Experimental and Modeling Studies of SO3 Homogeneous Formation in the Post-Flame Region

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ABSTRACT

SO3 exists in the atmosphere in the form of sulfuric acid aerosol, heavily polluting the environment and decreasing the safety of boiler equipment. This study focuses on the homogeneous formation mechanism of SO3 in the post-flame region. We conducted experiments and simulations to investigate the influence of various combustion parameters on SO3 generation. The formation of SO3 was affected by factors such as temperature and the concentrations of O2, SO2, NO, and H2O. With a rise in temperature, the SO3 concentration initially increased but then decreased, reaching its maximum at about 1000°C, which indicates that SO2 can promote the formation of SO3 over a certain temperature range. An increase in the O2 concentration promoted the formation of O and OH radicals, which enhanced the generation of SO3 from SO2. The presence of NO resulted in direct and indirect interactions between NOx and SOx species for different reaction sets, potentially enhancing SO3 generation. With an increase in the H2O concentration, SO3 formation initially increased rapidly before plateauing. ROP (rate of production) and sensitivity analyses suggest that adding H2O will produce O and OH, which strongly influence SO3 formation. Furthermore, the sensitivity analysis indicated that radicals and the direct reaction between SO2 and NO2 play significant roles in SO3 formation.

Keywords: Sulfuric acid aerosol; Chemical kinetics; Mechanism analysis; ROP analysis; Sensitivity analysis.

INTRODUCTION

SO2 is the atmospheric pollutant emitted from the combustion of fossil fuel. The main source of SO2 is the combustion of coal (Kato et al., 2016). A small amount of SO2 will subsequently be oxidized to SO3. SO2 causes serious damage to the equipment and environment of the boiler tail. Kagawa (2014) deemed that the growth of coal combustion has led to greater amounts of S emitted to the atmosphere. At temperatures above 200°C, as long as there is about 8% moisture in the flue gas, 99% of SO3 will be converted into sulfuric acid vapor. SO2 has always been in the atmosphere in the form of sulfuric acid aerosol (the diameter is generally 0.4–1.2 µm) (Hardman et al., 1988). When the flue gas temperature is lower than the acid dew point, low temperature corrosion may occur on the air preheater and low temperature economizer. SO3 can react with NH3, generating NH4HSO4 which will obstruct the air preheater. Furthermore, SO3 also reduces the rate of mercury removal from flue gas (Moser, 2007).

Mist particles are emitted into the atmosphere, which gives smoke its blue color, and the minimum concentration of SO3 causing this phenomenon is related to atmospheric conditions. In general, if the content of SO3 in flue gas is above 10 ppm, smoke opacity will be significant. When the SO3 concentration is 5 ppm, plume opacity can be as high as 20%. When the SO3 concentration is more than 10 ppm, smoke will be visibly blue, increasing the H2SO4 aerosol concentration near the power plant (Srivastava et al., 2004). A U.S. EPA report showed that SO3 and H2SO4 aerosols may be associated with a series of adverse health effects, including respiratory tract irritation and difficulty breathing (Walsh et al., 2006).

The concentration of SO3 in flue gas is related to SO2 concentration, the excess air coefficient, flue gas temperature, fly ash composition, and other factors (Lou, 2008). The conversion rate of SO2 to SO3 is about 0–2%. Kio (2001) determined that oxygen atoms in the high temperature combustion zone of a furnace react with SO2 to form SO3:

$$\text{SO}_2 + \text{O} (+\text{M}) \leftrightarrow \text{SO}_3 (+\text{M}) \quad (R1)$$

The formation of SO3 was shown by Fleig et al. (2009) to be the primary SO3 formation pathway at 1000–1400°C:
SO₂ + O ⇌ SO₃ (R1')

At 700–1000°C, SO₃ formation occurs via HOSO₂:

SO₂ + OH ⇌ HOSO₂ (R2)

HOSO₂ + O₂ ⇌ SO₃ + HO₂ (R3)

It has been confirmed that (R2) and (R3) are insignificant above 1000°C, because of the low stability of HOSO₂ (Alzueta et al., 2001). According to Han (2015), SO₃ formation is mainly controlled by thermodynamic equilibrium at high temperatures, and by reaction kinetics (Monckert et al., 2008) at low temperatures.

