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Combustion chemistry of COS and occurrence of intersystem crossing

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1. Introduction

The presence of sulfur impurities in bio and fossil fuels affects the combustion process, requiring detailed understanding of the oxidation reactions to design air-purification devices to avoid pollution. However, present models of sulfur combustion fail to explain the behaviour observed in experiments, especially the flammability and fire hazard of sulfur species. Sulfur may comprise up to several percent by weight in coals, natural gas (the so-called sour gas), coal seam gas and syngas. In energy industry, the conversion of H2S into solid-state sulfur during Claus treatment leaves small amounts of unconverted CS2 and COS in natural gas. Significant quantities of CS2 and COS also materialise during the thermal-oxidative reaction of sulfur-containing species in presence of hydrocarbons, such as in fuel-rich oxidation of methane seeded with H2S during the pyrolysis of ethylene doped with SO2.

Commercial grades of natural gas contain typically 5.5 mg·m−3 sulfur species, in which the odourant mercaptan (CH3SH) contributes 4.5 mg·m−3 as indicator of leakage. Further oxidation of CH3SH present in natural gas also leads to formation of H2S, CS2 and COS as intermediates in the combustion process. Municipal waste releases polyaromatic hydrogen (PAH), NOx, as well as sulfur containing species as pollutants during waste to energy conversion.

Additionally, the reduced sulfur species (H2S, CS2, COS and CH3SH) display high flammability and explosion hazard, which demand strict safety procedures during storage, transportation and processing in fuel industry. Especially, the low-cost and environmentally-friendly lithium-sulfur batteries may engender hazards in their manufacturing and recycling, due to the flammability of sulfur species. In the environment, COS exists as the most abundant sulfur carrier in the atmosphere, as well as sulfur containing species as pollutants. Municipal waste releases polyaromatic hydrogen (PAH), NOx, as well as sulfur containing species as pollutants during waste to energy conversion.

Despite the important role of reduced sulfur species in the energy and environmental fields, studies on combustion chemistry of CS2 and COS remain limited. Since COS appears as an intermediate in the oxidation of CS2, the COS/O2 sub-mechanism imposes a substantial influence on this
process [34]. By conducting a critical review and quantum chemical calculations, Glarborg and Marshall proposed a comprehensive oxidation mechanism for COS [35] and CS₂ [36]. The reaction scheme of Glarborg and Marshall overestimates the ignition temperature of both CS₂ and COS as measured in a tubular-flow reactor [37,38], at temperatures below 1400 K, by 260 K and 140 K, respectively, under the stoichiometric condition. This disagreement has important safety implications as CS₂ and COS may appear safer than indicated by their kinetics. Similarly, Abián et al. [39] reported a discrepancy between the predictions from this mechanism and the results of experiments performed under moist atmosphere in a tubular-flow reactor.

We have recently revised the oxidation mechanism of CS₂ based on the results of both experiments and quantum chemical calculations (at CBS-QB3 level), improving the important elementary reactions [26,40]. Conversion of COS has been captured as a critical intermediate in oxidation of CS₂ [40]. The crossing-over between the triplet (ground state) and singlet (excited state) reaction surfaces prevails in oxidation of reduced sulfur species, including the reactions of $\text{H}_2\text{S} + \text{O}_2$ [41], $\text{SH} + \text{SH}$ [42], $\text{CS}_2 + \text{O}_2$ [36], $\text{CS} + \text{O}_2$ [26], $\text{COS} + \text{O}_2$ [40], $\text{S} + \text{O}_2$ [43] and $\text{SO} + \text{O}_2$ [26]. The intersystem crossing (ISC) represents the transition between triplet and singlet pathway, to avoid the high activation barrier on traditional triplet surface, offering lower activation energy from 134.3 kJ mol$^{-1}$.

Reaction R1 initially changes its path from a triplet to singlet surface to activate the oxidation energy of 134.3 kJ mol$^{-1}$. It then proceeds on the singlet surface until completion to produce $\text{CO}$ and $\text{SO}_2$, both species detected in experiments. While it is possible that, a reaction may switch more than once between two spin surfaces, the results of the experiments tell us that the reaction does not return to its triplet pathway. Had the reaction switched back to the triplet pathway, it would have produced $\text{CO}_2$ and $\text{SO}_2$. However, we have detected no CO (only CO) in the experiments [40]. This occurred despite the products of the triplet pathway displaying lower energy by 15.4 kJ mol$^{-1}$.

