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Modeling of the reactions of a calcium-based sorbent with sulfur dioxide

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Abstract: A mathematical model of calcium sorbent reactions for the simulation of sulfur dioxide reduction from pulverized coal combustion flue gasses was developed, implemented within a numerical code and validated against available measurements under controlled conditions. The model attempts to resemble closely the reactions of calcination, sintering and sulfation occurring during the motion of the sorbent particles in the furnace. The sulfation was based on the partially sintered spheres model (PSSM), coupled with simulated particle calcination and sintering. The complex geometry of the particle was taken into account, with the assumption that it consists of spherical grains in contact with each other. Numerical simulations of drop down tube reactors were performed for both CaCO₃ and Ca(OH)₂ sorbent particles and results were compared with experimental data available from the literature. The model of the sorbent reactions will be further used for simulations of desulfurization reactions in turbulent gas–particle flow under coal combustion conditions.

Keywords: lime; particle; desulfurization; flue gas; model.

INTRODUCTION

In order to investigate in detail the possible reduction of sulfur oxides in flue gas by injection of a pulverized sorbent into coal-fired boiler furnaces, a model of sorbent reactions is required. In the literature, various models are available that can be roughly divided into groups according to the way they treat the sorbent particles. The simplest of them are shrinking unreacted core models, such as the one described by Borgwardt.¹ More complex and computationally demanding models are the partially sintered spheres model (PSSM),^{2–5} the pore model,^{2,3} the network model^{2,3} and their variations. The PSSM and pore models have a certain

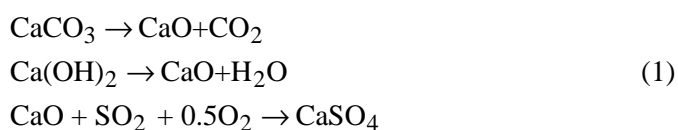
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level of similarity, both observing the particle structure during reactions and highly depending on particle transformation over time.

The Borgwardt model was implemented in previous research in a numerical model and used to simulate reactions of larger particle fractions (around 90 μm and a few larger and smaller fractions) in a fixed bed reactor as a method of validation⁶ and in a complex model of the boiler furnace.⁷ Implementation showed good agreement with experimental results, however, due to the short particle residence time, effects of sulfur reduction were not sufficient, and sorbent utilization was low. For this reason, the possible use of finely pulverized particle fractions (smaller than, or around 10 μm) had to be analyzed. Due to the lack of data and different reaction mechanism, this model could not be used to describe the reaction of smaller particles at high temperatures. Experimental studies conducted by Borgwardt,⁸ Flament,⁹ Miline,¹⁰⁻¹² Silcox,¹³ Fan¹⁴ and Chen¹⁵ showed the great potential for the use of finely pulverized sorbent particles when the sorbent is injected directly into the boiler furnace. Several models are available in literature.^{2-5,8,10-14}

The most used sorbents are calcium-based, *i.e.*, CaCO_3 and $\text{Ca}(\text{OH})_2$, due to their availability and good reactivity with sulfur oxides under combustion conditions. Reactions of particles consist of calcination, sintering and sulfation. During the calcination process, CaCO_3 is converted to CaO whereby the BET surface available for reaction increases greatly.^{8,9,13} If the reactant in use is $\text{Ca}(\text{OH})_2$, then during a short period, a dehydration reaction occurs^{9,14} that is followed by a rapid increase in the BET surface, much faster in comparison with the development of the surface obtained by calcination of calcium carbonate. These reactions are shown in Eq. (1).

At high temperatures together with calcination, sintering of the particles occurs, which leads to rapid loss of BET surface.^{8,9,13} The final reaction that occurs together with the two previous ones is sulfation of sorbent in atmospheres containing sulfur oxides:



THE SORBENT REACTIONS MODEL, ITS NUMERICAL IMPLEMENTATION AND EXPERIMENTAL

The model is based on the sulfation PSSM approach combined with the calcination model, both presented by Alvfors⁵ for a single particle. A brief description of the model is presented, with most significant equations given for reference. Further details on the model for single particle sulfation can be found in the papers by Lindner,² Kocafe³ and Alvfors.^{4,5} This model is implemented and used with a complex numerical code for the simulations. The particle calcination model, used to determine the development of the particle surface during

reaction time, was first introduced by Alvfors⁵ in combination with the PSSM. Alvfors⁵ showed that the expression given by Beruto,¹⁶ together with the German–Munir sintering formula,¹⁷ could give good agreement with the measured⁹ particle calcination and surface development.⁹

Expression used for the calcination model given by Beruto¹⁶ describes the extent of calcination at a given time:

$$\ln(1 - X_c(t)) = -k_c M_{M, CaCO_3} S_{CaCO_3} t \quad (2)$$

The extent of calcination was determined by expressing $X_c(t)$ from Eq. (2) used to calculate surface area of the calcium sorbent given later in Eq. (4).

