

Reduction and evaluation of the dimethyl sulfide and methanethiol oxidation mechanism

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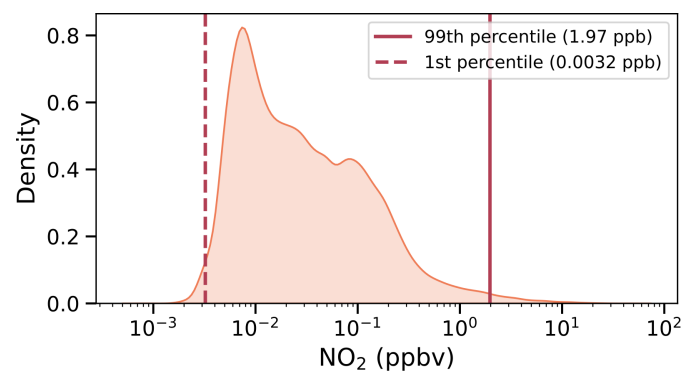


Figure S1. The distribution of NO₂ monthly average surface marine mixing ratios from UKCA (October 2013 to September 2014). The 1st and 99th percentiles are indicated by the dashed and solid lines, respectively.

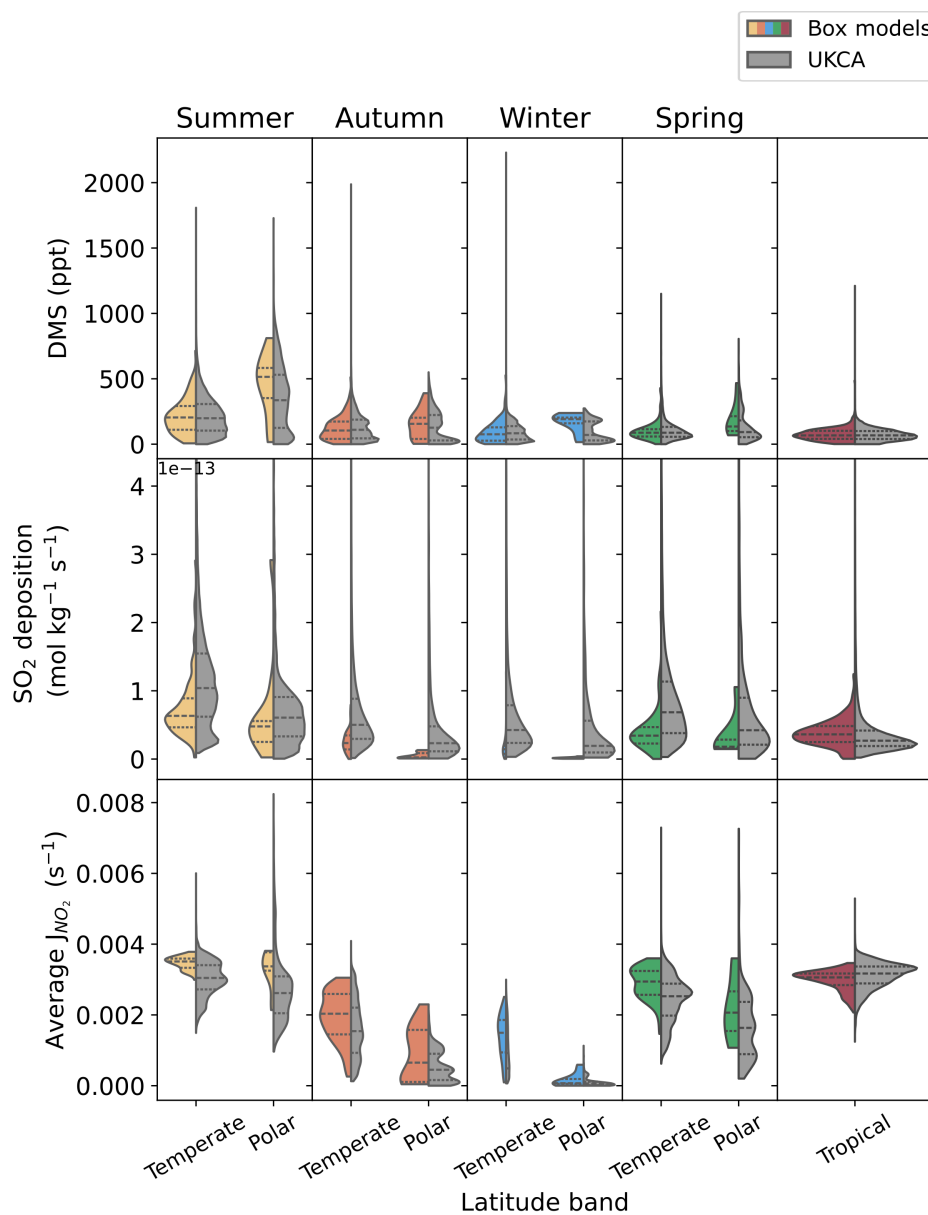


Figure S2. The mixing ratio of DMS, the dry deposition of SO₂, and the average photolysis rate constant of NO₂ in the 1000 marine box models, compared to UKCA (surface level monthly averages over the ocean), separated by seasons and latitude bands.