This study conducts direct experimental measurements of oxidation of COS in a jet-stirred reactor (JSR), to further improve our previously-proposed mechanism for COS oxidation [40]. Using the infrared spectroscopy, we carefully determine the conversion of COS to produce CO and $\text{SO}_2$, in the industrially-relevant temperature window of 550–1400 K, under ambient pressure and at a constant residence time of 1.88 s. We examine the performance of the previously-proposed kinetic mechanism and conduct a sensitivity analysis on the conversion of COS to identify the governing elementary reactions for its oxidation. Furthermore, by considering the oxidation of COS as a single step reaction, we fit the Arrhenius parameters for Reaction R1 directly from our experimental measurements. Finally, we validate the updated mechanism against the experimental measurements of other researchers and discuss the influence of moisture in the oxidation of COS.

2. Methodology

The following text provides a concise account of our jet-stirred reactor (JSR) system, with the experimental set-up described in detail in reference [45]. Fig. 1 illustrates the schematic diagram of the apparatus, including the temperature profiles in the electrically-heated single-zone furnace deployed in this study. Table S1 in Supplementary data lists the flow rates implemented in the experiments.

The jet-stirred reactor [46,47], built by Monash Scientific, Melbourne, Australia, incorporates four nozzles, each with 0.3 mm ID, hosted in a spherical space. This design induces a high Reynolds number of around 1990 for the inlet flow through the nozzles into the reactor, providing mixing and eliminating the temperature and species gradients in the reactor [48]. For this reason, the jet-stirred reactor approximates well the ideal continuous stirred tank reactor (CSTR), with CSTR named as the perfectly-stirred reactor (PSR) in the combustion literature [46]. Ultra-high purity quartz (99.99%) is used to construct the reactor to minimise the surface reaction as Wang et al. [49] reported the order of catalytic activity of CaO > Fe₂O₃ > Al₂O₃ > SiO₂ (at 313 K) for oxidising CS₂ on atmospheric particles. Additionally, the spherical jet-stirred reactor minimises the surface to volume ratio compared to the tubular flow reactor.

A Fourier transform infrared (FTIR, Perkin Elmer, U.S.) spectrometer facilitated online monitoring and quantitating the gas species exiting JSR, by averaging 8 individual spectra, each requiring approximately 15 s to collect. Thus, each IR spectrum presented in this contribution signifies about 2 min of data acquisition. QASoft software (Infrared Analysis Inc., U.S.) served to quantitate the species concentration, with the following limits of detection (LOD): $[\text{SO}_2] = 5$ ppm, $[\text{CO}] = 20$ ppm, $[\text{CO}] = 9$ ppm, using the IR bands for each of these gases (2086.1–2111.6 cm$^{-1}$ for COS, 1400.9–1302.2 cm$^{-1}$ for SO₂ and 2226.7–2144.7 cm$^{-1}$ for CO). Due to the low detection limit of CO, we have also conducted a calibration for the FTIR with standard CO gas (BOC, Australia, see Section S13 in Supplementary data). No CO₂ formed in the experiments, as revealed by lack of detection of this gas at the reactor outlet.

We adopted the COS/O₂ sub-mechanism included in our previous mechanism for CS₂ oxidation [26], which in turn had been based on the work of Glarborg et al. [35,36]. The mechanism involves the improved COS/O₂ subset that features the intersystem crossing. Finally, Chemkin-Pro [50] afforded the implementation of a perfectly stirred reactor to model the species concentrations in the exhaust stream from the reactor, while the sensitivity analysis served to locate the controlling steps for the COS conversion. Because of mixing of its contents, the concentrations of species in the reactor and in the outlet are the same.

