Supplementary Material

Kinetic Model

Below, the kinetic mechanism for simulating sulfuric acid formation during the cyclohexene ozonolysis is presented. An OH yield of 50% (average of results of this study and previous work) is assumed and implemented as a prompt Criegee Intermediate (CI) decomposition channel. A 5 % fraction of stabilised CI and 45 % fraction of isomerisation channels without OH formation are assumed. These assumptions, however, do not influence the model predictions. The same holds for most of the reactions belonging to the oxy-hydrogen chemistry, which are included as a sub-mechanism in order to account for OH loss different from reactions with hydrocarbons and sulfuric acid.

Table 1 List of the reactions considered in the kinetic model, with $\rightleftharpoons$ depicting a reversible reaction, $\longrightarrow$ an irreversible reaction and M a bath gas molecule

Nr.	Reaction	$A/cm^3\,mol^{-1}\,s^{-1}$	n	$E_a/kJ\,mol^{-1}$	Reference
1	$O_2 + H \rightleftharpoons OH\cdot + O$	$2.0\cdot10^{+14}$	0.0	70.3	Baulch et al. [1]
2	$H_2 + O \rightleftharpoons OH\cdot + H$	$5.1\cdot10^{+04}$	2.67	26.3	Baulch et al. [1]
3	$H_2 + OH\cdot \rightleftharpoons H_2O + H$	$1.0\cdot10^{+08}$	1.6	13.8	Baulch et al. [1]
4	$OH\cdot + OH\cdot \rightleftharpoons H_2O + O$	$1.5\cdot10^{+09}$	1.14	0.42	Baulch et al. [1]
5	$H + O_2 + M \rightleftharpoons HO_2\cdot + M$	$2.3\cdot10^{+18}$	-0.8	0.0	Maas et al. [2]
6	$HO_2\cdot + H \rightleftharpoons OH\cdot + OH\cdot$	$1.5\cdot10^{+14}$	0.0	4.2	Maas et al. [2]
7	$HO_2\cdot + H \rightleftharpoons H_2 + O_2$	$2.5\cdot10^{+13}$	0.0	2.9	Maas et al. [2]
8	$HO_2\cdot + H \rightleftharpoons H_2O + O$	$3.0\cdot10^{+13}$	0.0	7.2	Baulch et al. [1]
9	$HO_2\cdot + O \rightleftharpoons OH\cdot + O_2$	$1.8\cdot10^{+13}$	0.0	-1.7	Maas et al. [2]
10	$SO_2 + OH\cdot \longrightarrow HOSO_2\cdot$	$1.00\cdot10^{+12}$	0.0	0.0	Somnitz et al. [3]
11	$HOSO_2\cdot + O_2 \longrightarrow SO_3 + HO_2\cdot$	$2.59\cdot10^{+11}$	0.0	0.0	Atkinson et al. [4]
12	$SO_3 + H_2O \longrightarrow H_2SO_4$	$7.23\cdot10^{+8}$	0.0	0.0	Reiner et al. [5]
13	$OH\cdot + H_2SO_4 \longrightarrow HOSO_3 + H_2O$	$9.03\cdot10^{+09}$	0.0	0.0	Anglada et al. [6]
14	$HOSO_2\cdot \longrightarrow SO_2 + OH\cdot$	$2.30\cdot10^{-05}$	0.0	0.0	Somnitz et al. [3]
15	$O_3 + C_6H_{10} \longrightarrow C_6H_{10}O_3$	$5.10\cdot10^{+07}$	0.0	0.0	this work
16	$C_6H_{10}O_3 \longrightarrow OH\cdot + C_6H_9O_2$	$0.50\cdot10^{+06}$	0.0	0.0	see text
17	$C_6H_{10}O_3 \longrightarrow SCI$	$0.05\cdot10^{+06}$	0.0	0.0	see text
18	$C_6H_{10}O_3 \longrightarrow$ decomposition products	$0.45\cdot10^{+06}$	0.0	0.0	see text
19	$SCI \longrightarrow$ decomposition products	$5.00\cdot10^{+01}$	0.0	0.0	Nguyen et al. [7]
20	$OH\cdot + C_6H_{10} \longrightarrow C_6H_9\cdot + H_2O$	$4.09\cdot10^{+13}$	0.0	0.0	Wolf [8]
21	$OH\cdot + C_6H_{10} \longrightarrow C_6H_{11}O$	$3.63\cdot10^{+13}$	0.0	0.0	Peeters et al. [9]
22	$C_6H_9\cdot + O_2 \longrightarrow C_6H_9O_2$	$1.80\cdot10^{+12}$	0.0	0.0	Wu et al. [10]

$k = A \cdot T^n \cdot exp(-E_a / RT)$, the unity of A is s^{-1} for unimolecular reactions.