Loss of surface due to sintering of a particle is modeled by the German–Munir formula:¹⁷

$$\left[\frac{S_0 - S}{S_0} \right]^\gamma = K_s t \quad (3)$$

Equation (3) assumes the particle consists of spherical grains connected by necks between neighboring grains, and when sintering occurs, the necks connecting the grains begin to overlap.

Surface area of calcium sorbent, expressed in $m^2 cm^{-3}$, at a given time step consists of a $CaCO_3$ part and a CaO part, depending on the extent of calcination $X_c(t)$:

$$S_{0, Ca}^n = \frac{(X_c(t_n) S_{CaO}^n M_{M, CaO} + (1 - X_c(t_n)) S_{CaCO_3} M_{M, CaCO_3}) (1 - \epsilon_{Ca})}{X_c(t_n) V_{M, CaO} + (1 - X_c(t_n)) V_{M, CaCO_3}} \quad (4)$$

At a given time step, the surface area of the calcium oxide part, derived from Eqs. (2) and (3), is:

$$S_{CaO}^n = \sum_{k=1}^n S_{0, CaO} (1 - (K_s(T_k) t_n)^{1/\gamma(T_k)}) (X_c(t_k) - X_c(t_{k-1})) \quad (5)$$

As suggested by Alvfors,⁵ the PSSM should take into account the development of the BET surface, obtained by application of the calcination and sintering model, and use it as the basis for the determination of the sulfation rate.

The coefficients for calcination of $CaCO_3$, given by Alvfors,⁵ show good agreement with the available experimental data for small particles; however, the development of the BET surface is significantly slower, compared to the experimental one. Due to this, the calcination and sintering coefficients for $CaCO_3$ given by Borgwardt^{8,5} are used. For temperatures above 950 °C, the calculated BET surfaces show excellent agreement with the experimental data. The porosity of the particle is considered to be initially small, but afterwards, the porosity of the particle increases during the reaction.

The model for the development of the BET surface of $Ca(OH)_2$ particles given by Fan¹⁴ is more complex compared to the one described above. In order to simplify the calculations, the above model was used and the experimental data given by Fan¹⁴ were fitted with it. The coefficients used for the calculations of k_c , K_s and γ are given in Table I. The initial porosity of $Ca(OH)_2$ was considered to be high, and to decrease with time.

Sulfation model used was the PSS model introduced by Lindner² and further described in the literature.²⁻⁵ The model assumes that a sorbent particle consists of small non-porous spherical grains in contact with m other grains (Fig. 1). During the initial time step, all grains

are the same and have radius r_0 . When reaction begins, unreacted core reduces in size and its radius changes to r_2 (in dimensionless form $g_2 = r_2/r_0$), while the product layer increases in size and has radius r_1 (in dimensionless form $g_1 = r_1/r_0$). The change of the unreacted core over time, due to conversion, can be given by the differential equation:

$$\frac{dg_2}{dt^*} = \frac{S_0}{S_2} \bar{r} \quad (6)$$

TABLE I. Coefficients used for the calculations of calcination and sintering of the sorbent particle, and the particle porosity

Coefficient	Sorbent	
	CaCO ₃ (Borgwardt ¹⁸)	Ca(OH) ₂ (Fan ¹⁴)
$k_c / \text{mol m}^{-2} \text{s}^{-1}$	$3.405 \times 10^7 e^{\frac{-201}{RT_p}}$	$2.2 \times 10^6 e^{\frac{-141}{RT_p}}$
K_s / s^{-1}	$e^{\frac{6.735 - 11660}{T_p}}$	$e^{\frac{-1.4 - 2000}{T_p}}$
γ	$e^{0.0018T_p + 0.8154}$	$e^{0.002T_p + 0.89694}$

Conversion is obtained by comparing the initial and sulfated particle geometries, and it can be expressed by:

$$X_s = 1 - \frac{g_2^3 - \frac{m}{4} F(g_2, \lambda)}{1 - \frac{m}{4} (1 - \lambda)^2 (2 + \lambda)} \quad (7)$$