3. Results and discussion

3.1. Experimental results for oxidation of COS

Figures 2 and S1 illustrate the direct measurements of the FTIR spectra for the oxidation of COS under stoichiometric (Fig. 2, $\lambda = 1.00$) and near-stoichiometric (Fig. S1, $\lambda = 1.30$, 1.15, 0.85 and 0.70) conditions, with the individual spectra spaced every 20 K, for the residence time of 1.88 s. The peaks at 2071.3 cm$^{-1}$, 2131.8 cm$^{-1}$ and 1336.7 cm$^{-1}$ identify COS, CO and $\text{SO}_2$, respectively. In agreement with the previous experiments [34,38], oxidation of COS does not produce CO₂. Thus, we define the stoichiometric condition for the oxidation of COS as:

\[
\text{COS} + \text{O}_2 = \text{CO} + \text{SO}_2
\]

Rstoichiometry

The oxidation of COS commences at a significantly low temperature. Under the stoichiometric condition ($\lambda = 1.00$) and the residence time of 1.88 s, the oxidation (Fig. 2) sets off at 610 K, with COS completely converted to CO and $\text{SO}_2$ at around 1230 K. For the fuel-lean mixture ($\lambda = 1.30$, Fig. S1(a)), the reaction arises at 570 K and finalises at 1190 K; i.e., at a lower temperature than for the stoichiometric condition, because of the abundance of oxygen. However, under the fuel-rich condition ($\lambda = 0.70$, Fig. S1(d)), no complete conversion of COS comes to pass at temperatures up to 1310 K. For temperature above 1210 K, we highlight
a significant drop in the concentration of COS that occurs after the complete depletion of O\textsubscript{2} (as illustrated in Fig. S2(b) in Supplementary data). This is because, for temperatures above 1210 K, the pyrolysis process prompts the further consumption of COS.

We conducted three repeat experiments for each condition, achieving reproducibility within 5\% for the peak absorption of each species for all experimental temperatures and oxygen-fuel equivalence ratios. Supplementary data provide a comparison of the results from these experiments (Table S2). The experimental uncertainty originates from the accuracy of mass flow controllers (\(\pm 2\%\)), the error range for temperature in the reaction zone (\(\pm 2.5\ K\)), fluctuation of room temperature (295 K–299 K) and the online FTIR measurement of species concentration (\(\pm 2\%\)) due to background noise. While the error in the concentration of the purchased mixture of COS/N\textsubscript{2} (\(\pm 30\ ppm\) COS) does not affect the precision of the present measurements, it influences their accuracy. QASoft software [51] enabled the quantitation of COS, CO and SO\textsubscript{2} for all spectra measured with 0.1 m cell. The elemental balances for sulfur and carbon correspond to 100 \(\pm 10\%\) and 100 \(\pm 4\%\), respectively, with the elevated uncertainty for sulfur due to the unaccounted S formed along the pyrolysis pathway after the depletion of O\textsubscript{2} in the fuel-rich experiments.

### 3.2. Kinetic modelling of oxidation of COS

Fig. 3 contrasts the Chemkin modelling results of Glarborg and Marshall’s mechanism [25] with the species concentrations at the outlet from our jet-stirred reactor for the oxidation of COS under stoichiometric \(\lambda = 1.00\), for fuel-lean \(\lambda = 1.30\) and fuel-rich \(\lambda = 0.70\) conditions, see Fig. S2 of Supplementary data. The production of CO and SO\textsubscript{2} follows the ratio of 1:1, that is, [CO] \(\approx\) [SO\textsubscript{2}], as quantitated from the experimental IR spectra of the exhaust gases. This explains why the CO and SO\textsubscript{2} symbols overlap each other in Fig. 3. The equal production rates of CO and SO\textsubscript{2} reinforce the adopted definition of the stoichiometry (Reaction R\textsubscript{stoichiometry}). We also express the oxidation of COS as a single

Fig. 4. Sensitivity analysis for [COS] at different stage of the oxidation process, from 600 K to 1400 K. As the concentration of COS decreases during the oxidation, and the key reaction steps consume COS, the sensitivity coefficients are all negative.
3.5 Revised rate constant in the updated mechanism.