During combustion, the S element in the fuel is partially converted to SO₂, and if oxygen is excessive, some SO₂ will be further oxidized to SO₃ (Lee et al., 1967). Previous studies have shown that the primary condition for SO₃ production is excess O₂. If O₂ concentrations are below 3%, SO₃ production is sensitive to the O₂ concentration. But above this concentration, an increase in O₂ concentration has little effect on the formation of SO₃. Combustion and flue gas cooling cover a large range of temperatures. At high temperatures (above 1300°C), formation of SO₃ can reach equilibrium within 2 s, while at low temperatures (i.e., 300–700°C), equilibration may take days to years. Temperature directly affects homogeneous SO₃ formation by changing the reaction rate and the equilibrium point of the reaction. The oxidation rate declines with the increase of temperature. It can be concluded SO₃ is mainly formed at intermediate temperatures of about 1000°C, given the residence time of flue gas in each temperature section. Glarborg et al. (1996) studied the reaction characteristics of SO₂ and found that peak SO₃ formation occurred around 950°C. On the other hand, Bayless et al. (2000) found that at low temperatures if free radicals (O, H, etc.) are abundant, a certain amount of SO₃ can also be obtained to maintain the performance of ESP. In addition, Merryman (1979) studied staged combustion, assuming that temperature and O atom concentration were the main factors affecting formation of SO₃, and suggested that temperature affects oxidation of SO₂ by changing the concentration of O atoms. Therefore, temperature not only affects SO₃ formation by changing the reaction equilibrium (the rate of SO₃ decomposition and formation), but also via important indirect effects.

Currently, most research is focused on the generation mechanism of SO₂ and NOₓ, ignoring SO₃ generation. In this paper, homogeneous formation of SO₃ and its influencing factors were studied by experiments and simulations, and the homogeneous formation mechanism of SO₃ in post-flame region was clarified.

**EXPERIMENTAL AND MODELING**

**Introduction of Experimental Equipment**

The experimental device is shown in Fig. 1. The setup consists of three major sections: burner, reactor, and sample collector. The inlet gas composition is SO₂, N₂, O₂, CO₂, NO and H₂O. Gas is mixed into flue gas analyzer (testo 350). After the gas content is measured, the first three-way valve is adjusted to make N₂ and CO₂ enter the ultrasonic atomizer to carry H₂O. Then adjust the second three-way valve to make all gases enter the reactor, which is heated by a tubular resistance furnace (SK-2.5-13TS). Exhaust gas then passes through a serpentine condenser tube. Using a digital display thermostatic water bath (HH-1), the condenser temperature is maintained at 80°C. The SO₃ concentration is measured by the U.S. EPA method 8A. The ideal one-dimensional flow reactor model is adopted, with a residence time of 4 s and a pressure of 1 atm.

The quartz tube reactor is 1065 mm long, with an outer diameter of 28 mm and an inner diameter of 24.4 mm. The total flow of the reaction gas is 3 L min⁻¹, and the reaction gas composition is shown in Table 1.

![Fig. 1. Schematic diagram of experimental apparatus.](image-url)
Simulation Methods and Models

A detailed gas-phase kinetic model was utilized to discuss the measured SO$_3$ concentrations. The calculations were carried out by CHEMKIN-IV software. This combined model considers C, H, O, N, and S, include 694 reactions. But heterogeneous chemistry is not included in the mechanism. And the interactions between sulfur and chlorine are not included. The mechanism includes the oxidation of hydrocarbons based on the work of Glarborg et al. (1998, 2003) and Alzueta et al. (2008). The nitrogen chemistry and the interactions between hydrocarbons and nitrogen species are based on the work of Glarborg et al. (1998) and Dagaut et al. (2008). The sulfur chemistry in the mechanism is described in the work by Alzueta et al. (2001) and Giménez-López et al. (2011). Moreover, the reactions of sulfur-containing elements are more comprehensive in this model than previously. And the direct interactions between SO$_x$ and NO$_x$ species were considered in this model.