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**Influence of humidity on sulfuric acid formation**

The kinetic model presented on the preceding pages was used to simulate sulfuric acid formation for different humidity. Ozonolysis reactions in gas mixtures similar to the experiments were modelled. Only for the driest conditions (1 ppm H_2O) a slight retardation of H_2SO_4 formation is predicted. Above 10 ppm further increasing the humidity does only marginally influence H_2SO_4 concentration-time profiles. Assuming $x(H_2O)$ to be above 1 ppm, the low humidity is not critical for sulfuric acid formation. This is in agreement with the experimental observations.
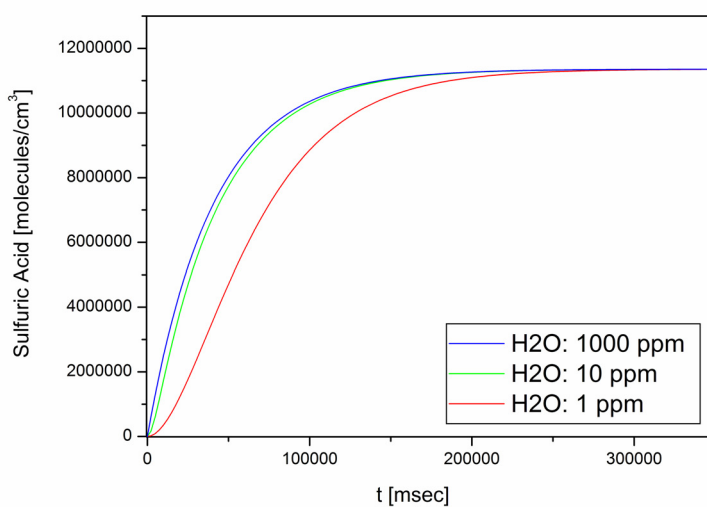
$x_0(CHEX)=10$ ppm, $x_0(O_3) = 1$ ppm.

Simultaneous formation of sulfuric acid and consumption of ozone

The simulation of ozone consumptions and H_2SO_4 formation in a typical experiment. Kinetic modeling shows that sulfuric acid formation and intermediate ozonolysis chemistry run in parallel. Therefore cross reactions such as $CI + H_2SO_4$ are possible.
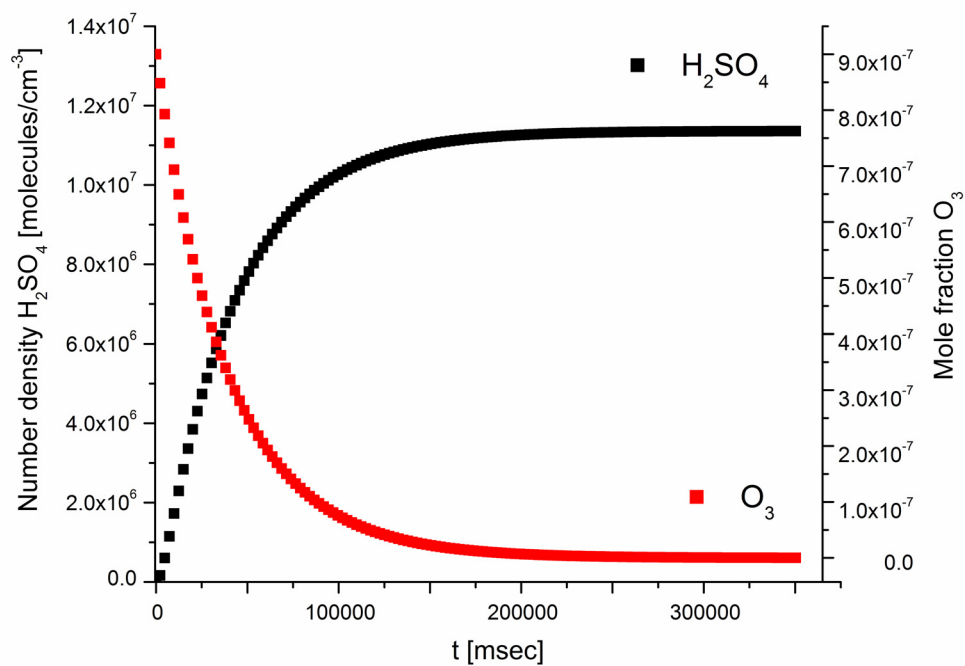
$x_0(CHEX)=10$ ppm, $x_0(O_3) = 1$ ppm, $x_0(H_2O) = 5$ ppm.