

K–Cl–S chemistry in air and oxy-combustion atmospheres

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Abstract

This paper studies the consequences on high temperature corrosion when biomass is co-fired with coal in oxy-fuel combustion, a concept that would enable negative CO₂ emissions by combining renewable fuels with CO₂ capture. The particular focus of the work is the sulphation of alkali chlorides which is studied by means of experiments and modelling. The melting point of alkali sulphates is higher than for alkali chlorides and a high degree of alkali sulphation is hence a measure to reduce issues related to high-temperature corrosion. In the experiments a propane flame was doped with SO₂ and KCl (in solution) in air and oxy-fuel atmospheres. Two alternative measurement principles were applied to quantify potassium sulphation and the paper thereby contributes with a novel experimental approach as well as unique experimental data for turbulent diffusion air and oxy-fuel flames. The degree of sulphation of the injected KCl increases substantially in oxy compared to air combustion conditions, a fact which favours the use of biomass in oxy-combustion. This is mainly due to the increased concentration of SO₂ due to flue gas recycling in oxy-combustion, but also chemical effects introduced by the CO₂ as well as a small effect resulting from an increased residence time in the combustor. © 2016 by The Combustion Institute. Published by Elsevier Inc.

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1. Introduction

The anthropogenic use of fossil fuels is widely accepted to be the main reason for global warming. The interest in alternative energy resources, such as biomass and waste derived fuels, has therefore

increased in recent years. An alternative path to reduce the emission of carbon dioxide (CO₂) from fossil fuels is to apply the concept of carbon capture and storage (CCS). The present work will focus on one of the main CCS technologies, oxy-fuel combustion, in which the fuel is combusted in a mixture of pure oxygen and recycled flue gas in order to obtain a high CO₂ concentration in the flue gas. The use of biomass in CCS processes (BECCS) has been discussed in the literature as an option to create a carbon sink in order to reduce

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the atmospheric concentration of CO_2 , see e.g. Ref. [1]. With this background, the present work studies the use of biomass in oxy-fuel combustion; in particular, the K-Cl-S chemistry is studied by means of modelling and experiments.

In relation to coal, biomass is usually considered as a fuel of lower quality, e.g. with respect to lower heating value and higher contents of alkali metals (sodium and potassium) and chlorine [2,3]. The alkali metals tend to react with chlorine and the product may cause issues with high temperature corrosion (HTC) on heating surfaces in a boiler. Compounds containing alkali metals and chlorine are among the most problematic HTC related compounds. Due to this, HTC is primarily a problem for power plants fired with biomass rather than coal [4]. One way of mitigating the HTC related issues is to introduce sulphur, for example by means of a second fuel with higher sulphur content. In such an environment, in which significant amounts of sulphur is present, the alkali chlorides can be converted into sulphates, whose melting temperatures are higher and which are less problematic from a HTC perspective [3,5]. It is therefore of interest to study how the degree of sulphation can be controlled both with respect to fuels and fuel mixtures as well as combustion parameters and design.

In oxy-fuel combustion the replacement of nitrogen with recirculated flue gases causes a difference in flue gas composition. As a consequence, the SO_2 concentration is typically more than three times higher in oxy-fuel combustion compared to air combustion [6,7]. As discussed in our previous modelling work, the increase in SO_2 will influence the homogenous sulphation process and in general the sulphation of alkali is substantially enhanced in oxy-fuel compared to air-fuel combustion [8]. The present work aims to examine this process further by means of a combined experimental and modelling approach; the overall aim is to assess the gas phase K-Cl-S chemistry including the overall degree of potassium sulphation. The sensitivity to CO_2/N_2 atmospheres, sulphur to potassium ratios injected to the combustor and residence time is analysed and discussed.