Table 1

| Reaction   | Source | A               | n  | \(E_a\)  |
|------------|--------|-----------------|----|----------|
| \(1^{16}\text{COS} + ^3\text{O}_2 \rightarrow ^{16}\text{CO} + \text{O} \) | [35]   | \(8.5 \times 10^{13}\) | 0.0 | 135.0    |
| \(1^{16}\text{COS} + ^3\text{O}_2 \rightarrow ^{16}\text{CO} + \text{O} \) | [40]   | \(3.5 \times 10^{12}\) | 0.0 | 85.4     |
| This work  |        | \(3.0 \times 10^{12}\) | 0.0 | 70.1     |

3.4. Validation of updated mechanism with literature data

This section tests the updated mechanism with the experimental measurements of Abián et al. [39] for the moist oxidation of COS in a tubular-flow reactor, discussing the effect of humidity. Direct fission of a \(\text{H}_2\text{O}\) molecule into \(\text{H}\) and \(\text{OH}\) entails a high activation energy of 446 kJ-mol\(^{-1}\) [53]. The hydrolysis of COS features a moderate activation energy of 152 kJ-mol\(^{-1}\), as calculated by Ling et al. [54]. Here, we implement Reaction R6 in our updated mechanism, using the rate parameters calculated by Ling et al. [54], and express the reaction rate as

\[
\frac{\text{d}\left[^{16}\text{COS} \rightarrow ^{16}\text{CO} + \text{S}\right]}{\text{d}t} = -5.0 \times 10^{13} \exp\left(-152.4 \text{kJ} \cdot \text{mol}^{-1} / (RT)\right) \cdot \text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}
\]

and for the trend in the conversion of COS. For the fuel-rich condition of \(\lambda = 0.70\), the updated kinetic model captures well the pyrolysis above 1210 K, also confirming the robustness of the pyrolysis mechanism.

Fig. 7 compares the experimental measurements and the results of the kinetic modelling of Abián et al. [39] with the predictions of the updated mechanism proposed in this work, for the stoichiometric condition of Ref. [39]: \(\lambda = 1.0\) ((COS) = 545 ppm, \([\text{O}_2]\) = 815 ppm, \([\text{H}_2\text{O}]\) = 5000 ppm) within the context of a plug-flow reactor model. Abián et al. performed their experiments with a constant total flow in a tubular flow reactor. To simplify the fluid-dynamic considerations, we model the reactor as perfectly turbulent and perfectly laminar; for the latter, providing the illustrative results along the centreline and near the wall. As expected, the species profiles obtained for the plug flow reactor reside between the two curves corresponding to the laminar conditions, as illustrated in Fig. S5 in Supplementary data. As the differences are small (within 30 K), we base our further discussion on the results obtained for the plug-flow reactor. A plausible explanation for this small difference may stem from high diffusion rates of product species compared to the convective flow rate, as follows from the calculations of the Péclet number for mass transfer, outlined in Supplementary data.

During the oxidation of COS under wet conditions at less than 1000 K, our model predicts no \(\text{CO}_2\) formation. Sensitivity analysis concluded that, Reaction R6 does not operate over the entire temperature window of the present study. This also means that, moisture does not affect the combustion chemistry of COS, in agreement with the analogous behaviour observed in combustion of natural gas [56]. At temperatures in excess of 1025 K, one observes the conversion between CO and \(\text{CO}_2\). Both modelling and experiments capture well this comportment.

The present mechanism improves the onset temperature for the oxidation of COS from 1160 K (Abián’s et al. model) to 940 K (this work), because of the increased rate induced by the updated constants of Reaction R1. However, our model under-estimates the ignition points by 80 K compared to the experimental results. Two possible explanations are provided here: (1) The updated reaction rate of R1 based on experiments at 600 K–800 K in a jet-stirred reactor involves a higher ratio of singlet pathway with lower activation energy. With ignition temperature increasing to 1000 K in tubular flow reactor (TFR), the triplet pathways become the predominant channel for the reaction of COS + \(\text{O}_2\) that displays a higher activation barrier, thus, leading to a higher reaction rate as expected. Fig. S6 in Supplementary data illustrates a comparison of the COS fraction at the outlet of the modelled reactors as a function of the temperature, either for a singlet or triplet pathway, as calculated in [40]. The experimental results fall between the modelling results obtained for the singlet and triplet pathways, respectively. The ratio between these two channels, through intersystem crossing,
deserves further study. (2) With a higher surface to volume ratio, the quartz surfaces in the tubular flow reactor (TFR) could remove more radical species than those in the jet-stirred reactor (JSR), thus inhibiting the ignition of COS. Fig. S7 in Supplementary data displays a semi-quantitative estimation of the effect of removal of radicals by the reactor walls on the mole fraction of species at the reactor outlet. In future, we expect more studies of COS oxidation, reporting oxidation of COS on catalytic surfaces and detailed theoretical calculations of intersystem-crossing, to fill the gap between modelling prediction and experimental measurements.