When the values of g_2 and X_s are known, the following volumetric balance can be used to determine value of g_1 if the molar volume ratio (α) between the solid product and solid reactant is known:

$$g_1^3 - g_2^3 - \frac{m}{4} ((g_1 - \lambda)^2 (2g_1 + \lambda) - F(g_2, \lambda)) = \alpha X_s \left(1 - \frac{m}{4} (1 - \lambda)^2 (2 + \lambda) \right) \quad (8)$$

The reaction rate on the particle surface can be given by $r_A = -k c_{A,s} S_2$, while the diffusion through product layer is $r_A = -D_s (c_A - c_{A,s}) S_{\text{avg}} / L$. From these two equations, an expression for local reaction rate is derived:

$$-\bar{r} = \frac{-r_A}{k c_{A0} S_0} = \frac{C}{S_2 + \frac{Da L S_0}{l_0 S_{\text{avg}}}} \quad (9)$$

The interaction between the local kinetics and pore diffusion is obtained by differential mass balance for the gaseous reactant, assuming pseudo steady state conditions:

$$\frac{1}{z^2} \frac{d}{dz} \left(z^2 \delta \frac{dC}{dz} \right) = -\Phi_{\text{Th}}^2 \frac{C}{S_0 / S_2 + Da L S_0 / l_0 S_{\text{avg}}} \quad (10)$$

From Eq. (9), the average reaction rate in the particle, which depends on pore diffusion, is obtained. Furthermore, it is used to determine the rate of sulfur oxide depletion from the surrounding gas.

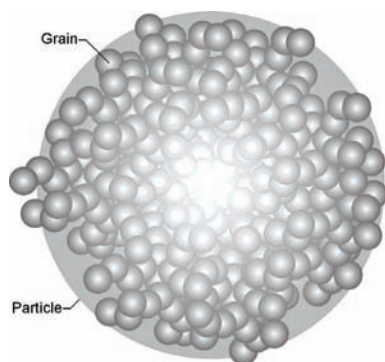


Fig. 1. Model of a sorbent particle.

A particle is considered to consist entirely of calcium. The initial particle parameters used are the ones given for the experimental data described in the literature:^{5,8,9} BET = 0.9 m² g⁻¹, $\varepsilon_0 = 3\%$, $S_{0,\text{CaO}} = 104 \text{ m}^2 \text{ g}^{-1}$ and $\lambda = 80\%$. Sulfation rate coefficients, and diffusion coefficients are the ones given by Alvfors⁴, as follows: $k = 20\exp(-25/RT_p)$, m s⁻¹; $D_0 = 1.5 \times 10^{-4}(T_p/1123)^{1.7}$, m² s⁻¹, and $D_s = 1.913 \times 10^{-5}\exp(-125/RT_p)$, m² s⁻¹.

Two drop down tube reactors were modeled in a 2D model with a grid of 600 cells×30 cells in size (estimated to provide stable numerical solutions). The system of gas phase transport equations of momentum, continuity and energy in an Eulerian field were solved by using the control volume numerical method. The fluid flow equations were coupled with the chemical reactions equations. The general form of the conservation equations used in the model could be written in index notation as:

$$\frac{\partial}{\partial x_j}(\rho U_j \Phi) = \frac{\partial}{\partial x_j} \left(\Gamma_\Phi \frac{\partial \Phi}{\partial x_j} \right) + S_\Phi + S_p^\Phi \quad (11)$$

Φ represents a general variable, such as U , V , W , x_{O_2} , x_{N_2} , x_{CO_2} , $x_{\text{H}_2\text{O}}$, x_{SO_2} , etc. Terms in Eq. (11) from left to right are convection, diffusion, source term for variable Φ , and additional source term due to particles.

The tubes considered in the simulations had the same dimensions and gas phase flow conditions as in the experiments conducted by Flament⁹ with CaCO₃ and Fan¹⁴ with Ca(OH)₂. Gas mixture components and their concentrations used in the simulations correspond to those found in experiments^{9,14}. The conditions are also similar to the flue gas composition that can be found during the pulverized coal combustion, providing useful data in simulations of large boiler furnaces.

Sorbent particles are injected at the beginning of a reactor tube. Their velocity is determined from gas velocity field in the reactor, and interphase slipping is considered to have no influence on particle velocity. Particles are tracked in Lagrangian system.

