

## 4.039 Heterogeneous reaction of SO<sub>2</sub> with soot: the role of the chemical composition of soot in surface sulfates formation.

Early Career Scientist

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Abstract:

It has been found that soot can catalyze the oxidation of SO<sub>2</sub> to form sulfates in the presence of O<sub>2</sub> and water<sup>1, 2</sup>. A linear relationship has been observed between NO<sub>2</sub> uptake and the content of reduced organic carbon in soot prepared under different combustion conditions<sup>3</sup>. However, the effect of the chemical composition of soot on the adsorption or further oxidation of SO<sub>2</sub> on the surface of soot is still poorly understood. In this study, soot samples with different fractions of unsaturated hydrocarbons and oxygen groups were prepared by combusting n-hexane under well-controlled conditions. The heterogeneous reaction of SO<sub>2</sub> with soot at ambient pressure and ambient relative humidity (RH) was investigated using *in situ* attenuated total internal reflection infrared (ATR-IR) spectroscopy, ion chromatography (IC) and a flow tube reactor. We observed that the surface properties of soot, which were governed by combustion conditions, played an important role in the heterogeneous reaction of SO<sub>2</sub> with soot. This role was found to greatly depend on RH. At low RH, soot produced with high fuel/oxygen ratio exhibited high reactivity toward SO<sub>2</sub>, because it contained a large amount of unsaturated hydrocarbons which acted as the active site for SO<sub>2</sub> adsorption. At moderate RH, water and SO<sub>2</sub> both participated in the reaction. Soot produced with moderate fuel/oxygen ratio showed high reactivity toward SO<sub>2</sub>, since it contained appropriate amounts of unsaturated hydrocarbons and oxygen groups, which led to optimal surface concentrations of SO<sub>2</sub> and water, respectively.

### REFERENCES

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