Fig. 6. Comparison between experimental measurements (symbols) and modelling results with the updated mechanism for oxidation of COS under fuel-lean ((a) \( \lambda = 1.30 \), (b) \( \lambda = 1.15 \)), stoichiometric ((c) \( \lambda = 1.00 \)) and fuel-rich ((d) \( \lambda = 0.85 \), (e) \( \lambda = 0.70 \)) conditions, at a fixed residence time of 1.88 s. We applied the experimental results for \( \lambda = 0.70 \), 1.00 and 1.30 to derive the Arrhenius constants in \( k_{R1} \) and then tested the predictions of the model against the experimental measurements for \( \lambda = 0.85 \) and 1.15.
4. Conclusions

This contribution reported new experimental measurements for oxidation of COS from a jet-stirred reactor system operated in the temperature range from 550 K to 1400 K at a fixed residence time of 1.88 s, under atmospheric pressure, and oxygen-fuel equivalence ratio of 0.70, 0.85, 1.00, 1.15 and 1.30. Through kinetic modelling, the sensitivity analysis for [COS] located the controlling step for oxidation (Reaction R1: \(^1\text{COS} + \text{O}_2 \rightarrow \text{CO} + \text{SO}_2\)) of COS. By considering the oxidation of COS as a single step reaction, we fitted the Arrhenius expression of \(k = (3.0 \pm 0.3) \times 10^{12} \times \exp(-70.1 \pm 2.9 \text{kJ} \cdot \text{mol}^{-1}/(RT)) \text{cm}^3 \cdot \text{mol}^{-1} \cdot \text{s}^{-1}\), from 550 K to 1150 K. As expected, the fitted activation energy of 70.1 kJ mol\(^{-1}\) agrees with the outcome of the crossing-point calculation performed at the Hartree-Fock level of theory, between the triplet and singlet pathways of 85.4 KJ mol\(^{-1}\), as reported in literature. We have also validated the updated mechanism with the results of experiments conducted using a tubular-flow reactor in the presence of moisture and discussed the influence of H\(_2\)O on the oxidation of carbonyl sulfide. The effect of moisture is limited to the conversion of CO to CO\(_2\) at temperatures in excess of 1025 K. The proposed kinetic model for the oxidation of COS will assist in the design of SO\(_2\) mitigation processes and in the development of safe industrial systems for extracting sulfur impurities from fossil fuels. We also highlight the occurrence of the inter-system crossing process in the oxidation of COS, as investigated in this work and the previous publication. Attention should be paid to the crossing-over between electronic states when examining the oxidation processes of sulfur-containing species. We recommend future calculations to be performed at a higher level of theory, to locate the crossing-over points, as well as to experimentally detect and establish the spin states of S, S\(_2\), SO and O.

CRediT authorship contribution statement

Zhe Zeng: Conceptualization, Investigation, Writing - original draft, Writing - review & editing. Bogdan Z. Dlugogorski: Conceptualization, Methodology, Investigation, Resources, Supervision, Writing - review & editing. Ibukun Oluwoye: Investigation, Writing - review & editing, Validation. Mohammednoor Altarawneh: Investigation, Methodology, Supervision, Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fuel.2020.119257.

