Model study of chamber photochemical experiments of Sulfur Mass-Independent Fractionation under reducing conditions

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We have developed a 1D isotopic photochemical model and applied it to chamber experiments of sulfur dioxide (SO₂) and carbon monoxide (CO) irradiated with ultraviolet light. We incorporated the most relevant chemical reactions of the chamber experiment in the model and estimated sulfur isotopes from species products such as residual SO₂ and carbonyl sulfide (OCS). The main pathway of OCS production was elucidated by analysis of reaction rates. The model also showed good agreement in the concentration change of chemical species over time. The simulated Sulfur Mass-Independent Fractionation (S-MIF) δ^{34} S, Δ^{33} S and Δ^{36} S showed the same trend with experimental values in the literature although δ^{34} S and Δ^{36} S magnitudes were larger and the Archean slope Δ^{36} S/ Δ^{33} S was accurately reproduced. Moreover, the physical processes responsible for producing Archean S-MIF and the contribution of the Inter-System Crossing (ISC) effect to the S-MIF were also confirmed to contribute but significantly. Therefore, the model can be applied to simulate the atmospheric sulfur cycle, the chemical species formation and evolution in reducing conditions, and estimate each spectrum range contribution to the total S-MIF.

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