2. Theory

In a solid-fuel fired combustion system, both potassium (K) and sodium (Na) are typically present but potassium is usually the main alkali specie. In addition, sodium has been reported to follow a similar reaction mechanism as potassium [3,9]. In this work, potassium was therefore chosen to represent both alkali metals. Potassium and chlorine are released from the fuel to the gas phase during devolatilization and combustion. The chlorine is mainly released as HCl, KCl or chlorinated hydrocarbons. The chlorinated hydrocarbons react soon after the release with subsequent formation

of HCl during combustion. As long as chlorine is present, the potassium is released as KCl, otherwise it is released either as atomic potassium (K) or as hydroxide (KOH) [10–12]. Due to the number of reactions and general complexity, the release of inorganic compounds and ash reactions are neglected in this work, which instead focuses entirely on the gas phase chemistry and its potential to convert potassium chloride into potassium sulphate. The chlorinated form of potassium, KCl, is the main potassium compound released to the gas phase. KCl may, however undergo sulphation during combustion to form potassium sulphate (K_2SO_4). At temperatures lower than 450°C , sulphated potassium may be found as pyrosulphate ($\text{K}_2\text{S}_2\text{O}_7$) [13]. Such low temperatures are however not relevant for this work. The sulphation of potassium chloride is suggested to follow one of two possible paths: homogenous sulphation where the sulphates are formed in the gas phase (and are condensed after its formation), or heterogeneous sulphation which includes surface reactions of non-gaseous chloride particles. The heterogeneous sulphation of KCl was proposed by Steinberg and Schofield [14] as a surface reaction phenomenon taking place under post flame conditions. In their work with hydrogen and propane flames, they concluded sodium sulphate to be too unstable during flame conditions to be responsible for the observed sulphation [14,15]. Experimental results presented by others have, on the other hand, showed that the heterogeneous path is too slow to describe the sulphation typically occurring in industrial scale boilers [16,17]. Therefore, this work focuses entirely on homogenous sulphation of KCl.

The theory which suggests that gas phase reactions control the sulphation process is in agreement with several experimental studies [16–18]. In the present work, we aim to examine if the homogeneous chemistry can explain the potassium sulphation also in an 80 kW turbulent propane diffusion flame. The sulphation of KCl may follow one of the reaction routes available including reactions with both SO_2 and SO_3 (see Table 1). Regardless of the route, the final step is the condensation of gaseous K_2SO_4 , which first is formed in reaction between KHSO_4 and KCl or KOH (R1 and R2). There are mainly four routes which concerns the formation of KHSO_4 including either SO_2 or SO_3 . SO_3 may react directly with KOH (R3) or through a two-step reaction starting with KCl (R4 and R5). KHSO_4 may then also be formed via SO_2 in a three-step reaction starting with K (R6–R8) or starting with KSO_3 (R9), which may form from either KO (R10) or K (R11) involving SO_2 and SO_3 , respectively. KCl, KOH, KO and $\bar{\text{K}}$ are key components in the sulphation process. These compounds are coupled via several reactions; the most important ones are listed in Table 1. This list is based on the result in our previous work [8]. KOH may form from KCl via a reaction with water (R12), KOH may

Table 1

List of the most active reactions containing potassium taking part in the sulphation of KCl.