References

[1] Selim H, Al Shoaibi A, Gupta AK. Effect of H\(_2\)S in methane/air flames on sulfur chemistry and products spectrum. Appl Energy 2011;88(8):2353–60.
[2] Williams A, Jones JM, Ma I, Pourkashanian M. Pollutants from the combustion of solid biomass fuels. Prog Energy Combust Sci 2012;38(2):113–37.
[3] Johnsson JE, Glarborg P. Pollutants from combustion-formation mechanisms and impact on atmospheric chemistry. Klawer Academic Publisher; 2000.
[4] Chun C-L. Sulfur in coals: a review of geochemistry and origin. Int J Coal Geol 2012;100:1–13.
[5] Burgers WFJ, Northrop PB, Keshghi HS, Valencia JA. Worldwide development potential for sour gas. Energy Procedia 2011;4:2178–84.
[6] Rodriguez JA, Brink J. Interaction of sulfur with well-defined metal and oxide surfaces: Unraveling the mysteries behind catalyst poisoning and desulfurization. Acc Chem Res 1999;32:719–28.
[7] Jüngst E, Nehb W. Hydrogen sulfide to sulfur (Claus Process). In: Handbook of Heterogenous Catalysis, Wiley-VCH Verlag GmbH & Co.; 2008.
[8] Karan K, Mehrzad AK, Behie LA. A high-temperature experimental and modeling study of homogeneous gas-phase COS reactions applied to Claus plants. Chem Eng Sci 1999;54(15-16):2999–3006.
[9] Karan K, Behie LA. CS\(_2\) formation in the Claus reaction furnace: a kinetic study of methane–sulfur and methane–hydrogen sulfide reactions. Ind Eng Chem Res 2004;43:3304–13.
[10] Selim H, Al Shoaibi A, Gupta AK. Fate of sulfur with H\(_2\)S injection in methane/air flames. Appl Energy 2012;92:57–64.
[11] Selim H, Al Shoaibi A, Gupta AK. Experimental examination of flame chemistry in hydrogen sulfide-based flames. Appl Energy 2011;88:2601–11.
[12] Colom-Díaz JM, Leciteseina M, Pelazar A, Abián M, Millera A, Bilbao R, et al. Study of the conversion of CH\(_4\)S\(_2\) mixtures at different pressures. Fuel 2020;262:116484.
[13] Colom-Díaz JM, Abián A, Millera A, Bilbao R, Alzueta MU. Influence of pressure on H\(_2\)S oxidation: experiments and kinetic modeling. Fuel 2019;258:116145.
[14] Viteri F, Abián M, Millera A, Bilbao R, Alzueta MU. Ethylene–SO\(_2\) interaction under sooting conditions: PAH formation. Fuel 2016;184:966–72.
[15] Zeng Z, Altarawneh M, Oluwoye I, Glarborg P, Dlugogorski BZ. Inhibition and promotion of pyrolysis by hydrogen sulfide (H\(_2\)S) and sulfanilyl radical (S\(_2\);). J Phys Chem A 2016;120(45):8941–8.
[16] Adánez-Rubio I, Viteri F, Millera A, Bilbao R, Alzueta MU. S–PAH, easy–PAH and EPA–PAH formation during ethylene–SO\(_2\) pyrolysis. Fuel Process Technol 2018;182:68–76.
[17] Viteri F, Sánchez A, Millera A, Bilbao R, Alzueta MU. Effect of the presence of hydrogen sulfide on the formation of light gases, soot, and PAH during the pyrolysis of ethylene. Energy Fuel 2016;30(11):9745–51.
[18] North American Energy Standards Board, Natural Gas Spees Sheet, Page 5, https://www.naesb.org/pdf2/wg2_bpg_6005w2.pdf.
[19] Colom-Díaz JM, Alzueta MU, Zeng Z, Altarawneh M, Dlugogorski BZ. Oxidation of H\(_2\)S and CH\(_3\)SH in a jet stirred reactor: Experiments and kinetic modeling. Fuel 2020 (in press, JPUR,119258).
[20] Alzueta MU, Pernins R, Abián M, Millera A, Bilbao R, CH\(_3\)SH conversion in a tubular flow reactor. Experiments and kinetic modeling. Combust Flame 2019;203:23–30.
[21] Colom-Díaz JM, Alzueta MU, Fernandes U, Costa M. Emissions of polycyclic aromatic hydrocarbons from a domestic pelleted-ﬁred boiler. Fuel 2019;247:108–12.
[22] Colom-Díaz JM, Millera A, Bilbao R, Alzueta MU. High pressure study of H\(_2\)S oxidation and its interaction with NO. Int J Hydrogen Energy 2019;44:6235–32.
[23] Zhang H, Schuchardt F, Li G, Yang J, Yang Q. Emission of volatile sulfur compounds during composting of municipal solid waste (MSW). Waste Manage 2013;33(3):957–63.
[24] Song Y, Marrodan L, Vin N, Herbinet O, Asaf E, Pfitzchen C, Stagni A, Faravelli T, Alzueta MU, Battin-Leclere F. The sensitizing effects of NO\(_2\) and NO on methane low temperature oxidation in a jet stirred reactor. Proc Combust Inst 2018;37(1):607–75.
[25] Ismail TM, Yoshikawa K, Sherif H, Abd El-Salam M. Hydrothermal treatment of municipal solid waste into coal in a commercial plant: numerical assessment of process parameters. Appl Energy 2019;250:653–64.
Zeng Z, Dlugogorski BZ, Altarawneh M. Flammability of CS$_2$ and other reduced sulfur species. Fire Saf J 2017;91:226–34.