Conservation equation for every gaseous component in fluid mixture can be written in a form derived from the general Eq. (11). In this form, Γ_A is a transport coefficient for variable "A":

$$\frac{\partial}{\partial x_j}(\rho U_j \chi_A) = \frac{\partial}{\partial x_j} \left(\Gamma_A \frac{\partial \chi_A}{\partial x_j} \right) + S_{p,A}^m \quad (12)$$

Here the "A" represents O₂, N₂, CO₂, H₂O, SO₂ and other components if needed. The source term for these gaseous components represents their generation or depletion in a two-phase

flow due to particle reactions. The conservation equation for the SO_2 component of a gas mixture has two source terms due to the particles; one is from combustion of coal particles, while the other is due to absorption of SO_2 by the CaO particle:

$$\frac{\partial}{\partial x_j} (\rho U_j \chi_{\text{SO}_2}) = \frac{\partial}{\partial x_j} \left(\Gamma_{j,\text{SO}_2} \frac{\partial \chi_{\text{SO}_2}}{\partial x_j} \right) + S_{p,\text{SO}_2} + S_{p,\text{SO}_2}^{\text{CaO}} \quad (13)$$

For each time step, the particle obtains information about the temperature and gas concentration in the cell corresponding to the particle position at the given time.

After obtaining these values as input for the particle reactions model, the BET surface is calculated. The most important influential factor in determining the BET surface is the particle temperature. For this temperature, the calcination rate, and sintering parameter and exponent are determined for each time step. After this, for the current time step, the surface of the calcium oxide part is determined using Eq. (5), with respect to the thermal history of the particle from previous time steps. With knowledge of extent of calcination, we can estimate the particle porosity can be estimated. After this, a specific particle surface is determined using Eq. (4). Knowing this particle surface, the sulfation reaction is calculated for the same time step.

The sulfation model considers the reactions of a single grain in the particle with an averaged reaction rate over the entire particle. Particle temperature is considered the same as the temperature of surrounding gas;¹⁴ this approximation is valid due to the rapid heating rate of the particle. The particle velocity in the reactor tube is considered to be the same as gas velocity.¹⁴ Particle position in the axial direction at each time step is determined from the previous position and time of the particle. Reaction rate constant and diffusion coefficients are determined for the current temperature of the particle and surrounding gas. The concentration of sulfur dioxide at the surface is calculated based on the numerical grid cell in which the particle currently is. The dimensionless time step is calculated using the particle parameters: grain radius, sulfur dioxide and calcium oxide concentration. Specific surfaces are determined using expressions given in the literature;^{2,3} these expressions are derived from the assumed particle geometry. Dimensionless unreacted core radius, g_2 , is determined from dimensionless rate and dimensionless time using Eq. (6). This is employed to determine further the extent of sulfation, X_s (Eq. (7)). When the dimensionless unreacted core radius and extent of sulfation are known, the dimensionless radius of reaction products, g_1 , can be estimated using Eq. (8). From this radius, the current porosity can be determined, and from it the effective diffusion. With this data, the differential Eq. (10) is used to determine concentration profile within the particle, from which the overall reaction rate is obtained, Eq. (9). This reaction rate is used to estimate the sulfur reduction for given trajectory, in a given cell during the residence time of the particle in the reactor.

RESULTS AND DISCUSSION

Comparison of calculated particle calcination showed that the Alvfors⁵ calcination rate constant provided better agreement with the experimental data than the ones given by Borgwardt;^{8,5} however, the results for the simulation of BET surface development, shown in Fig. 2A, suggest that use of the combined calcination and sintering models with the Borgwardt coefficients gave a faster surface development and better agreement with the experimental data. The results suggest that simulated surface for temperatures below 950 °C would give poor

agreement with experimental data. Due to relatively high local temperatures in pulverized coal-fired boiler, this will probably not be a problem but it could be overcome by switching between the use of Alvfors and Borgwardt coefficients, depending on whether the current temperature is below or above 950 °C.