R1	$\text{KHSO}_4 + \text{KCl} \rightleftharpoons \text{K}_2\text{SO}_4 + \text{HCl}$	R11	$\text{K} + \text{SO}_3(+\text{M}) \rightleftharpoons \text{KSO}_3(+\text{M})$
R2	$\text{KHSO}_4 + \text{KOH} \rightleftharpoons \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$	R12	$\text{KCl} + \text{H}_2\text{O} \rightleftharpoons \text{KOH} + \text{HCl}$
R3	$\text{KOH} + \text{SO}_3(+\text{M}) \rightleftharpoons \text{KHSO}_4(+\text{M})$	R13	$\text{KOH} + \text{OH} \rightleftharpoons \text{K} + \text{H}_2\text{O}$
R4	$\text{KCl} + \text{SO}_3(+\text{M}) \rightleftharpoons \text{KSO}_3\text{Cl}(+\text{M})$	R14	$\text{KCl}(+\text{M}) \rightleftharpoons \text{K} + \text{Cl}(+\text{M})$
R5	$\text{KSO}_3\text{Cl} + \text{H}_2\text{O} \rightleftharpoons \text{KHSO}_4 + \text{HCl}$	R15	$\text{KCl} + \text{H} \rightleftharpoons \text{K} + \text{HCl}$
R6	$\text{K} + \text{SO}_2 \rightleftharpoons \text{KSO}_2$	R16	$\text{KOH} + \text{H} \rightleftharpoons \text{K} + \text{H}_2\text{O}$
R7	$\text{KSO}_2 + \text{O}_2(+\text{M}) \rightleftharpoons \text{KSO}_4(+\text{M})$	R17	$\text{KOH}(+\text{M}) \rightleftharpoons \text{K} + \text{OH}(+\text{M})$
R8	$\text{KSO}_4 + \text{H}_2\text{O} \rightleftharpoons \text{KHSO}_4 + \text{OH}$	R18	$\text{KO} + \text{O} \rightleftharpoons \text{K} + \text{O}_2$
R9	$\text{KSO}_3 + \text{OH} \rightleftharpoons \text{KHSO}_4$	R19	$\text{KO} + \text{CO} \rightleftharpoons \text{K} + \text{CO}_2$
R10	$\text{KO} + \text{SO}_2 \rightleftharpoons \text{KSO}_3$	R20	$\text{KO} + \text{SO}_2 \rightleftharpoons \text{K} + \text{SO}_3$

then react further to KO (R13). K is formed directly from KCl (R14 or R15) or indirect via KOH or KO (R16–R20). The present work focuses entirely on homogenous alkali sulphation, as described by the reactions shown in Table 1. Thus, this forms the basis for the modelling results of the alkali chemistry presented in this paper.

3. Method

As mentioned previously, this paper focuses on the homogenous gas phase chemistry related to sulphation of KCl. The gas phase composition derived from combustion of a solid fuel process will depend on the ash composition via both the release and retention processes. These effects will complicate the assessment of the transformation of organic and inorganic species in the gas phase. In the present work, experiments were conducted using a propane flame doped with SO_2 and $\text{KCl}(\text{aq})$ in order to avoid unnecessary heterogeneous effects. The experiments were conducted in the Chalmers 100 kW test unit presented in Fig. 1a, which was carefully cleaned before the start of the test campaign. The unit has a top fired propane burner and can be operated in both air- and oxy-fuel mode [19]. In all experiments performed in this work, the amount of propane fed to the burner is kept constant at 1.73 g/s (corresponding to 80 kW) whereas the oxidizer is adjusted to a stoichiometric ratio of 1.15.

The unit is equipped with injection systems for both SO_2 and KCl (the location of both systems are indicated in Fig. 1a) The SO_2 is fed as a gas directly into the oxidizer upstream the split of the primary and secondary register streams. The KCl is sprayed in the form of an aqueous solution directly into the flame. The system consists of a storage tank, a metering pump and an injection probe. The storage tank is equipped with an internal recirculation pump, which minimizes the risk of salt precipitation. In this work, the $\text{KCl}(\text{aq})$ solution has a concentration of 3.4 wt% of KCl which is fed by the metric pump at a constant flow rate of 0.9 l/h corresponding to a theoretical flue gas concentration of 100 ppm KCl during air combustion. The injection probe is inserted through the furnace ceiling.

The spray nozzle in the tip of the probe has a spray angle of 15° and the solution is sprayed directly into the flame.

