

Sulfur retention by ash during coal combustion. Part II. A model of the process

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Abstract: An overall model for sulfur self-retention in ash during coal particle combustion is developed in this paper. It is assumed that sulfur retention during char combustion occurs due to the reaction between SO₂ and CaO in the form of uniformly distributed non-porous grains. Parametric analysis shows that the process of sulfur self-retention is limited by solid diffusion through the non-porous product layer formed on the CaO grains and that the most important coal characteristics which influence sulfur self-retention are coal rank, content of sulfur forms, molar Ca/S ratio and particle radius. A comparison with the experimentally obtained values in a FB reactor showed that the model can adequately predict the kinetics of the process, the levels of the obtained values of the SSR efficiencies, as well as the influence of temperature and coal particle size.

Keywords: coal combustion, sulfur retention by ash, modelling.

INTRODUCTION

During coal combustion, SO₂ produced from sulfur-containing organic and non-organic species reacts with base oxides contained in the mineral impurities. This process, due to which a part of the SO₂ is retained in ash, is designated as sulfur self-retention (SSR). The most important base oxide for SSR is CaO, formed as a result of CaCO₃ decomposition and combustion of organic groups containing Ca.¹ SSR is influenced by various factors,^{1,2} which depend on the coal properties (Ca/S mole ratio, particle size, content of sulfur forms and coal rank) and on the combustion conditions (temperature, residence time of ash particles, air excess ratio, *etc.*).

The reaction of SO₂ with CaO (designated as sulfation) is first order with respect to SO₂ and zero order with respect to O₂.³ There are numerous expressions for sulfation kinetics in the literature, ranging from empirical ones⁴ up to expressions of the Arrhenius

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type.⁵ Values of the kinetic parameters (pre-exponential factor and activation energy) differ significantly, depending on the kind of physical model used. The basic difference between the various models of sulfation is whether the formation of a solid product layer of CaSO_4 , as well as diffusion through this layer,⁶ is taken into account. In this case, the sulfation rate is diffusion limited.⁷

In the existing models^{8,9} of SSR, the sulfation rate is taken into account in a simplified manner. Yeh *et al.*⁸ take the char pore surface area as a measure of the surface of CaO available for sulfation reaction, while Chen and Kojima⁹ take into account the concentration of CaO in the coal briquette. In both cases, these simplifications are somewhat corrected by assuming that the sulfation rate decreases proportionally with the conversion degree of CaO.

The sulfation reaction has been mostly investigated in the case of SO_2 retention by CaCO_3 as a sorbent.¹⁰ This process is mostly used in the case of fluidized bed combustion (FBC) of coal since it enables sulfation to take place in the optimum temperature range (800–900 °C). In this paper a novel approach has been applied for modeling SSR, closely related to the grain model¹¹ used for SO_2 retention by CaCO_3 .

SULFUR SELF-RETENTION MODEL

The combustion of coal particles takes place in two successive steps: devolatilization and char combustion. Both of these processes must be considered since they determine the relevant conditions that influence the process of SSR. Devolatilization is a process significantly shorter than char combustion and during which unfavourable conditions for SSR prevail (reducing atmosphere and lower temperatures). Our experimental investigations have shown that it is possible to predict the amount of sulfur that remains in char after devolatilization using the following correlation¹²:

$$S_{\text{Ch}} = 0.5 S_{\text{p}} + S_{\text{o}} \cdot C_{\text{fix}} / (1 - \text{Ash}) + S_{\text{s}} \quad (1)$$

Char combustion

Most of SSR takes place during char combustion. It is assumed that the combustible sulfur, *i.e.*, the part of it that remained after devolatilization, is solely converted to SO_2 and that the rate of its formation is proportional to the rate of carbon conversion.^{8,9,13} The applied model for char combustion belongs to the microscopic intrinsic models and has been presented in detail in previous papers.^{13,14} The model describes the dynamic behaviour of a porous char particle during combustion, *i.e.*, spatial and temporal changes of all important physical properties of the char particles (porosity, internal specific surface area, thermal conductivity) and process parameters (temperature, gas concentrations, effective diffusivity, conversion degree).