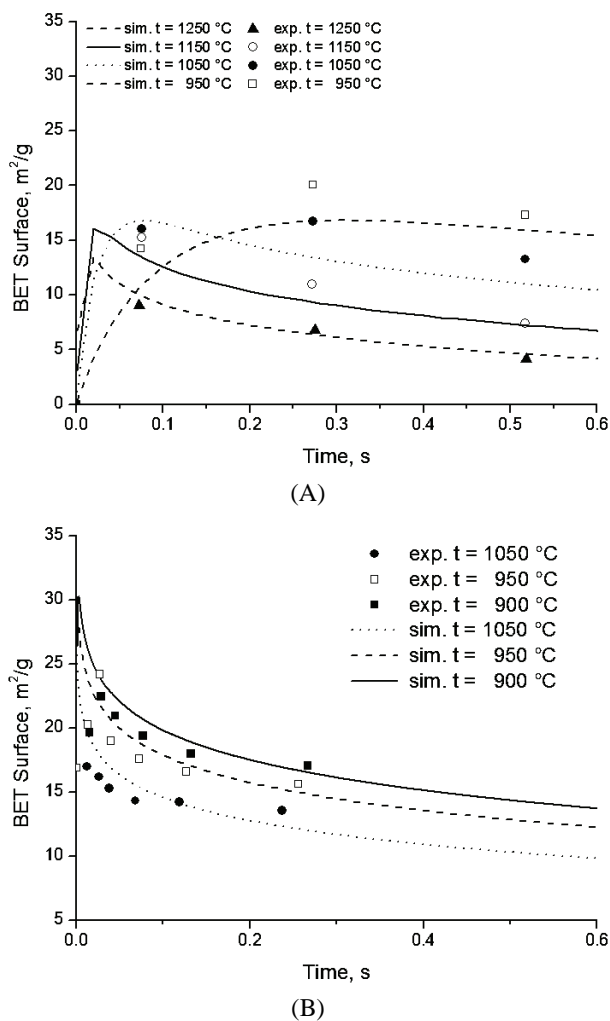


Fig. 2. Development of the BET surface – simulated with coefficients calculated by Borgwardt for CaCO₃, compared to experimental data of Flament and with fitted coefficients for Ca(OH)₂ sorbent, based on experimental data by Fan.¹⁴

The calculated calcination rates for calcium hydroxide are higher, compared to the ones obtained in the experiments by Fan,¹⁴ but the calculated BET surface development agrees well with the experimental data. The fitted data for BET

surfaces when calcium hydroxide was used as the sorbent for the simulations of the reactor used by Fan are shown in Fig. 2B.¹⁴ For the entire temperature range considered, the calculated data is in good agreement with the experimental data, especially when the residence time of the sorbent particle was longer than 0.1 s. It should be stressed that the typical residence time of a sorbent particle within a pulverized coal-fired furnace is around 2 to 5 s, or longer, depending on the sorbent injection location and aerodynamic conditions in the furnace. As expected, the BET surface was lower for higher temperatures, due to more intensive sintering reactions.

The sulfur dioxide concentration field along the simulated experimental IFRF reactor tube is shown in Fig. 3. It is noticeable that fastest reduction is achieved near the center of the reactor, while it is slower near the walls, but as the fluid flow develops, concentration level evens out over the tube cross-section.

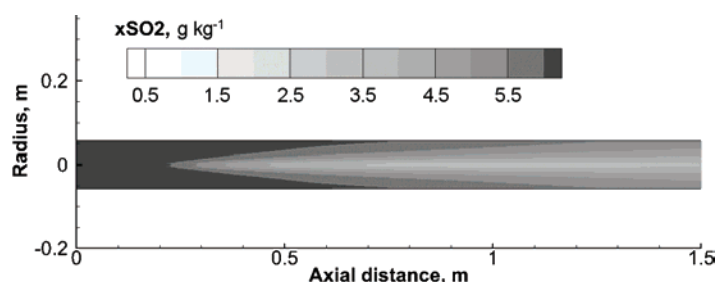


Fig. 3. Axial SO₂ concentration profile over the simulated IFRF reactor (total simulated length 3 m, sorbent CaCO₃).

Extent of calcination, shown in Fig. 4A, follows well the trend of experimental data in the case of CaCO₃ sorbent, giving better agreement when reaction temperatures were higher, while in the case of Ca(OH)₂ sorbent, the predicted calcination (Fig. 4B) was lower than the experimentally one obtained in the experiments by Fan,¹⁴ suggesting that corresponding reaction model used for Ca(OH)₂ needs to be improved – an initial surface development model is required to provide higher initial BET surfaces in order to properly simulate the more intensive initial sulfur capture.