Since the injection of $\text{KCl}(\text{aq})$ is kept constant, the S/K ratio in the system is varied by changing the amount of injected SO_2 . During oxy-fuel combustion flue gas recirculation is applied, which includes SO_2 as one of the recirculated species. A small amount of sulphur leaving the furnace is lost in the flue gas system before the recirculation due to absorption in the condenser and reactions in the filters etc. This loss of sulphur varies with time, but is monitored continuously and compensated for by adjusting the SO_2 injection to keep the SO_2 concentration constant in the oxidant. The running conditions are summarized in Table 2.

The gas composition is measured using standard gas analysers for CO , CO_2 , O_2 and SO_2 . The concentration of HCl was measured using an FTIR (Bomem MB9100) designed for gas composition analysis. For all gas composition measurements sampling gas is extracted using a water cooled suction probe. The measured HCl concentration in the flue gas exit (M8) is used to determine the degree of sulphation. The degree of sulphation has also been determined by the use of the IACMTM (in situ alkali chloride monitor) system in measurement port M7 (Fig. 1a) by means of measuring the KCl concentration. The measurement principle is based on absorption of UV-light [20] and a schematic drawing of the setup is presented in Fig. 1b. The system uses light from a 150 W intensity UV-light source (1). The light was passed through an aperture (2) and was collimated in a 90° off-axis parabolic mirror (3) with UV-enhanced aluminium coating. The collimated UV light beam is subsequently passed through another aperture (4) before reaching the flue gas channel (6). At the opposite side, the light passes a second window before the detector (8) which consists of a UV-enhanced aluminium reflective collimator equipped with a SMA connector for the optical fibre. The collected UV light was then analysed in a spectrometer (10). The collected spectrum was evaluated by means of the Differential Optical Absorption Spectroscopy (DOAS) technique in order to obtain the KCl concentration in the flue gas [21,22].

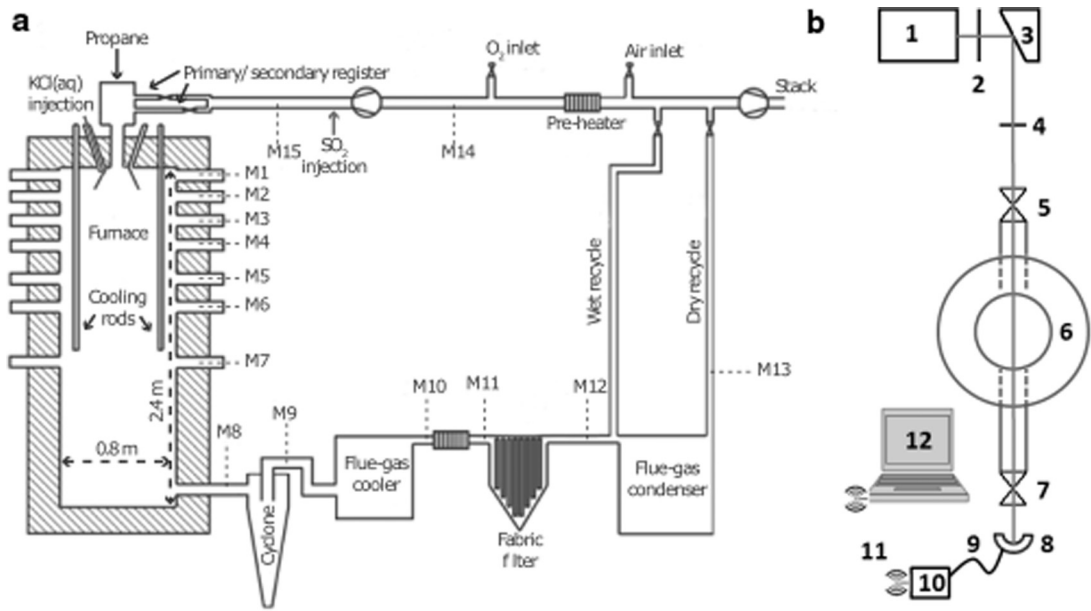


Fig. 1. (a) Schematic drawing of the 100 kW test unit at Chalmers University of Technology. The locations of the 15 measuring ports are indicated as M1–M15. (b) The set-up of the IACMTM system used. (1). UV light source, (2). Aperture, (3). Parabolic mirror, (4). Aperture, (5). Ball valve with an optical window and purge gas (N₂) connector, (6). Cross-section drawing of the furnace at the measuring point, (7). Ball valve with an optical window and purge gas connector, (8). Detector (collimator), (9). Optical fiber, (10). Spectrometer, (11). Connection between the spectrometer and the computer, (12). Computer.