During char combustion the process of SO_2 formation, sulfation and CaSO_4 decomposition take place simultaneously, and thus the mass balance partial differential equation for SO_2 has the following form:

$$\frac{1}{r^2} \cdot \frac{\partial}{\partial r} \cdot \left(r^2 \cdot D_{\text{eff}} \cdot \frac{\partial c_{\text{SO}_2}}{\partial r} \right) + \mathfrak{R}_f + \mathfrak{R}_s + \mathfrak{R}_d = \frac{\partial c_{\text{SO}_2}}{\partial \tau} \quad (2)$$

Sulfation

It is assumed that the active part of CaO in coal, formed as a result of CaCO_3 decomposition and combustion of Ca-containing organic compounds, is the only base oxide that contributes to sulfur retention. Calcium present in clays and silicates can not react with SO_2 under FBC conditions,^{1,2} since in this temperature range these Ca-containing compounds cannot decompose to CaO. It is also assumed that after devolatilization all of the active Ca is present in the form of non-porous CaO grains of the same initial radius ($R_{g0} \approx 1 \mu\text{m}$), which are uniformly distributed throughout the char volume. A changing size grain model was adopted for the following reaction between the CaO grains and SO_2 :



A partially sulfated CaO grain is shown in Fig. 1. It consists of an unreacted core, of radius r_c , surrounded by a non-porous product layer of CaSO_4 . As the process of sulfation progresses, the size of the grains increases ($R_g > R_{g0}$) due to the larger molar volume of CaSO_4 compared to CaO. It is assumed that Ca^{2+} ions (and O^{2-} in a coupled manner to sat-

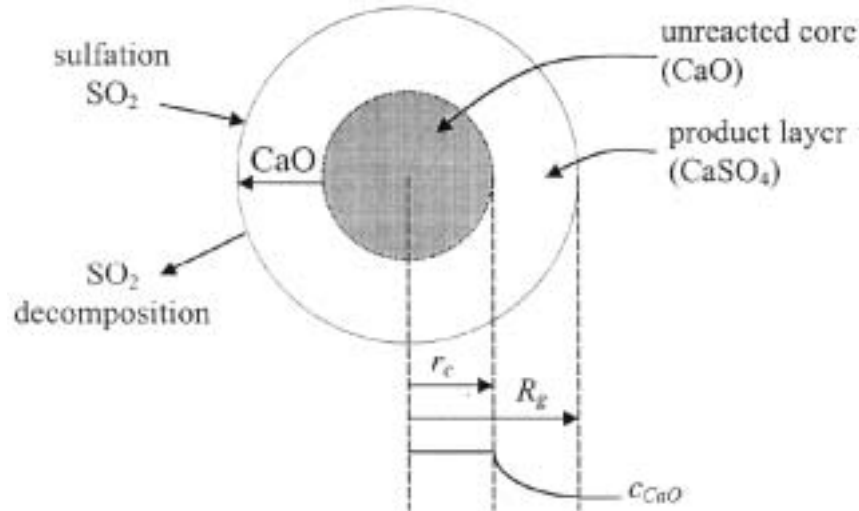


Fig. 1. Schematic representation of a partially sulfated CaO grain.

isfy local mass and charge balances) migrate outward through the non-porous product layer. This mechanism of product layer diffusion was proposed by Hsia *et al.*^{15,16} based on their experimental investigations and is used for modeling the CaO– SO_2 reaction.¹⁷ The values of the product layer (solid) diffusion coefficient (D_{CaO}) cited in the literature show considerable variation and its value is known to depend on the choice of the model. In the case of the grain model, with the coupled diffusion of Ca^{2+} and O^{2-} ions, its value is of the

order of 10^{-16} m²/s. The product layer diffusion activation energy is about 120 kJ/mol, which is typical for an ionic diffusion mechanism.¹⁷ The existence of an unreacted CaO core is the consequence of such a low value of D_{CaO} , even though the CaO–SO₂ reaction does not take place at its surface but rather at the surface of the grains. The reaction rate and the rate constant are defined by the following expressions:

$$\mathfrak{R}_s = \frac{\partial c_{\text{SO}_2}}{\partial t} = -k_s \cdot S_{\text{CaO}} \cdot c_{\text{CaO}} \cdot c_{\text{SO}_2} \quad (4)$$

$$k_s = A_s \cdot \exp\left(-\frac{E_s}{R_g \cdot T}\right) \quad (5)$$

Taking into account the content of Ca in the char particle, CaO grain dimensions and the properties of the char particle, the specific surface for the sulfation reaction (m² of CaO grains per m³ of char) is derived as:

$$S_{\text{CaO}} = 3 \cdot Y_{\text{CaO}} \frac{\rho_{\text{Ch}}}{\rho_g} \cdot \frac{R_g^2}{R_{g0}^3} \quad (6)$$