RESULTS AND DISCUSSION

Gas-phase coal combustion experiments were performed to obtain speciation data of SO$_x$ under a variety of operating conditions. Sampling temperature ranged from 400°C to 1300°C within the reactor. Other factors included O$_2$, SO$_2$, NO, and H$_2$O concentrations.

Effect of Temperature on SO$_3$ Formation

The experimental conditions were 550 ppm NO, 2000 ppm SO$_2$, 2.22% H$_2$O, and 5% O$_2$ (Fig. 2).

As shown in Fig. 2, the experimental results and simulated data indicated that the concentration of SO$_3$ first increased, but then decreased with increasing temperature. The maximum SO$_3$ concentration was around 1000°C. At 400–1000°C, the concentration of SO$_3$ increases with an increase in temperature, and the concentration of SO$_3$ decreased with an increase in temperature when the temperature is higher than 1100°C. When the temperature was below 700°C, the SO$_3$ concentration was very near or below the limit of detection. Wang (2015) also observed a similar trend in SO$_3$ concentration with temperature. This model is modified to ensure that the modeling results in the middle temperature region (800–1200°C) are consistent with the experimental results, but the discrepancy in the low temperature region (400–700°C) cannot be completely eliminated.

Through ROP analysis, the main reactions of SO$_3$ were (R1)–(R4).

SO$_2$ + NO$_2$ $\leftrightarrow$ NO + SO$_3$ (R4)

When the resistance furnace wall temperature is between 600°C and 800°C, the base reaction for SO$_3$ formation is (R4). The wall temperature of the resistance furnace increases the concentration of activated molecules in the reaction gas, and decomposition of H and OH with H$_2$O increases. According to the literature (Mantashyana, 2014), O radicals are mainly produced by (R5) and decomposition of O$_2$. The concentration of H radical increased in this temperature range, which promoted the formation of O radical. The concentration of NO$_2$ also increased by (R6), and the rate of formation of (R4) increased as well. Higher concentrations of NO$_2$ result in (R4) playing a decisive role in the generation of SO$_3$.

O$_2$ + H $\leftrightarrow$ OH + O (R5)

NO + O (+M) $\leftrightarrow$ NO$_2$ (+M) (R6)

As temperature increases, the total formation rate of SO$_3$ increases rapidly. Fleig (2013) measured the formation of SO$_3$ by introducing different gas components into a one dimensional furnace. Results showed that NO promoted SO$_3$ formation at low temperatures.

| Test | N$_2$ (%) | CO$_2$ (%) | SO$_2$ (ppmv) | NO (ppmv) | O$_2$ (%) | H$_2$O (%) |
|------|-----------|------------|---------------|-----------|-----------|------------|
| 1    | 77.525    | 15         | 2000          | 550       | 5         | 2.22       |
| 2    | 81.525    | 15         | 2000          | 550       | 1         | 2.22       |
| 3    | 79.525    | 15         | 2000          | 550       | 3         | 2.22       |
| 4    | 75.525    | 15         | 2000          | 550       | 7         | 2.22       |
| 5    | 73.525    | 15         | 2000          | 550       | 9         | 2.22       |
| 6    | 77.675    | 15         | 500           | 550       | 5         | 2.22       |
| 7    | 77.625    | 15         | 1000          | 550       | 5         | 2.22       |
| 8    | 77.575    | 15         | 1500          | 550       | 5         | 2.22       |
| 9    | 77.475    | 15         | 2500          | 550       | 5         | 2.22       |
| 10   | 77.425    | 15         | 3000          | 550       | 5         | 2.22       |
| 11   | 77.48     | 15         | 2000          | 0         | 5         | 2.22       |
| 12   | 77.4546   | 15         | 2000          | 254       | 5         | 2.22       |
| 13   | 77.3814   | 15         | 2000          | 986       | 5         | 2.22       |
| 14   | 79.645    | 15         | 2000          | 550       | 5         | 0          |
| 15   | 67.445    | 15         | 2000          | 550       | 5         | 12.2       |
| 16   | 61.545    | 15         | 2000          | 550       | 5         | 18.1       |
| 17   | 46.445    | 15         | 2000          | 550       | 5         | 33.2       |

Table 1. Gas composition in experiments.
Fig. 2. Relationship between SO$_3$ concentration and temperature.

