

**Supplementary information for**  
**A new diagnostic for tropospheric ozone production**

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The new  $P_sO_3$  diagnostic has been implemented via the tracking of reactions by type in the GEOS-Chem chemical mechanism file. Table S1 describes the tags used. This tracking of reactions enables the fate of all oxidisable bonds as well as the production and loss of all  $RO_2$  within the model to be determined using the GEOS-Chem production and loss diagnostic (standard diagnostic number ND65). This diagnostic was also used to track the production of CO and the chemical losses of  $RO_{2y}$ , as well as a check on the reaction tagging. Standard GEOS-Chem diagnostics were used to calculate species emission and deposition rates. Methane emissions were calculated using the  $CH_4 + OH$  reaction, as this is the only loss for  $CH_4$  in the model and in a constant concentration field is thus equal to the effective emission. In addition to  $CH_4$  there are 6 other species that have prescribed concentrations instead of emissions (ACTA, EOH,  $H_2$ , HCOOH, MOH, and RCOOH). The production and loss of these species was also tracked to calculate an effective emission and loss.

Reaction type	Example reaction	
Bonds produced by errors in chemistry scheme	ISNOOA + NO --> NO2 + R4N2 + CO + HO2	[3]
Peroxy radicals from oxidisable bonds broken by photolysis	CH2O + hv --> 2HO2 + CO	[2]
Oxidisable bond loss via non-OH chemical reaction (e.g. O3, NO, RO2, etc.)	Isoprene + NO3 --> INO2	[1]
Oxidisable bond loss via OH chemical reaction	Isoprene + OH --> RIO2	[1]
Oxidisable bond loss to photolysis	ALD2 --> MO2 + HO2 + CO	[1]
Photolysis reactions that yield 2 peroxy radicals	CH2O + hv --> 2HO2 + CO	[1]
Parent peroxy radicals back from peroxides	MP + OH --> MO2 + H2O	[1]
Peroxy radical loss	O3 + HO2 --> OH + O2	[1]
Decompositional bond loss after photolysis	MP + hv --> CH2O + HO2 + OH	[1]
Peroxy back from nitrate	PAN --> MCO3 + NO2	[1]
HO2/RO2 + NO --> NO2	HO2 + NO --> NO2 + OH	[1]
Inorganic peroxy source	O3 + OH --> HO2 + O2	[1]
Bonds lost by errors in chemistry scheme	ISNOOA + NO2 --> PMN	[2]
Emitted bond to peroxy by chemistry	CO + OH --> HO2 + CO2	[1]
OH + CH4	OH + CH4	[1]

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RO2 → Peroxide	MO2 + HO2 → MP	[1]
Parent RO2 back from peroxide	MP + OH → MO2 + H2O	[1]
Chemical or photolysis loss of peroxide	MP + OH → CH2O + OH	[1]
RO2 + NO → HO2 + NO2 + carbonyl	ETO2 + NO → ALD2 + NO2 + HO2	[1]
RO2 + NO → Nitrate	ATO2 + NO → 0.96NO2 + 0.96CH2O + 0.96MCO3 + 0.04R4N2	[0.04]
RO2 lost to carbonyl forming peroxy radical self reactions	MO2 + MO2 → MOH + CH2O	[2]
RO2 + NO2 → PAN	HO2 + NO2 → HNO4	[1]
PAN → RO2 + NO2	HNO4 → HO2 + NO2	[1]
PAN loss	HNO4 + OH → H2O + NO2 + O2	[1]
RO2 loss	OH + HO2 → H2O + O2	[1]
RO2 + NO3 → HO2 + NO2 + carbonyl	ISNOOB + NO3 → R4N2 + GLYX + 2xNO2	[1]
HO2 → Peroxide	MO2 + HO2 → MP	[1]
bond + hv → 0 rads	CH2O + hv → H2 + CO	[2]
bond + O3 → 0 rads	ISOP + O3 → 0.244MVK + 0.325MACR + 0.845CH2O + 0.11H2O2 + 0.522CO + 0.204HCOOH + 0.199MCO3 + 0.026HO2 + 0.27OH + 0.128PRPE + 0.051MO2	[3.523]
bond RO2 + RO2 → 0 rads	MO2 + MO2 → MOH + CH2O + O2	[1]
bond + OH → 1 rad (RO2)	OH + H2 → HO2 + H2O	[1]
bond + OH → 1 rad (OH)	MP + OH → CH2O + OH + H2O	[1]
bond + OH → 1 rad (other)	PROPNN + OH → NO2 + MGLY	[1]
bond + RO2 (incl. RO2 + NO) → 1 rad (RO2)	MO2 + NO → CH2O + HO2 + NO2	[1]
bond + RO2 (incl. RO2 + NO) → 1 rad (OH)	MRO2 → CO + HAC + OH	[1]
bond + RO2 (incl. RO2 + NO) → 1 rad (other)	PRN1 + NO → 2NO2 + CH2O + ALD2	[1]
bond + other (incl. RO2 + O3/NO3) → 1 rad (RO2)	O3 + MO2 → CH2O + HO2 + 2O2	[1]
bond + other → 1 rad (other)	ISNOOB + NO3 → R4N2 + GLYX + 2NO2	[1]
bond + hv → 2 rad (RO2)	CH2O + hv → 2HO2 + CO	[0.5]
bond + hv → 2 rad (OH)	MP + hv → CH2O + HO2 + OH	[0.5]
bond + hv → 2 rad (other)	MPN + hv → CH2O + NO3 + HO2	[0.5]
bond + O3 → 2 rad (RO2)	MOBA + O3 → OH + HO2 + CO2	[0.5]
bond + O3 → 2 rad (OH)	MOBA + O3 → OH + HO2 + CO2	[0.5]
bond + O3 → 2 rad (other)	PMN + O3 → NO2 + 0.6CH2O + HO2	[0.5]
bond RO2 + RO2 → 2 rad (RO2)	HC5OO + HO2 → 0.1IAP + 0.9OH + 0.9MGLY + 0.9GLYC + 0.9HO2	[0.45]
bond RO2 + RO2 → 2 rad (OH)	HC5OO + HO2 → 0.1IAP + 0.9OH + 0.9MGLY + 0.9GLYC + 0.9HO2	[0.45]
bond RO2 + RO2 → 2 rad (other)	R4N1 + MCO3 → MO2 + NO2 + 0.39CH2O + 0.75ALD2 + 0.57RCHO + 0.3R4O2	[0.15]

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**Table S1 | P<sub>s</sub>O<sub>3</sub> implementation.** Tracked reaction types (left column) used in the GEOS-Chem chemistry scheme to follow the processing of oxidisable bonds. Examples of each reaction type are given in the right column of the table, with multiple of tracked quantity for example reaction shown in parenthesis.