The CaO concentration (c_{CaO}) in Eq. 4 is related to the surface of the CaO grains where the sulfation reaction takes place and it is determined using the pseudo-steady-state condition:

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial c_{\text{CaO}}}{\partial r} \right) = 0 \quad (7)$$

with the following boundary conditions:

$$c_{\text{CaO}}|_{r=r_c} = \frac{\rho_g}{M_{\text{CaO}}} \quad \text{and} \quad -D_{\text{CaO}} \left(\frac{\partial c_{\text{CaO}}}{\partial r} \right)_{r=R_G} = k_s \cdot c_{\text{CaO}} \cdot c_{\text{SO}_2} \quad (8)$$

The solution of the partial differential Eq. (7) with the boundary conditions (8) gives the CaO concentration profile in the product layer of the reacting CaO grain (Fig. 1). At the grain surface, the value of the CaO concentration is:

$$c_{\text{CaO}} = \frac{\rho_g}{M_{\text{CaO}}} \cdot \frac{D_{\text{CaO}}}{D_{\text{CaO}} + R_g \cdot k_s \cdot c_{\text{SO}_2} \left(\frac{R_g}{r_c} - 1 \right)} \quad (9)$$

The solid diffusion coefficient through the product layer is of the Arrhenius type⁷:

$$D_{\text{CaO}} = A_D \cdot \exp\left(-\frac{E_D}{R_g T}\right) \quad (10)$$

CaSO₄ decomposition

There is sufficient experimental evidence that the degree of CaO conversion goes through a maximum as the temperature increases.^{8,11} This means that at higher temperatures the process of product decomposition takes place (a kind of a reverse reaction to the sulfation reaction). There are different explanations for this phenomenon in the literature: thermal decomposition,³ reductive decomposition¹⁸ (due to the higher CO concentrations) or sintering¹⁹ (due to which the exposed surface of the CaO grains decreases). In this model the decomposition process is taken into account with the following expression for the decomposition rate:

$$\mathfrak{R}_d = \frac{\partial c_{\text{SO}_2}}{\partial \tau} = k_d \cdot S_{\text{CaO}} \quad \text{where} \quad k_d = A_d \cdot \exp\left(-\frac{E_d}{R_g \cdot T}\right) \quad (11)$$

SOLUTION PROCEDURE

The initial conditions (temperatures, gas concentrations, CaO grain radius) are given as the input to the model and the initial values of all parameters are constant along the radius of the char particle. The amount of sulfur that remains in the char, after devolatilization, is calculated by Eq. 1. The processes of char combustion and sulfur retention are treated simultaneously. For numerical purposes, the char particle is subdivided into segments (usually more than 100) of equal volume. The method of control volumes²⁰ is used for solving the system of partial differential equations that treat char combustion^{13,14} and sulfur self-retention (Eqs. 2, 4–11).

After each time interval, a new set of values for the temperature and gas concentrations along the char particle radius is obtained. For each char particle segment, a new value of the unreacted core radius is determined, solving the following differential equation:

$$\frac{dr_c}{d\tau} = \frac{M_{\text{CaO}}}{\rho_g} \cdot \frac{R_g^2}{r_c^2} \cdot (k_d - k_s \cdot c_{\text{CaO}} \cdot c_{\text{SO}_2}) \quad (12)$$

which takes into account the net effect of sulfation and decomposition.

The determined values of r_c enable the calculation of the degree of CaO conversion and, in turn, the value of the partially sulfated CaO grain radius for each char particle segment:

$$x_s = 1 - \frac{r_c^3}{R_{g0}^3} \quad (13)$$

$$R_g^3 = r_c^3 + z \cdot x_s \cdot R_{g0}^3 \quad (14)$$

where z represents the molar volume ratio of CaSO₄ and CaO ($z = 3.09$).