The simulation results obtained for sulfur capture with CaCO₃ using the diffusion rates and reaction rate constant suggested by Alvfors,⁵ are compared with the experimental results of Flament⁹ in Fig. 5A for a range of Ca/S mole ratios. Figure 5B shows the results for simulated sulfur capture when Ca(OH)₂ was used as sorbent are presented in Fig. 5B for a range of temperatures with a fixed Ca/S mole ratio = 2.0. From Fig. 5, it is clear that reactivity of Ca(OH)₂ was significantly higher during the initial period compared to the reactivity of CaCO₃ for the same Ca/S mole ratios. This could be attributed to the faster development of the BET surface of Ca(OH)₂ in this initial period. However, at

higher temperatures, Ca(OH)_2 lost its reactivity more rapidly due to the rapid loss of internal surface. The calcination and sintering surface area development were simulated using the data of Borgwardt data for the calcination and sintering rate coefficients in the case of CaCO_3 and with the use of fitted data based on the experimental data of Fan¹⁴ in the case of the Ca(OH)_2 reactor. Using these data in the model, good agreement was obtained between the experimental and simulated reduction of sulfur oxides, but it is expected that with further improvements, the calculated sulfation of Ca(OH)_2 would be more accurate.

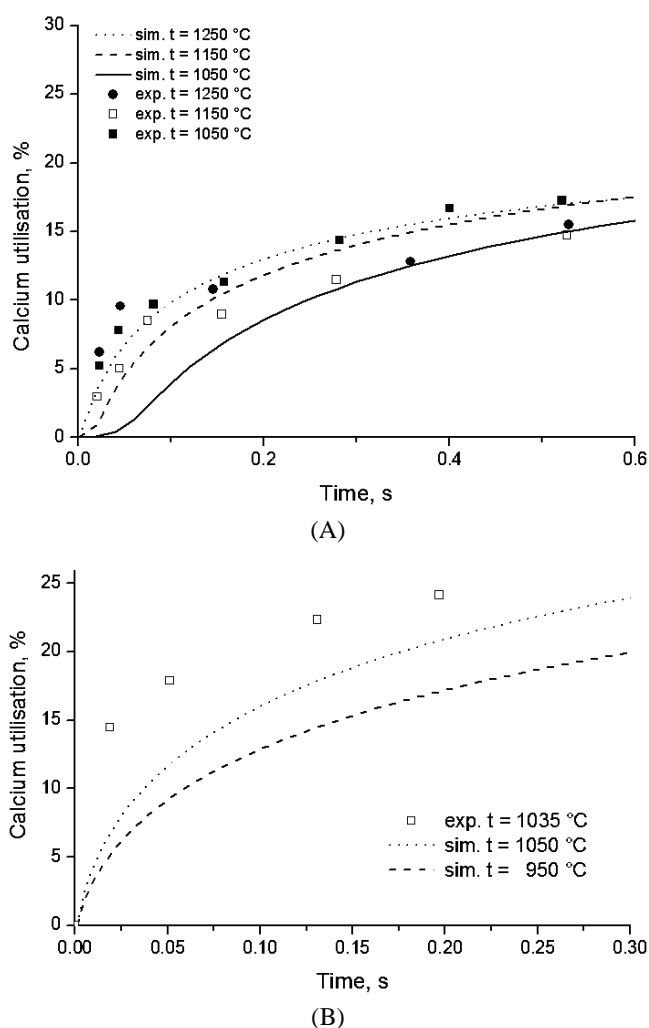


Fig. 4. Simulated extent of calcination of sorbent compared to experimental results by Flament (CaCO_3 sorbent)⁹ and experimental results by Fan (Ca(OH)_2 sorbent).¹⁴