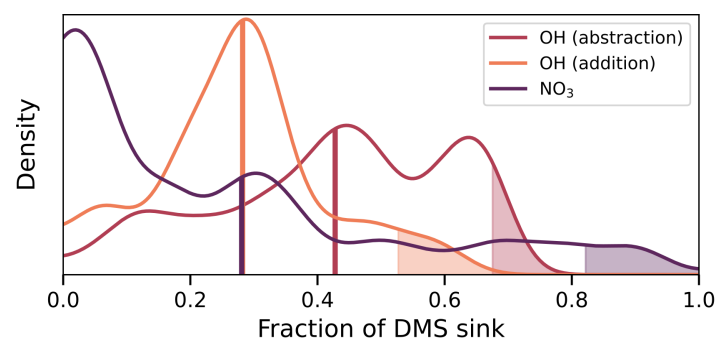


Figure S3. The distribution of the sink ratios calculated for DMS across the 100 randomised box models of the marine surface atmosphere. The coloured vertical lines indicate the mean sink ratio for each pathway, while the shaded region represents values above the 95th percentile (i.e. the highest 5% of sink ratio values). For clarity, the minor oxidation pathways of DMS (oxidation via $O(^3P)$ and CH_3SO_3) have been excluded.

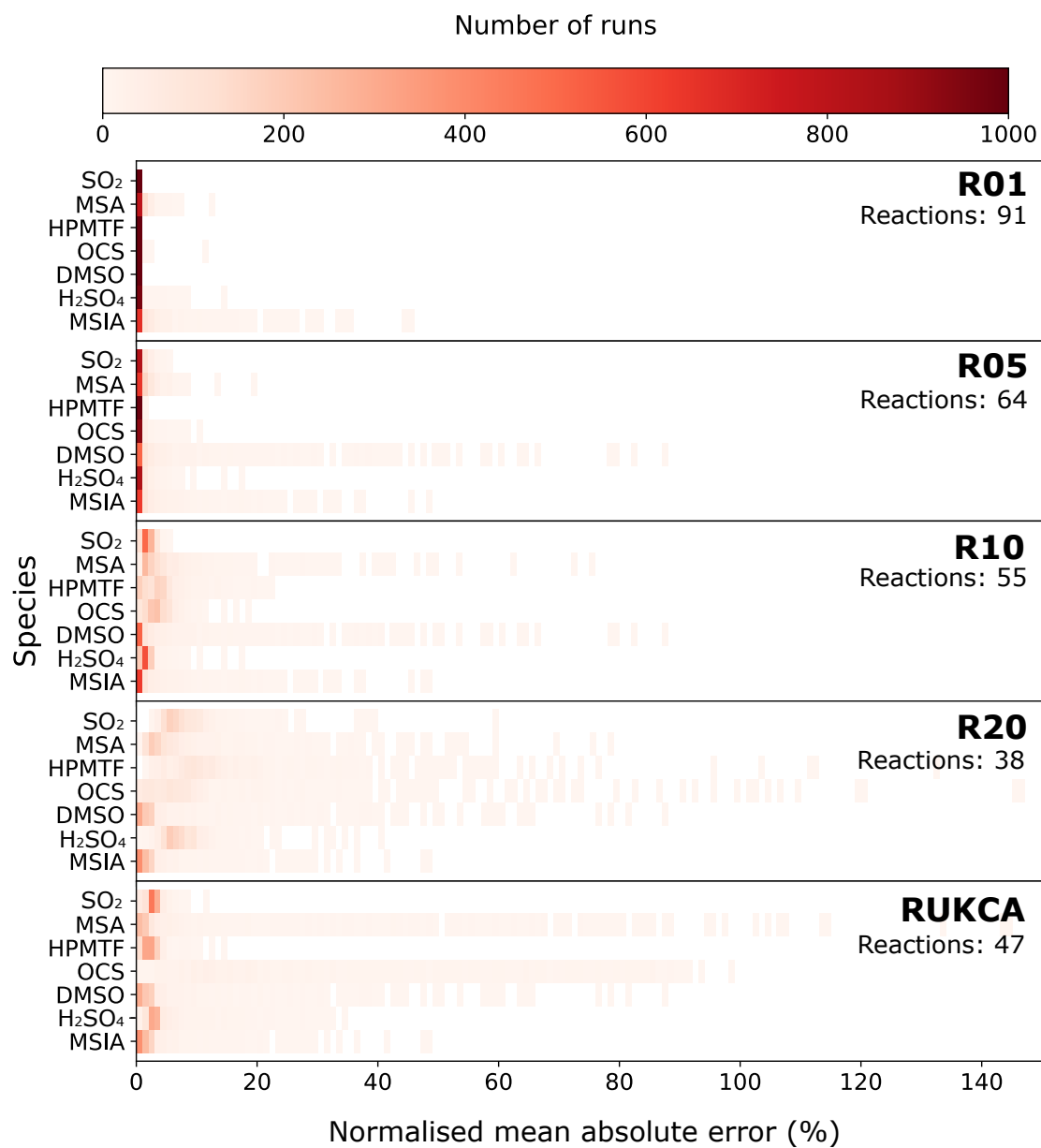


Figure S4. A heatmap of the normalised mean absolute error for SO₂, MSA, HPMTF, OCS, DMSO, H₂SO₄ and MSIA from the reduced mechanisms evaluated against the full mechanism for each marine box model, using a bin size of 1%.

Table S1. The average normalised mean absolute error and normalised mean bias (given as percentages), and their 90% confidence intervals for SO₂, MSA, HPMTF, OCS, DMSO, H₂SO₄ and MSIA from the reduced mechanisms: R01 (91 reactions), R05 (64 reactions), R10 (55 reactions), R20 (38 reactions) and RUKCA.

Species	R01		R05		R10		R20		RUKCA	
	Error	Bias	Error	Bias	Error	Bias	Error	Bias	Error	Bias
SO ₂	0.0 ^{+0.1} _{-0.0}	-0.0 ^{+0.0} _{-0.1}	0.7 ^{+1.5} _{-0.5}	-0.7 ^{+0.5} _{-1.5}	1.9 ^{+1.6} _{-1.2}	-1.9 ^{+1.2} _{-1.6}	8.1 ^{+6.6} _{-3.9}	-8.1 ^{+3.9} _{-6.6}	2.8 ^{+1.8} _{-1.9}	-2.8 ^{+2.1} _{-1.9}