The total conversion degree of the CaO in the char particle is obtained by integrating the local degrees of CaO conversion along the char particle radius:

$$X_s = \frac{3 \int_0^{R_{\text{Ch}}} x_s(r) \cdot r^2 dr}{R_{\text{Ch}}^3} \quad (15)$$

PARAMETRIC ANALYSIS

The characteristics of the model were determined using computer simulations. Firstly, the influence of the kinetic parameters was investigated. For this purpose, calculations were performed with the following set of data: $R_{Ch} = 2$ mm, $Ash = 20$ %, $C_{fix} = 80$ %, initial porosity 50 %, initial specific surface area 200 m²/cm³, $S_{Ch} = 2$ %, $Ca/S = 1$, $T = 800$ °C and the surrounding gas is air ($c_{O_2} = 21$ %). The sensitivity of the model to variations of k_s and D_{CaO} , for different values of R_{g0} , is shown in Fig. 2a. It may be seen that the variation of k_s , in the range of values reported in the literature,^{5,21} does not significantly influence the calculated SSR efficiency. On the other hand, the influence of D_{CaO} and R_{g0} is quite noticeable. This shows that the process of SSR is limited by solid diffusion through the product layer and that D_{CaO} and R_{g0} are important model parameters whose values should be chosen by comparing model results with experimental data. For further analysis in this work the following values of these parameters were assumed: $D_{CaO} = 10^{-10} \cdot \exp(-125000/R_gT)$, $k_s = 7.7 \cdot 10^{-3} \cdot \exp(-67000/R_gT)$ and $R_{g0} = 0.5$ μm.

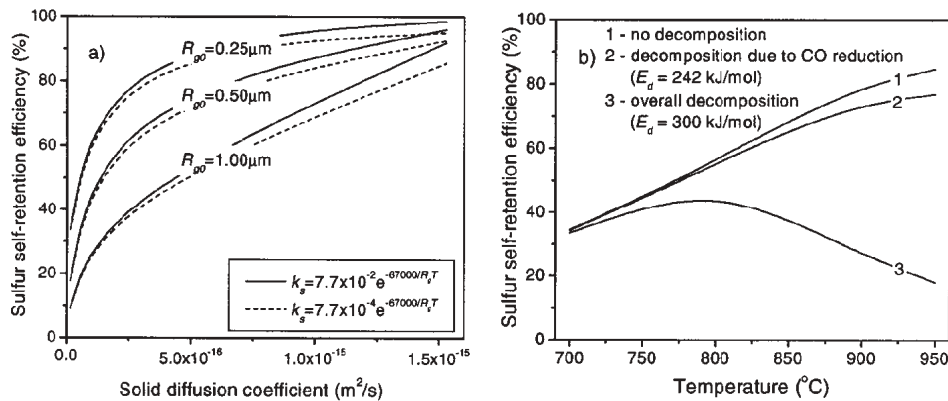


Fig. 2. Sensitivity of the model to variations of the main kinetic parameters: a) k_s and D_{CaO} , b) E_d .

The sensitivity of the model to variations of k_d is shown in Fig. 2b. If it were assumed that there were no decomposition, the SSR efficiency would continually increase with surrounding temperature (curve 1). As previously stated, this is not in accordance with the experimental data available in the literature which show that there is an optimal temperature after which the SSR efficiency decreases. If only reduction with CO is assumed, using the corresponding E_d ,²² the SSR efficiency maximum would be at much higher temperatures (curve 2) than reported in the literature (around 850 °C in the case of limestone). For further analysis in this work a greater value for E_d was assumed which leads to a temperature maximum at around 800 °C (curve 3). It should be noted that the temperatures inside the char particle are somewhat higher than these of the surrounding.

The sensitivity of the model to variations of the molar Ca/S ratio and char particle radius is shown in Fig. 3. Higher values of Ca/S lead to higher SSR efficiencies, as is well known from the literature.²³ Also, the model predicts that increasing the values of Ca/S