When the resistance furnace wall temperature is between 800°C and 1600°C, the basic reactions for SO$_3$ formation are (R3) and (R4). With an increase in temperature, H and OH production is enhanced by H$_2$O decomposition. An increase in the concentration of H radicals promotes formation of O radicals, enhancing (R7) and leading to an increase in OH concentration. A combination of H and OH will promote (R2), which will facilitate (R3).

$$O + H_2O \leftrightarrow 2OH \quad (R7)$$

The concentration of OH radical is higher than NO$_2$, so the effect of reaction (R3) is greater than that of (R4).

When the resistance furnace wall temperature is 1100°C, as the temperature continues to rise, the reaction rate of (R6) is accelerated and the concentration of NO$_2$ begins to decline. N$_2$ reacts with O$_2$ to generate large amounts of NO, and higher concentrations of NO inhibit (R4). Above 1100°C, the free radical HOSO$_2$ begins to decompose in the reaction gas.

Fleig et al. (2009) pointed out that formation of SO$_3$ in a power plant boiler mainly occurs between 900 and 1300°C, which is approximately consistent with the average temperature range of SO$_3$ generation.

**Effect of O$_2$ on SO$_3$ Formation**

The O$_2$ concentration of the combustible mixture was varied from 1% and 9% in simulations and experiments. Other inlet gas content remained unchanged.

Fig. 3 shows the outlet concentration of SO$_3$ derived for different concentrations of O$_2$ in the inlet gas. The SO$_2$ concentration was 2000 ppm in all experiments. SO$_2$ formation was favored by high O$_2$ concentrations, as well as by temperature. The concentration of SO$_3$ increased with increasing O$_2$, but the degree of influence gradually decreased. Duan (2015) also demonstrated that oxygen enrichment enhances SO$_3$ formation. When the concentration of O$_2$ is less than 7%, the increase in O$_2$ concentration promotes the formation of SO$_3$. On the contrary, the influence on the formation of SO$_3$ is reduced. As shown in (R5), with increasing O$_2$ concentration, a higher concentration of O and OH radicals is expected, which contributes to higher SO$_3$ formation. Due to the fixed content of SO$_2$, when O$_2$ concentration is low, increasing the oxygen content can rapidly increase SO$_3$ formation. However, the O$_2$ that can participate in the reaction is affected by SO$_2$ concentration and temperature, so the effect of oxygen content on the SO$_3$ production rate gradually decreases.

ROP analysis was performed on reactions (R1)–(R4). When the concentration of O$_2$ increases, both (R3) and (R4) play a major role in the formation of SO$_3$. An increase in O$_2$ concentration promoted (R5) to produce more free radical O and OH, and then promoted (R6), such that (R3) plays a decisive role in the formation of SO$_3$.

**Effect of SO$_2$ on SO$_3$ Formation**

The experimental and modeling conditions were 550 ppm NO, 2.22% H$_2$O, 5% O$_2$, and a residence time of 4 s, SO$_2$ concentration ranged 500–3000 ppm. Fig. 4 shows the experimental and simulated SO$_3$ concentrations for different inlet SO$_2$ concentrations.

As shown in Fig. 4, both the experimental and modeling results show that the concentration of SO$_3$ increased with an increase in SO$_2$. A similar trend was observed in a study (Belo et al., 2014) investigating gas-phase conversion of SO$_2$ to SO$_3$ in a simulated oxy-combustion environment, which was explained by the dependency of the reaction order on SO$_2$ concentration.

The simulation process analyzed by ROP shows that the most important reactions for SO$_3$ formation are (R3) and (R4) with increasing SO$_2$ concentrations. Increasing the concentration of SO$_2$ promotes reaction (R2), thus promoting (R3).
Effect of NO Concentration

NO concentrations between 0 and 1000 ppm were analyzed in simulations and experiments to investigate the effect of NO on the final SO$_3$ concentration (Fig. 5).