Table 2
Running conditions of the experimental cases.

	Fuel feed (g/s)	O ₂ /fuel ratio (-)	O ₂ oxidizer (% dry)	O ₂ stack (% dry)
Air	1.73	1.15	21	2.95
OF25	1.73	1.15	25	3.57
S/K (injected)	KCl(aq) (l/h)	SO ₂ injection* (g/h)	SO ₂ oxidant Air	(ppm dry) OF25
1	0.9	26.5	107	485
2	0.9	53.0	215	1126
4	0.9	106.0	429	2345
6	0.9	159.0	644	3559
8	0.9	212.0	859	–

* Varied to keep the inlet concentration constant.

3.1. Data evaluation

The degree of sulphation is defined as the ratio between the amount of potassium bound as sulphates and the total amount of potassium in the system (Eq. (1)).

$$\frac{2n_{K_2SO_4}}{n_K^{inlet}} = \text{degree of sulphation} \quad (1)$$

The concentration of K₂SO₄ cannot be measured with the present set-up. The total amount of potassium is assumed to be the same as the amount of KCl fed to the system since this is the only source of potassium to the system. The concentra-

tion of K₂SO₄ is estimated by two different measurements: HCl concentration and KCl concentration using FTIR and the IACMTM system, respectively. Both methods are based on the assumption that all potassium will be found as either KCl or K₂SO₄. The degree of sulphation based on HCl and KCl measurements is then estimated according to Eqs. (2) and (3), respectively.

$$\frac{n_{HCl}}{n_{KCl}^{inlet}} \approx \text{degree of sulphation} \quad (2)$$

$$\frac{n_{KCl}^{inlet} - n_{KCl}}{n_{KCl}^{inlet}} \approx \text{degree of sulphation} \quad (3)$$

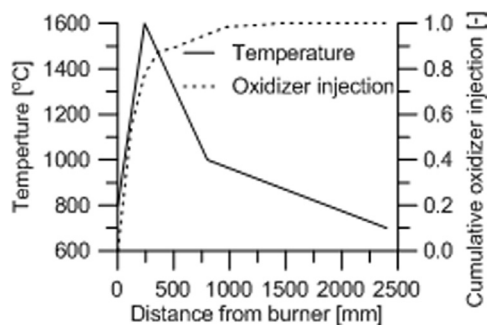


Fig. 2. The temperature profile (solid line) and cumulative oxidizer injection profile (dashed line) used in the modelling.

3.2. Modelling

The chemistry of importance for sulphation of KCl is described in the work of Hindiyarti et al. [9] and the mechanism presented in that work includes the following subsets: CO/H₂, S, Cl and K, which were validated using experiments from Refs. [17,18]. In the present work, an additional subset was added to estimate the condensation of K₂SO₄ which has been presented by Li et al. [23]. This mechanism is derived for post flame conditions and does not include any reactions describing the combustion of hydrocarbons. In addition, a second mechanism was also applied in this work in which three subsets describing the oxidation of C1, C2 and C3 are included [24–26]. The two mechanisms are combined into one single mechanism which is used for comparison with the experimental results. The modelling is used in order to simulate the entire combustion process in the experimental unit for both the Air and OF25 case; the modelling results are given the index M (Air_M and OF25_M, respectively). It should be noted that the combined mechanism used in this work has not been validated by any additional lab-scale experiments. However, the effect of adding the C1–C3 subset to the sulphation mechanism has been evaluated as part of this work; no significant effect was found during isothermal conditions above 700 °C. At lower temperatures, the sulphation was observed to be slightly faster when the C1–C3 subset was included, but the effect is minor and will not significantly influence the modelling results of this work.