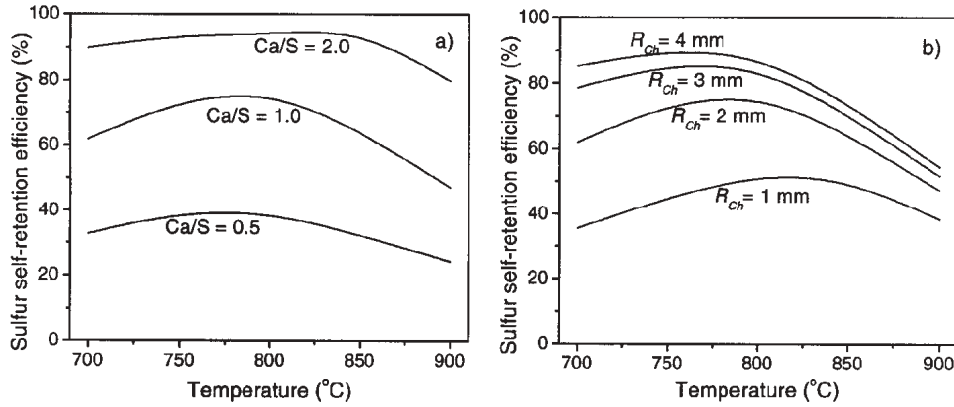


Fig. 3. Influence of Ca/S (a) and R_{ch} (b) on sulfur self-retention (model predictions).

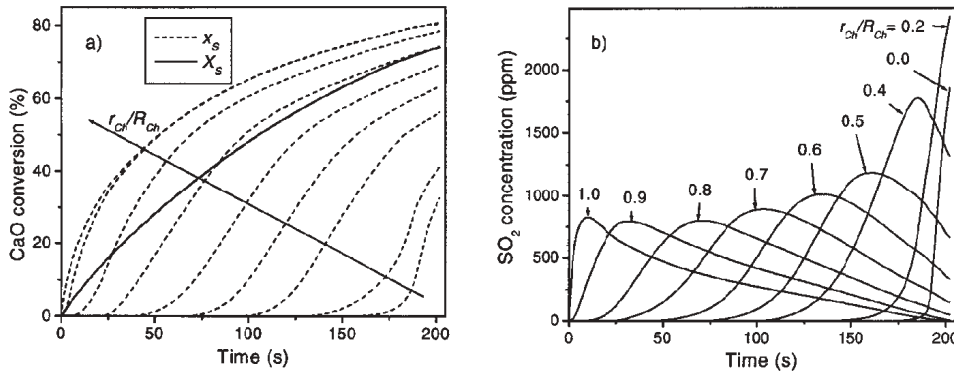


Fig. 4. Model predictions of spatial and temporal changes of the CaO conversion (a) and SO₂ concentration (b) inside a char particle during combustion.

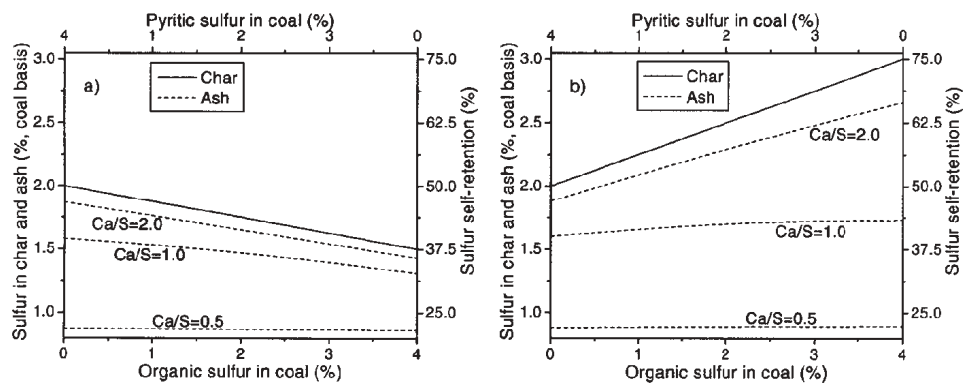


Fig. 5. Overall model predictions in the case of a low rank coal (a) and a high rank coal (b).

shifts the temperature maximum towards higher temperatures. This is a consequence of the still available CaO in the outer layers of the char particle which retain SO₂ at lower temperatures (close to the surrounding conditions) and where the effect of decomposition is, thus, relatively smaller. With increasing char particle radius the residence time of SO₂ inside the char particle increases, which leads to higher SSR efficiencies. The shift of the temperature maximum is a consequence of the higher temperatures inside the larger char particles.¹⁴

The process of SSR during char combustion may be analysed through the spatial and temporal changes of the CaO conversion which are shown in Fig. 4a. Initially, only the CaO in outer layers contribute to the SSR. As the combustion proceeds, the SO₂ concentration increases inside the char particle, Fig. 4b, due to which the CaO conversion gradually progresses towards the centre of the char particle. The final local CaO conversion differs along the char particle radius, decreasing towards the particle centre.