NO is known to affect the amount of SO$_3$ produced in this system. Increasing NO concentration, an increase in SO$_3$ concentration was observed for both experiments and simulations. When the NO concentration is below 600 ppmv, there are some differences between experimental data and simulated data. However, for NO concentration above 600 ppmv, the experimental results are basically consistent with simulated results. In a previous investigation, Fleig et al. (2011) showed that small amounts of NO can result in increased SO$_3$ generation during combustion.

ROP analyses showed that the following reactions were important to SO$_3$ formation: (R1), (R3), (R4), and (R8). (R3) and (R4) were determined to be most important for SO$_3$ generation.

\[
\text{SO}_3 + \text{OH} \leftrightarrow \text{SO}_2 + \text{HO}_2 \quad \text{(R8)}
\]

The NO inlet concentration influenced the SO$_3$ outlet concentration, because NO acts on the radical pool through (R6) and (R9).

\[
\text{NO} + \text{HO}_2 \leftrightarrow \text{NO}_2 + \text{OH} \quad \text{(R9)}
\]

(R9) increases OH production, which can promote (R2).
and (R3), and results in higher production rates of SO$_3$ from SO$_2$ via HOSO$_2$. However, as (R6) indicates, when NO is converted into NO$_2$, O is consumed. This reaction is in competition with (R1). But the most important direct interaction between NO$_x$ and SO$_x$ species is (R4), although (R6) consumes O and affects SO$_3$ generation, the SO$_2$ generated by (R6) will eventually generate SO$_3$ through (R4). Thus, the production of SO$_3$ increases with an increased NO concentration. A computational parametric study conducted by Choudhury et al. (2016) also concluded that the direct interaction between SO$_x$ and NO$_x$ mostly occurred via (R4), while indirect interactions changed the radical pool.

**Effect of H$_2$O Concentration**

In addition to obtaining the SO$_3$ content in coal combustion flue gas under different combustion parameters, the influence of H$_2$O was investigated through kinetic simulations and experiments (Fig. 6). There is a discrepancy between the experimental and modeling results. As far as the experimental results are concerned, the generation of SO$_3$ is very low when there is no H$_2$O. When the inlet gas contains 2.22% H$_2$O, the amount of SO$_3$ generation initially increases rapidly. Then with the increase of H$_2$O content, the generation of SO$_3$ remains constant. However, the simulation results demonstrate that the concentration of SO$_3$ increases gradually with the increase of H$_2$O content to 18.1%, and then remains unchanged. The reason for the discrepancy may be that the H$_2$O added in the experiment may not be vaporized in time. Anyway, the trend of the experimental and modeling results is consistent. H$_2$O has a positive effect on the formation of SO$_3$.

$$H_2O \leftrightarrow OH + H \quad (R10)$$

Most previous studies are on the effect of H$_2$O on SO$_3$ formation, but their conclusions are different. There is still no consistent conclusion about the effect of H$_2$O on SO$_3$ formation. Belo (2014) suggested that the conversion of SO$_2$ to SO$_3$ is independent of water content. He found that increasing the moisture concentration from 3% to 9% did not have a significant effect on the conversion of SO$_2$ to SO$_3$. Wang (2015) found that the outlet SO$_3$ concentration decreased drastically with the injection of steam, which indicated steam could inhibit SO$_3$ formation. Fleig et al. (2013) concluded that an increase in H$_2$O concentration clearly increased SO$_3$ formation, as evidenced by experimental measurements and model predictions.

**SENSITIVITY ANALYSIS**

In the current research, experimental results and simulation data of others are similar, with the exception of the effect of H$_2$O concentration. To study the effect of inlet H$_2$O concentration on SO$_3$ generation, a sensitivity analysis was carried out.