The modelling has been carried out using the software ChemkinPro. The input to the modelling work in terms of temperature profiles and residence times are based on data from our previous experimental work [27]. The temperature profile used in this work is presented in Fig. 2 together with the oxidant injection profile. The temperature profile is kept the same for both the Air_M and the OF25_M cases. Both cases also use the same oxygen mixing conditions, although the absolute mass flow of ox-

Table 3
Summary of the cases investigated during the sensitivity analysis.

Case	O ₂ (%)	N ₂ (%)	CO ₂ (%)	Residence time (s)
Air _M	21	79	0	4.4
Air _M (5.3)	21	79	0	5.3
Air _M (6.4)	21	79	0	6.4
OF25 _M	25	0	75	5.6
0% CO _{2M}	25	75	0	5.6
25% CO _{2M}	25	56.2	18.8	5.6
50% CO _{2M}	25	37.5	37.5	5.6
75% CO _{2M}	25	18.8	56.2	5.6

idant differs due to the difference in chemical composition between the cases. The injection profile is used to describe the influence of radial mixing in the flame zone of the furnace (assumed to be perfect in a PFR). The geometry of the reactor is set to the same as the experimental unit for both cases. This results in different total residence times for the Air_M and the OF25_M case which is 4.4 s and 5.6 s, respectively, which is due to the difference in volumetric flow. The inlet chemical composition is kept the same as in the experiments. In the model the KCl is fed as gaseous KCl and not as an aqueous solution.

In addition to the analysis of the influence of the S/K ratio the modelling was also used to investigate the effect of the residence time and change in oxygen and carbon dioxide concentration. The analysis includes two modified cases of the Air_M case where the residence is increased from the original 4.4 s to 5.3 and 6.4 s. Four cases are created based on the OF25_M case where the oxidizer concentration of carbon dioxide is set to 75, 50, 25 and 0% on an oxygen free basis and nitrogen is then set by difference. The characteristics of all cases investigated in the sensitivity analysis are summarized in Table 3.

4. Results and discussion

Figure 3a shows both experimental and modelling results of the sulphation of KCl during combustion of propane in the 100 kW test unit. Different S/K ratios were injected into the furnace and corresponding calculations were made using the described S/K/Cl/C1–C3 mechanism. As mentioned, the degree of sulphation was experimentally determined by means of two different measurement techniques, as represented by open (FTIR) and closed (IACMTM) symbols (see Eqs. (1)–(3) in the method section). As seen, the results show a good agreement between modelling and experiments for both combustion atmospheres. For the Air case, in which both measurement techniques were used, there is also a good agreement between the experimental methods. The IACMTM system tends