Chen W, Lei T, Wu C, Deng M, Gong C, Hu K, et al. Designing safe electrolyte systems for a high-stability lithium-sulfur battery. Advanc Energ Mat 2018;8:1702348.

Zhu J, Zhu P, Yan C, Dong X, Zhang X. Recent progress in polymer materials for advanced lithium-sulfur batteries. Prog Polym Sci 2019;90:118–63.

Goodenough JB, Kim Y. Challenges for rechargeable Li batteries. Chem Mater 2016;22(3):587–603.

Barkley MP, Palmer PI, Boone CD, Bernath PF, Suntharalingam P. Global distributions of carbonyl sulfide in the upper troposphere and stratosphere. Geophys Res Lett 2008;35(14).

Zeng Z, Altarawneh M, Dlugogorski BZ. Atmospheric oxidation of carbon disulfide (CS$_2$). Chem Phys Lett 2017;690:43–8.

North GR, John AP, Zhang F, editors. Biogeochemcial cycles - sulfur cycle, encyclopedia of atmospheric sciences, Vol. 1. Elsevier; 2014.

Camacho A. In: Encyclopedia of inland waters. Elsevier; 2009. p. 261–78.

Azatyan VV, Genshenson UM, Sarkissyan EN, Sachyan GA, Nalbandyan AB. Investigation of low-pressure flames of a number of compounds containing sulfur by the ESR method. Symp (Int) Combust 1969;12(1):989–94.

Glarborg P, Marshall P. Oxidization of reduced sulfur species: carbonyl sulfide. Int J Chem Kinet 2013;45(7):429–39.

Glarborg P, Halaburt B, Marshall P, Guillaory A, Tree J, Thellefson M, Christensen K. Oxidation of reduced sulfur species: carbon disulfide. J Phys Chem A 2014;118(34):6798–809.

Homan KH, Krome G, Wagner H. Carbon disulfide oxidation 3: the isothermal oxidation of carbon disulfide. Ber Bunsen Phys Chem 1970;74:74–9.

Homan KH, Krome G, Wagner H. Carbon disulfide oxidation 1: speed of elemental reaction. Ber Bunsen Phys Chem 1968;74:74–9.

Abdian M, Cebrian M, Millena A, Bilbao R, Alzueta MU. CS$_2$ and COS conversion under different combustion conditions. Combust Flame 2015;162(5):2119–27.

Zeng Z, Dlugogorski BZ, Altarawneh M. Combustion chemistry of carbon disulfide (CS$_2$). Combust Flame 2019;210:413–25.

Montoya A, Sendt K, Haynes BS. Gas-phase interaction of H$_2$S with O$_2$: a kinetic and quantum chemistry study of the potential energy surface. J Phys Chem A 2005;109:1057–62.

Zhou C, Sendt K, Haynes BS. Theoretical study of hydrogen abstraction and sulfur insertion in the reaction H + S + S. J Phys Chem A 2008;112(14):3239–47.