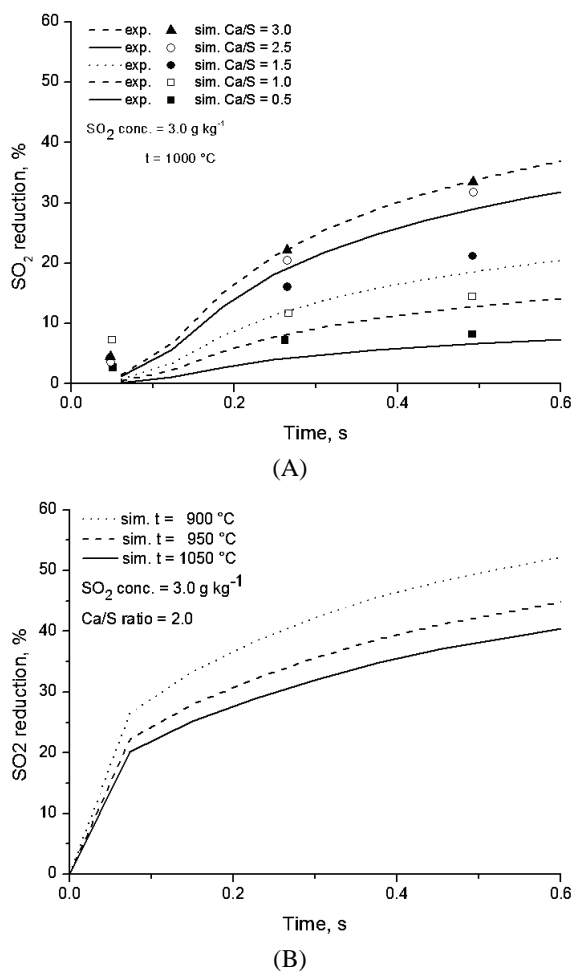


Fig. 5. Simulated data compared to experimental data from Flament for SO₂ reduction (CaCO₃ sorbent)⁹ and simulated data for SO₂ reduction (Ca(OH)₂ sorbent).

CONCLUSIONS

Simulations with selected models particle calcination, sintering and sulfation reactions of Ca-based sorbents, coupled with particle tracking in the gas phase of a referent drop down tube reactors, provided the basis for the validation of the model and showed a considerable reduction in sulfur oxides. In the case of CaCO₃, experimental and simulation data showed good agreement, while the simulation with Ca(OH)₂ underestimated calcium utilization at lower temperatures. This could probably be attributed to the BET surface development model not capturing the narrow time interval with extremely high BET surfaces. With high Ca/S mole ratios, the reduction was estimated to be up to 35 % during first

0.5 s of reaction for an initial sulfur concentration of 3.0 g kg^{-1} . With Ca/S molar ratios around 2.0, the simulated reduction at the reactor exit was over 25 % (when sorbent was CaCO_3), and over 30 % (for Ca(OH)_2 as the sorbent), with respect to the given temperature ranges in the simulations. Considering the obtained agreement with experimental results, the model will be further improved and adapted to be used in conjunction with a complex flow, heat transfer and combustion model of a pulverized coal-fired boiler furnace. Due to higher particle residence times, ranging from 2 to about 5 seconds in the boiler furnace, it is expected that with a proper distribution of particles over the furnace cross-section, sorbent injection would achieve good results in emission reduction of sulfur oxides.

The model for prediction of calcium sorbent particles reaction with sulfur dioxide, together with numerical code for fluid flow simulation could be used to obtain insight into the complex processes in boiler furnaces. The simulation results depend highly on the prediction of the development of the reactive (BET) surface. The model underestimates to some extent Ca(OH)_2 surface development, thus underestimating utilization of CaO obtained during calcination of Ca(OH)_2 . Consequently, this results in an underestimation of the final amount of reduced SO_2 with this sorbent. For CaCO_3 , the surface development estimation was in good agreement with experimental results, which influence the final results, giving good agreement with measured utilization of Ca and reduction of SO_2 . The model is intended to be used in the simulation of sorbent particles injection into utility boiler furnaces with pulverized coal combustion. For simulations of CaCO_3 , the model is usable in the temperature range from $950 \text{ }^\circ\text{C}$ to $1250 \text{ }^\circ\text{C}$, and results are in good agreement with the measured values, while for Ca(OH)_2 a sorbent, compared with available experimental results, the usable temperature range is from 950 to $1100 \text{ }^\circ\text{C}$, but it must be kept in mind that the predictions underestimated SO_2 reduction to a certain extent. With these limitations, the model could be used to simulate CaCO_3 sorbent injection into a boiler furnace, giving good qualitative and quantitative predictions, and in the case of Ca(OH)_2 sorbent, it could be used for qualitative analysis, but it should be further improved to provide better agreement, and to be able to give better quantitative predictions.