The overall predictions of the model, taking into account both devolatilization and char combustion, are shown in Fig. 5. Two sets of data for the coal characteristics are considered. One set corresponds to a lower rank coal ($C_{\text{fix}} = 30\%$, volatiles 50%), Fig. 5a, and the other to a higher rank coal ($C_{\text{fix}} = 60\%$, volatiles 20%), Fig. 5b. In both cases $Ash = 20\%$ and $S_{\text{O}} + S_{\text{P}} = 4\%$, while the Ca/S and $S_{\text{O}}/S_{\text{P}}$ ratios vary. The most noticeable difference for these two types of coal is the amount of sulfur that remains in the char after devolatilization (full lines). This difference increases as the $S_{\text{O}}/S_{\text{P}}$ ratio increases, as a consequence of the behaviour of the sulfur forms during devolatilization, which is taken into account by Eq. 1. The molar Ca/S ratio determines the amount of sulfur in the char that can be retained in the ash during char combustion. From the aspect of the overall SSR, the model predicts higher SSR efficiencies for higher rank coals. In the case of lower rank coals it is beneficial if the sulfur present in coal is in the form of pyritic sulfur while in the case of higher rank coals if it is in the form of organic sulfur. Also, the beneficial effect of higher values of Ca/S is relatively greater in the case of higher rank coals.

EXPERIMENTAL VERIFICATION

The results of batch combustion test runs were used for experimental verification of the model. Two coals were used, Kolubara and Bogovina, the characteristics of which are given in Tables I and II. The main differences between these two coals are their rank, sulfur content and molar Ca/S ratio (only the active part of the Ca is taken into account).

The batch combustion tests were carried out in a ϕ 80 mm fluidized bed (FB) reactor. The bed material was silica sand with a mean particle diameter of 0.5 mm, while the bed height was 60 mm. The fluidizing velocity was in the range of 0.45 – 0.55 m/s. The dry char particles were introduced into the hot FB and the bed temperature and gas concentrations immediately above the bed were continuously monitored during char combustion. The experiments were performed with three coal particle size fractions of the coal (4.0 – 7.0, 7.0 – 10 and 10 – 13 mm) with three bed temperatures (750, 800 and 850 °C). The SSR efficiency was determined taking into account the total content of sulfur in the coal and in the ash (S_{Ash}), after combustion: $\eta_{\text{SO}_2} = (S_{\text{Ash}}/S_{\text{T}}) \cdot 100$.

Figure 6a shows that a substantial part of the sulfur evolves during devolatilization and that the concentrations of SO₂, monitored at the top of the bed are significantly higher than during char combustion. Since the evolution of SO₂ during devolatilization is taken into account in the model by Eq. 1, the comparison between the experimental and model predicted SO₂ concentrations was done only during char combustion (Fig. 6b). It may be seen that the model can adequately predict the evolution of SO₂ during char combustion.

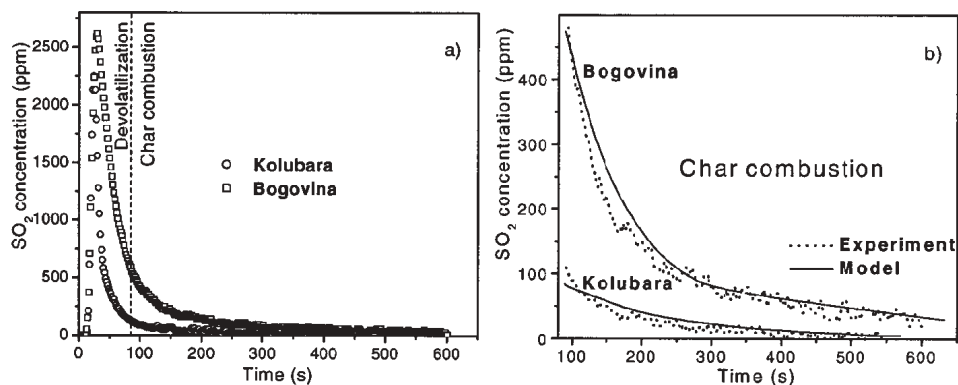


Fig. 6. SO_2 concentration at the top of the bed during batch combustion of coal, $T_{\text{bed}} = 750^\circ\text{C}$, $R_{\text{Ch}} = 2 - 3.5$ mm: a) experimental values during the whole combustion process, b) experimental values and model predictions during char combustion.