MSA	0.7 ^{+1.5} _{-0.5}	-0.5 ^{+0.5} _{-1.5}	1.2 ^{+3.5} _{-1.1}	-0.3 ^{+1.9} _{-2.4}	5.8 ^{+12.6} _{-4.7}	-5.5 ^{+4.5} _{-12.8}	7.6 ^{+15.0} _{-5.9}	-7.4 ^{+5.8} _{-15.2}	14.5 ^{+52.3} _{-13.9}	10.4 ^{+56.1} _{-17.5}
HPMTF	0.1 ^{+0.0} _{-0.0}	-0.0 ^{+0.0} _{-0.1}	0.1 ^{+0.4} _{-0.1}	0.1 ^{+0.5} _{-0.1}	4.1 ^{+7.3} _{-3.5}	4.1 ^{+7.3} _{-3.5}	14.7 ^{+23.9} _{-10.9}	14.7 ^{+23.9} _{-10.9}	2.4 ^{+1.9} _{-1.6}	2.4 ^{+1.9} _{-1.6}
OCS	0.1 ^{+0.2} _{-0.1}	0.0 ^{+0.1} _{-0.1}	0.4 ^{+1.1} _{-0.3}	0.4 ^{+1.1} _{-0.3}	3.5 ^{+3.8} _{-2.9}	3.2 ^{+4.1} _{-4.6}	11.6 ^{+27.0} _{-10.7}	5.0 ^{+32.9} _{-15.1}	34.6 ^{+48.2} _{-30.5}	-34.5 ^{+30.7} _{-48.3}
DMSO	0.0 ^{+0.0} _{-0.0}	0.0 ^{+0.0} _{-0.0}	5.8 ^{+25.0} _{-5.7}	5.8 ^{+25.0} _{-5.7}	5.8 ^{+25.0} _{-5.7}	5.8 ^{+25.0} _{-5.7}	6.1 ^{+24.5} _{-5.7}	4.5 ^{+25.4} _{-7.1}	6.1 ^{+24.5} _{-5.7}	4.5 ^{+25.4} _{-7.1}
H ₂ SO ₄	0.2 ^{+0.5} _{-0.2}	-0.1 ^{+0.3} _{-0.3}	0.8 ^{+2.2} _{-0.6}	-0.7 ^{+0.7} _{-2.0}	1.7 ^{+1.3} _{-1.3}	-1.5 ^{+1.9} _{-1.3}	7.6 ^{+5.0} _{-3.8}	-7.6 ^{+3.8} _{-5.0}	5.3 ^{+12.5} _{-3.9}	-5.2 ^{+4.0} _{-12.5}
MSIA	2.3 ^{+9.9} _{-2.2}	2.3 ^{+9.9} _{-2.2}	2.9 ^{+12.9} _{-2.8}	2.9 ^{+12.9} _{-2.8}	2.9 ^{+12.9} _{-2.8}	2.9 ^{+12.9} _{-2.8}	3.2 ^{+11.7} _{-2.9}	1.7 ^{+12.8} _{-4.2}	3.2 ^{+11.7} _{-2.9}	1.7 ^{+12.8} _{-4.2}