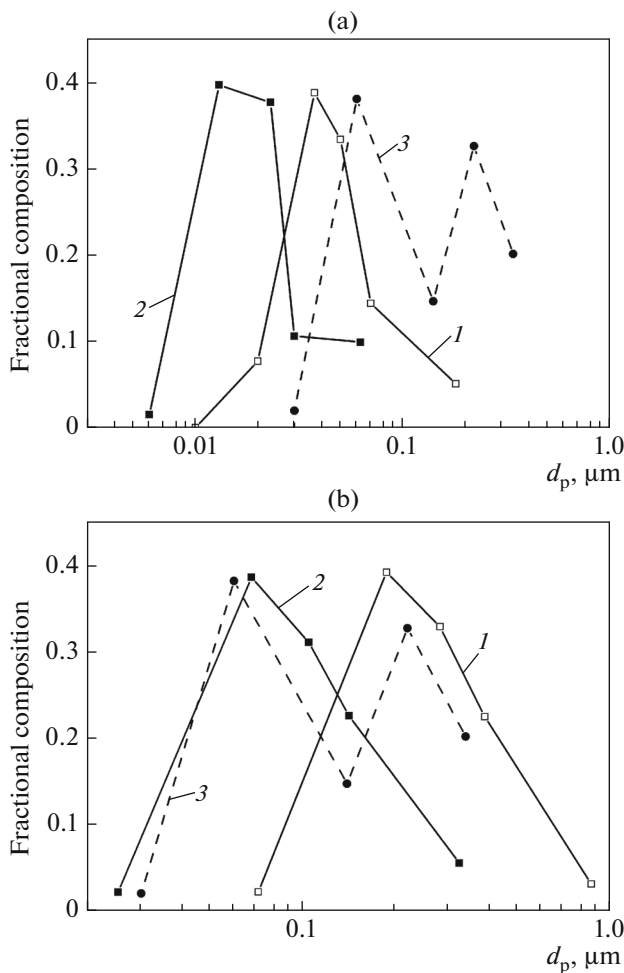
Fig. 6. Fractional composition of particles generated in burning coal no. 13. Solid curves represent the results of calculations carried out taking into account the generation of aluminosilicates and "freezing" at (a) $T_{fr} = 1700$ K and (b) $T_{fr} = 1900$ K for two values of the condensation coefficient: $\beta = 1$ (*1*) and $\beta = 0.3$ (*2*). Dashed curves *3* represent the experimental data of [2].

For comparison purposes, the calculated and experimental data on the fractional composition of particles generated in burning coal nos. 12 (Ca/Si = 1.4) and 13 (Ca/Si = 0.22) are shown in Figs. 5 and 6. The fractional composition was calculated as the ratio of particles with a certain size to the total mass of particles. For the possibility to carry out comparison, the experimental data from [2] were processed in a similar way. It can be seen that the calculation results obtained for coal no. 12 at $T_{fr} = 1700$ K (see Fig. 5a) can be approached to the experimental data with the condensation coefficient β [20] ranging from 0.3 to 1.0. At $T_{fr} = 1900$ K (see Fig. 5b), the corresponding condensation coefficient values are 0.1–0.3. At the same time, for coal no. 13 at $T_{fr} = 1700$ K (see Fig. 6a) the calculated particle sizes corresponding to the fraction composition maximum are smaller than their experi-

mental values even with the maximum possible value of $\beta = 1$. In all likelihood, better agreement between the calculated and experimental data could be obtained in this case by increasing T_{fr} with the corresponding increase of condensing substance concentration in the gaseous phase. Indeed, at $T_{fr} = 1900$ K (see Fig. 6b), better agreement between the calculated and experimental data on the fractional composition for coal no. 13 is reached already with a permissible value of the condensation coefficient $(0 < \beta \le 1)$ $\beta = 0.3$.

Thus, owing to the use of two variable parameters in the model, i.e., T_{fr} and β, it became possible to successfully describe enough the experimental data for two coals having different mineral part compositions and, primarily, the parameter Ca/Si [10].

CONCLUSIONS

(1) Thus, the proposed model describing the generation of submicron particles in burning coals according to the condensation mechanism rests on applying a combined thermodynamic and kinetic approach to describing the bulk condensation process in coal combustion products.

(2) The proposed model implemented by means of software opens the possibility to model the parameters of the particles being generated, namely, their concentration and distribution by sizes, proceeding from the reference data on coal composition.

(3) A comparison with the available experimental data for two coals shows that the predictions obtained using the model can be regarded as cues in setting up efficient trapping of submicron particles generated in firing coals from flue gases.

(4) It is necessary to carry out further investigations for sophisticating the model in regard of taking into account the compounds of potassium and sodium not only with sulfur but also with phosphorus. Further testing of the model should also be carried out.

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