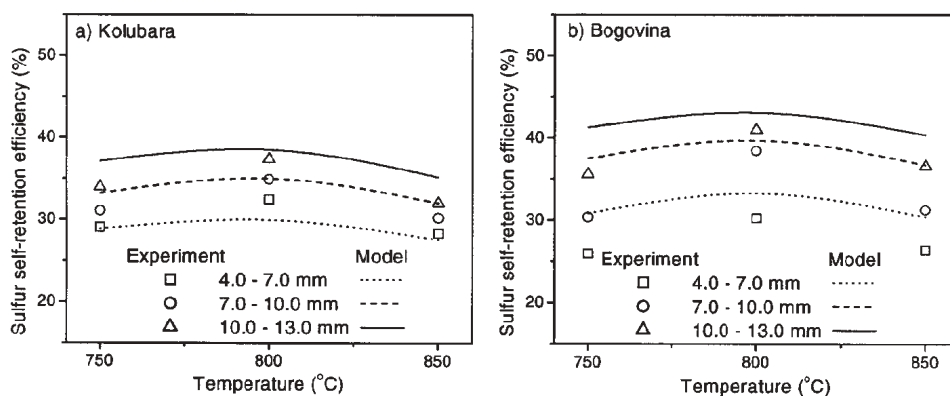


Fig. 7. Experimental values and model predictions of the overall sulfur self-retention efficiency for batch combustion of coals Kolubara and Bogovina in a FB reactor.

TABLE I. Proximate analysis and ultimate analysis of the coals^a

Coal	Proximate analysis				Ultimate analysis				
	Ash/%	VM/%	$C_{\text{fix}}/\%$	LHV/kJ/g	C %	H %	N %	S %	O %
Kolubara	16.34	47.69	35.97	15.14	52.69	4.62	0.62	0.82	24.89
Bogovina	19.75	39.21	41.04	15.76	54.38	4.73	0.92	4.16	16.06

^aAll values given on dry coal basis

Model predictions for the overall SSR efficiency are compared with the obtained experimental data in Fig. 7. It may be seen that the model predicts relatively well the levels of the SSR efficiencies, as well as the influence of particle size and temperature with the maximum values around 800°C . The increase of SSR efficiencies with increasing particle size was noticed in all cases and may be explained as being a consequence of the longer SO_2 diffusion paths in the larger particles. The existence of a SSR temperature maximum in the case of FBC conditions and the beneficial effect of particle size have also been reported by other authors.⁸

TABLE II. Sulfur and calcium^a analysis of the coals

Coal	$S_s/\%$	$S_p/\%$	$S_o/\%$	$S_T/\%$	$Ca_A/\%$	Ca_A/S
Kolubara	0.11	0.00	0.73	0.84	0.53	0.51
Bogovina	0.22	0.09	4.31	4.62	4.64	0.80

^aActive calcium content (Ca_A) determined by reported analytical procedure²

Although the model predicts relatively well the levels of SSR and the influence of temperature and coal particle size, differences between the model predictions and the experimentally obtained data are in some cases significant, especially in the case of coal Bogovina. Apart from the significant non-uniformity of the investigated coals,² the possible reasons for these differences can also be found in the simplifications adopted in the model, especially concerning the decomposition of $CaSO_4$. In the model this phenomenon is taken into account by the reaction rate, which depends only on temperature, disregarding the effect of the reducing conditions and/or sintering. Also, the assumption that all CaO grains have the same initial radius (R_{g0}), is in the case of both coals questionable. Investigations have shown that coals contain two different forms of active calcium: organic-bound and carbonate. Thus, the predictions of the model may be improved by including the effects of reductive decomposition, sintering and the presence of different forms of active calcium (presumably having different grain dimensions).