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NOMENCLATURE

BET = initial particle surface (measured), $\text{m}^2 \text{ g}^{-1}$
 c_{A0} , c_{B0} – concentrations of reactants (SO_2 and CaO), mol m^{-3}
 C – local reactant concentration at position z

- Da – Damköhler number, $Da = kl_0/D_s$
 D_{eff} – effective diffusion coefficient in the particle, $\text{m}^2 \text{s}^{-1}$
 D_0 – diffusion coefficient in the bulk gas phase, $\text{m}^2 \text{s}^{-1}$
 D_s – diffusion coefficient of the solid product layer, $\text{m}^2 \text{s}^{-1}$
 $F(g_2, \lambda)$ – structural function that depends on the extent of particle sulfation
 g_0, g_1, g_2 – dimensionless grain radius
 k – sulfation reaction rate constant, m s^{-1}
 k_c – calcination rate constant, $\text{mol m}^{-2} \text{s}^{-1}$
 K_s – sintering rate kinetic factor, s^{-1}
 l_0 – characteristic distance, m
 L – product layer thickness, m
 $M_{\text{M,CaCO}_3}$ – molar mass of calcium carbonate, g mol^{-1}
 $M_{\text{M,CaO}}$ – molar mass of calcium oxide, g mol^{-1}
 m – number of particles in contact
 r_0, r_1, r_2 – grain radius for initial time step, unreacted core and product layer, respectively, m
 S_{avg} – average specific surface area, $S_{\text{avg}}^2 = S_1 S_2$
 S – the surface after sintering, $\text{m}^2 \text{g}^{-1}$
 S_{CaCO_3} – surface of calcium carbonate part, $\text{m}^2 \text{g}^{-1}$
 S_{CaO}^n – surface area of calcium oxide part at a given time, $\text{m}^2 \text{g}^{-1}$
 S_0 – the initial specific surface of particle, $\text{m}^2 \text{m}^{-3}$
 $S_{0,\text{CaO}}$ – nascent calcium surface area, Borgwardt,¹⁸ $\text{m}^2 \text{g}^{-1}$
 S_1 – specific surface of product layer, $\text{m}^2 \text{m}^{-3}$
 S_2 – specific surface of unreacted core, $\text{m}^2 \text{m}^{-3}$
 $S_{\text{p,SO}_2}$ – source term for SO_2 due to particles
 t – reaction time, s
 t^* – dimensionless time, $t^* = (kc_{\text{A}0}t)/(r_0c_{\text{B}0})$
 U_j – velocity component, m s^{-1}
 $V_{\text{M,CaCO}_3}$ – molar volume of calcium carbonate
 $V_{\text{M,CaO}}$ – molar volumes of calcium oxide
 $X_c(t)$ – extent of calcination at a given time step, -
 $X_s(t)$ – extent of sulfation at a given time step, -
 χ_{SO_2} – concentration of component in gas phase, kg kg^{-1}
 z – dimensionless position inside the particle, -
 α – molar volume ratio
 γ – exponent
 Γ_A – Effective diffusion (transport coefficient for variable Φ)
 δ – relation between effective diffusivity at the beginning and at the current time step
 ε_{Ca} – particle porosity, influenced by sintering of particle
 λ – structural parameter, and depends on connected grains neck overlapping
 ρ – gas mixture density, kg m^{-3}
 Φ_{Th} – Thiele modulus, $\Phi_{\text{Th}}^2 = R_0^2 k S_0 / D_{\text{eff},0}$
 Φ – general scalar variable
Subscript
 n – a current time step at which the surfaces are calculated.

ИЗВОД
МОДЕЛОВАЊЕ РЕАКЦИЈА СОРБЕНТА НА БАЗИ КАЛЦИЈУМА СА
СУМПОР-ДИОКСИДОМ

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Математички модел реакција сорбента на бази калцијума ради симулације смањења емисије сумпор-диоксида из димних гасова при сагоревању спрашеног угља је развијен, уграђен у нумерички код и проверен поређењем са доступним мерењима под контролисаним условима. Модел би требало да детаљно опише реакције калцинације, синтеровања и сулфатизације, које се одвијају током кретања честица сорбента кроз ложиште. Модел сулфатизације је заснован на тзв. моделу делимично синтерованих сфера, повезаног са изабраним моделима калцинације и синтеровања. Модел узима у обзир сложenu геометрију честице, под претпоставком да се састоји од сферичних зрна у додиру. Нумеричке симулације реактора са вертикалном цеви су изведене за честице CaCO_3 и Ca(OH)_2 као сорбента и резултати су упоређени са доступним експерименталним подацима из литературе. Модел реакција сорбента ће бити даље коришћен за симулацију реакција одсумпоравања у турбулентном двофазном току гаса и честица у условима који владају при сагоревању угља.

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