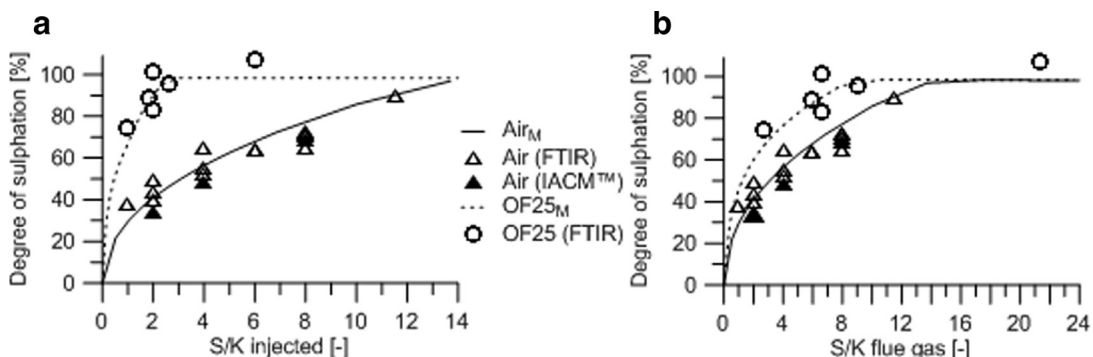


Fig. 3. Comparison between modelling and experimental results with respect to, (a) the injected sulphur to potassium ratio (S/K) and b) the S/K ratio in the flue gas. The solid and dotted line represent modelled values for the Air_M and OF25_M cases, respectively. Experimental values are indicated by symbols where open symbols represent FTIR measurements and closed symbols the IACMTM measurements.

to measure a slightly lower degree of sulphation compared to the HCl measurements. The IACMTM sampling position is located upstream of that of the FTIR, which is a plausible explanation for those minor differences; the modelling results indicate that the sulphation process might still be active at the measurement position of the IACMTM system. However, the difference is small and both methods agree well with the modelling results. Thus, both methods are considered to be valid for estimating the degree of sulphation. It should also be mentioned that the IACMTM always measured a KCl level above 95 ppm when no sulphur was added. This suggests that the loss of KCl, due to deposition on the walls, is small. Over time the sulphation of the deposited KCl may be more noticeable and this is one of the possible reasons for a measured degree of sulphation being slightly above 100% for the test cases with the highest sulphur concentration.

It is evident that the amount of sulphur available in relation to the amount of potassium (S/K-ratio) is an important parameter for the sulphation process which is shown to be valid for both air and oxy-fuel combustion atmospheres. Due to the recirculation of flue gas in oxy-fuel combustion the concentration of sulphur species is higher in the OF25 case compared to the Air case when the same amount of SO₂ is fed to the system. The degree of sulphation is always higher in the oxy-fuel than in the air-fired system for S/K injection ratios lower than 14. For injected S/K = 14, the Air case has reached almost complete sulphation which is achieved for S/K injected of about 3 during OF25. In Fig. 3b, the actual S/K ratio in the flue gases is presented for both cases; for a similar SO₂ concentration in both cases there is still a higher degree of sulphation obtained for OF25 compared to Air for flue gas S/K ratios lower than 14. This shows that the higher sulphur content is not the only explanation for a higher degree of sulphation in the oxy-fuel compared to the air-fuel atmosphere.

In our previous modelling work [8], it was observed that the overall reaction activity (defined as the integrated reaction rate with respect to residence time) of the sulphation process was increased in oxy-fuel conditions compared to air conditions. The main difference is the higher activity in the reactions in which at least one of the reactants contains sulphur. However, for high sulphur contents (S/K ratios above what is required for complete sulphation) there is also an increased reaction activity for R3, which includes also a backwards reaction, hence on-setting a reaction loop where the potassium is sulphated to KHSO₄ which to a large extent is decomposed back to KOH and which then can be sulphated again. However, we have not yet examined if the same phenomenon can be found in an atmosphere where the sulphur content is the same in oxy-fuel compared to air-fuel combustion. This decomposition is one example of a difference in sulphur chemistry between air and oxy-fuel combustion, a fact which is further discussed in our previous work [8].

Another parameter which is influenced by the flue gas recirculation and the use of pure oxygen is the residence time in the combustor; the total volumetric flow is reduced for an oxygen fraction of 25% (OF25) compared to air conditions. The effect of a change in residence time was modelled with results presented in Fig. 4. The effect of increasing the residence time for the Air_M case from 4.4 s to 5.3 and 6.3 s is shown together with a comparison with the OF25_M case for a total residence time of 5.6 s. As seen, the degree of sulphation is enhanced for an increased residence time, but the Air_M case with 6.3 s does not reach the same degree compared to the OF25_M case despite a longer residence time.