CONCLUSION

A developed overall model for sulfur self-retention in ash during coal particle combustion is presented in this paper. The amount of sulfur that remains in the char after devolatilization is predicted by an empirical equation. A novel approach has been applied for modeling the self-retention of sulfur during char combustion by assuming that the Ca in the char is present in the form of CaO grains. A changing grain size model is adopted for the reaction between the CaO grains and SO_2 . Our previously developed model for char combustion is used for the prediction of spatial and temporal changes of all important physical properties of the char particle and parameters needed for the model of sulfur self-retention.

The characteristics of the model, as well as its sensitivity to variations of the main parameters were determined by computer simulation. It is concluded that the process of sulfur self-retention is limited by solid diffusion through the non-porous product layer and that D_{CaO} and R_{g0} are the most important model parameters. The most important coal characteristics which influence sulfur self-retention are coal rank, content of sulfur forms, molar Ca/S ratio and particle radius.

The comparison with the experimentally obtained values in a FB reactor showed that the model can adequately predict the kinetics of the process, the levels of the obtained values of SSR efficiencies, as well as the influence of temperature and coal particle size.

NOMENCLATURE

Ash – ash content in coal, % (on dry coal basis)

A_s, A_d – pre-exponential factor for the sulfation and decomposition reaction, respectively, ($m^4/mol \cdot s$, $mol/m^2 \cdot s$)

A_D – pre-exponential factor for solid diffusion of CaO through $CaSO_4$, (m^2/s)

C_{fix} – fixed carbon content in coal, % (on dry coal basis)
 c_j – concentration of j -component, (mol/m³)
 D_{eff} – effective gas diffusion coefficient, (m²/s)
 D_{CaO} – solid diffusion coefficient of CaO through CaSO₄, (m²/s)
 E_{D} – activation energy for solid diffusion of CaO through CaSO₄, (J/mol)
 $E_{\text{s}}, E_{\text{d}}$ – activation energy of sulfation and decomposition reaction, respectively, (J/mol)
 $k_{\text{s}}, k_{\text{d}}$ – reaction rate constant for sulfation and decomposition, respectively, (m⁴/mol·s, mol/m²·s)
 M_j – molar mass of j -component, (kg/mol)
 r, R – current radius and particle radius, (m)
 r_{c} – unreacted core radius of CaO grain, (m)
 R_{g} – universal gas constant, (J/mol·K)
 S_{CaO} – specific surface for the sulfation reaction, (m² of Ca grains/m³ of char)
 S_{Ch} – total sulfur content in char, % (on dry coal basis)
 S_{O} – organic sulfur content in coal, % (on dry coal basis)
 S_{P} – pyritic sulfur content in coal, % (on dry coal basis)
 S_{S} – sulfate sulfur content in coal, % (on dry coal basis)
 T – temperature, (K)
 Y_{CaO} – mass fraction of CaO in char, (-)
 $x_{\text{s}}, X_{\text{s}}$ – local and total CaO conversion degree, respectively, (-)
 ρ – density, (kg/m³)
 \mathcal{R} – reaction rate, (mol SO₂/(m³ s))
 τ – time, (s)

Subscripts

0 – initial value

Ch – related to char particle

d – related to decomposition of CaSO₄f – related to formation of SO₂ due to combustion

g – related to CaO grain

s – related to sulfation

ИЗВОД

 ЗАДРЖАВАЊЕ СУМПОРА У ПЕПЕЛУ ТОКОМ САГОРЕВАЊА УГЉА. ДЕО II.
 МОДЕЛ ПРОЦЕСА

 ВАСИЛИЈЕ МАНОВИЋ¹, БОРИСЛАВ ГРУБОР², МЛАДЕН ИЛИЋ² и БРАНИМИР ЈОВАНЧИЋЕВИЋ^{3,4}

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У раду је приказан развијени модел задржавања сумпора у пепелу током сагоревања угља. Претпоставка модела је да се задржавање сумпора током сагоревања коксног остатка одиграва услед реакције SO₂ и CaO који је у облику равномерно распоређених зрна. Параметарска анализа је показала да је процес задржавања сумпора контролисан дифузијом кроз формирану слој чврстог продукта на зрнима CaO, као и да су ранг угља, садржај форми сумпора, моларни Ca/S однос и величина честице важне особине угља које утичу на процес. Поређење са експерименталним резултатима добијеним у реактору са флуидизованим слојем је показало да модел може адекватно да предвиди кинетику процеса, ефикасност задржавања сумпора у пепелу, као и утицај температуре и величине честице угља.

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