Sensitivity analyses were performed on the model to determine the rate dominating reactions for SO$_3$ formation. The sensitivity function in the CHEMKIN-IV software was used for this purpose and the data was analyzed based on normalized coefficients. Different sets of reactions were observed to play a role in SO$_3$ formation for this mechanism. The reactions (R2), (R11), (R12), (R3), (R4), (R1) and (R-6) were found to influence SO$_3$ formation.
The sensitivity coefficients of the most sensitive reactions of input gas containing H2O are shown in Fig. 7. The X-scale is the logarithmic sensitivity coefficient, which can be calculated as “$\frac{\partial \ln m}{\partial \ln k}$”. Where $m$ is SO3 concentration in flue gas and $k$ is the pre-exponential factor of the Arrhenius formula.

$$\text{NO}_2 + \text{O} \leftrightarrow \text{NO} + \text{O}_2 \quad (R11)$$

$$\text{OH} + \text{HO}_2 \leftrightarrow \text{H}_2\text{O} + \text{O}_2 \quad (R12)$$

Positive sensitivities towards SO3 generation were found for (R2), (R11), (R12), (R3), (R4), and (R1). Evolution of OH radicals and O through these reactions facilitates SO3 generation via (R1)–(R3). (R4) had a strong positive effect on SO3 generation by the direct interaction between SO2 and NO2. (R2) was found to affect SO3 formation to the greatest extent. Since the inlet gas contained water, a large amount of OH and O free radicals were generated by (R10), (R5), and (R7). So that, (R2), (R11), (R12), and (R1) were encouraged, enhancing the formation of SO3.

A negative influence was observed for (R-6) due to an increase in O free radical concentration. The sensitivity analysis showed that S formation is highly sensitive to reactions involving H, OH, and O radicals.

On the other hand, when the input gas did not contain H2O, the main reactions that affect SO3 generation were (R11), (R1), (R-6), (R4), and (R13). The sensitivity coefficients of the most sensitive reactions of input gas without H2O are shown in Fig. 8.

$$\text{SO}_2 + \text{O} (+\text{N}_2) \leftrightarrow \text{SO}_3 (+\text{N}_2) \quad (R13)$$

Obviously, (R11) was found to affect the SO3 formation to the greatest extent, instead of (R2). In this case, (R11), (R1), (R4), and (R13) had a positive effect on SO3 formation. On the contrary, (R6) still had a negative effect on SO3 formation. Compared with adding water, fewer reactions affect SO3 generation. Moreover, the negative effect of (R6) is greater than when water is added. The reason for this is that without water, relatively small amounts of OH and O form.

The simulation results therefore show that the direct reaction between SO2 and NO2 plays an important role in the formation of SO3, whether or not H2O is in the input gas.

SO3 gas generation experiments and chemical kinetic simulation results for the transformation of SO2 to SO3 are summarized in Fig. 9. Changing different factors influence processes (a), (b), and (c), affecting transformation of SO2 to SO3.

CONCLUSIONS

In this comprehensive study, sulfur chemistry, particularly SO3 generation in the post-flame region, was investigated by both modeling and experimental methods. In particular, the influence of flue gas conditions (temperature, O2, SO2, NO, and H2O) on the formation of SO3 was studied.

Modeling temperature ranged from 400°C to 1300°C. With an increase in temperature, the concentration of SO3 increased initially and then decreased, achieving its maximum value at around 1000°C. Additionally, the SO3 concentration increased with the SO2 concentration, and the outlet SO3 concentration increased with the NO and O2 concentrations. H2O also contributed to the formation of SO3.

To further study the effect of the influential factors on SO3 in flue gas, an improved kinetic mechanism was built based on previous research. The direct interactions between SOx and NOx species were addressed in this model, and it was found that significant SO3 formation occurs due to the direct interaction of SO2, NO, and NO2. ROP analyses revealed that reactions involving O, OH, and H dominated SO3 generation.
Sensitivity analysis was carried out for two cases: inlet gas with and without H\textsubscript{2}O. The direct reaction between SO\textsubscript{2} and NO\textsubscript{2} played an important role in the formation of SO\textsubscript{3}. Moreover, when the inlet gas contained H\textsubscript{2}O, the subsequently generated OH and O significantly affected the formation of SO\textsubscript{3}.

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