In the modelling, the temperature profile is fixed to the same conditions in both atmospheres, which enables an evaluation of possible direct chemical effects when switching from a N₂ to a CO₂ based atmosphere, see Fig. 5. The figure includes four

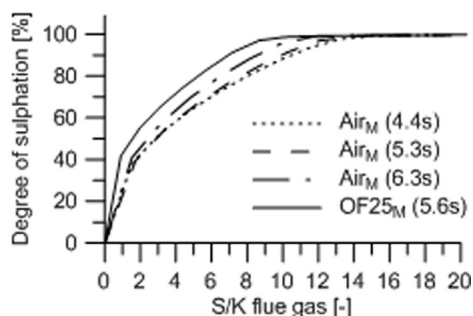


Fig. 4. The modelled degree of sulphation for the Air (4.4 s) and OF25 (5.6 s) case in comparison to Air_M (5.3 s) and Air_M (6.3 s).

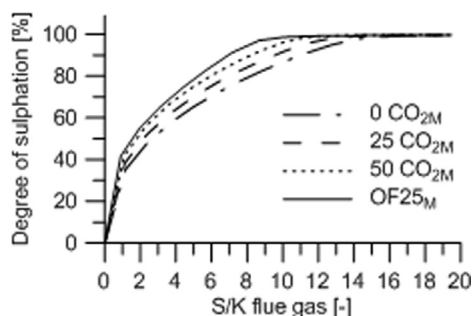


Fig. 5. Simulated degree of sulphation as a function of S/K-ratio in the flue gas for four cases with different flue gas compositions.

cases with 25% oxygen where the composition of the remaining 75% is varied from pure nitrogen to pure carbon dioxide. The latter case is then the same as OF25_M. All cases in the figure has a residence time of 5.6 s. Comparing the Air_M case and the 0% CO₂ case shows no significant effect of increasing the oxygen concentration with respect to the degree of sulphation and this case is therefore omitted in the figure. This indicates that the increase in oxygen concentration from 21 to 25% does not cause the degree of sulphation to change. However, it is evident that the degree of sulphation increases for a higher CO₂ concentration. When 75% of the N₂ is replaced with CO₂ (56% CO₂ and 19% N₂ including the oxygen) the same degree of sulphation is reached as in the OF25_M case (this result is also omitted in Fig. 5). In general, R19 is the only reaction among the 20 most active potassium reactions which includes CO₂ and according to our previous work [8] this reaction was suggested to be more active during oxy-fuel combustion compared to air combustion. On the other hand, higher CO₂ concentrations may also change the composition and activity of the radical pool via its reaction with atomic hydrogen (H) when forming carbon monoxide (CO) and hydroxide (OH); H and OH are represented in several

reactions with potassium as well as with sulphur and chlorine which could influence the overall sulphation. To further scrutinize the chemistry of the K/S/Cl in CO₂-based atmospheres, a more extensive modelling work combined with lab-scale experiments will be required, which is out of scope of the present study. It is however obvious that the sulphation process is strongly enhanced by the flue gas conditions in oxy-combustion and that the most influential parameter is the S/K ratio in the fuel/fuel blend added to the system and that this will be an advantage in co-combustion systems when oxy-combustion is applied.

5. Conclusions

The sulphation of KCl was studied during combustion of propane in a 100 kW test facility and experiments with both air and oxy-fuel combustion conditions were conducted. According to the results presented in this work, the sulphation of KCl is substantially enhanced in oxy-fuel combustion compared to air combustion. The experiments show that an increased concentration of SO₂ in oxy-fuel combustion is the main reason for the increased degree of sulphation, but modelling also shows that the elevated CO₂ concentration has a chemical influence, and, that a small effect is introduced by a change in combustor residence time. In addition, the satisfactory agreement between modelling and experiments suggests that the kinetic gas phase mechanism used is appropriate for describing the sulphation of KCl in the tested turbulent air-fuel and oxy-fuel flames.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.proci.2016.08.069](https://doi.org/10.1016/j.proci.2016.08.069).

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