Supporting Information:

A simplified parameterization of isoprene-epoxydiol-derived secondary organic aerosol (IEPOX-SOA) for global chemistry and climate models

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Table S1. Chemical reactions and dry deposition processes used in this study. The GEOS-Chem default chemistry mechanism is shown in the left column, and the corresponding lumped reactions used as the starting point of this work are shown in the right column.

#	Reactions (GEOS-Chem v11-02-rc)	Reaction rate	Reactions (Lumped)	Reaction rate
1	ISOP + OH $\rightarrow$ 1.0 ISOPO ₂	3.1E-11*exp(360/T)	ISOP + OH $\rightarrow$ 1.0 ISOPO ₂	3.1E-11*exp(360/T)
2	ISOP + O ₃ $\rightarrow$ other products	1.00E-14*exp(-1970/T)	ISOP + O ₃ $\rightarrow$ other products	1.00E-14*exp(-1970/T)
3	ISOP + NO ₃ $\rightarrow$ other products	3.5E-12*exp(-450/T)	ISOP + NO ₃ $\rightarrow$ other products	3.5E-12*exp(-450/T)
4	ISOP + Cl $\rightarrow$ 1.0 ISOPO ₂	7.60E-11*exp(500/T)	ISOP + Cl $\rightarrow$ 1.0 ISOPO ₂	7.60E-11*exp(500/T)
5	ISOPO ₂ + HO ₂ $\rightarrow$ 0.628 ISOPOOH_A + 0.272 ISOPOOH_B + 0.037 ISOPOOH_D	2.06E-13*exp(1300/T)	ISOPO ₂ + HO ₂ $\rightarrow$ 0.937 ISOPOOH	2.06E-13*exp(1300/T)
6	ISOPO ₂ + NO $\rightarrow$ 0.009 ISOPND + 0.081 ISOPNB	2.7E-12*exp(350/T)	ISOPO ₂ + NO $\rightarrow$ 0.009 ISOPND + 0.081 ISOPNB	2.7E-12*exp(350/T)
7	ISOPO ₂ + CH ₃ O ₂ $\rightarrow$ other products	8.37E-14	ISOPO ₂ + CH ₃ O ₂ $\rightarrow$ other products	8.37E-14
8	ISOPO ₂ + ISOPO ₂ $\rightarrow$ other products	2.30E-12	ISOPO ₂ + ISOPO ₂ $\rightarrow$ other products	2.30E-12
9	ISOPO ₂ + CH ₃ CO ₃ $\rightarrow$ other products	1.68E-12	ISOPO ₂ + CH ₃ CO ₃ $\rightarrow$ other products	1.87E-12
	ISOPO ₂ + CH ₃ CO ₃ $\rightarrow$ other products	1.87E-13		
10	ISOPO ₂ $\rightarrow$ other products	4.07E+08*exp(-7694/T)	ISOPO ₂ $\rightarrow$ other products	4.07E+08*exp(-7694/T)
11	ISOPOOH_A + OH $\rightarrow$ 0.750 ISOPO ₂	6.13E-12*exp(200/T)	ISOPOOH + OH $\rightarrow$ 0.652 ISOPO ₂	5.69E-12*exp(200/T)
	ISOPOOH_B + OH $\rightarrow$ 0.480 ISOPO ₂	4.14E-12*exp(200/T)		
	ISOPOOH_D + OH $\rightarrow$ 0.250 ISOPO ₂	5.11E-12*exp(200/T)		
12	ISOPOOH_A + OH $\rightarrow$ 0.578 IEPOX_A	1.70E-11*exp(390/T)	ISOPOOH + OH $\rightarrow$ 0.697 IEPOX	2.26E-11*exp(390/T)
	ISOPOOH_B + OH $\rightarrow$ 0.680 IEPOX_A + 0.320 IEPOX_B	2.97E-11*exp(390/T)		
	ISOPOOH_D + OH $\rightarrow$ 0.500 IEPOX_D	2.92E-11*exp(390/T)		
13	ISOPND + OH $\rightarrow$ 0.1 IEPOX_D	1.20E-11*exp(652/T)	ISOPND + OH $\rightarrow$ 0.1 IEPOX	1.20E-11*exp(652/T)
14	ISOPNB + OH $\rightarrow$ 0.067 IEPOX_A + 0.033 IEPOX_B	2.40E-12*exp(745/T)	ISOPNB + OH $\rightarrow$ 0.1 IEPOX	2.40E-12*exp(745/T)
15	ISOPND + O ₃ $\rightarrow$ other products	2.90E-17	ISOPND + O ₃ $\rightarrow$ other products	2.90E-17
16	ISOPNB + O ₃ $\rightarrow$ other products	3.70E-19	ISOPNB + O ₃ $\rightarrow$ other products	3.70E-19
17	IEPOX_A + OH $\rightarrow$ other products	3.73E-11*exp(-400/T)	IEPOX + OH $\rightarrow$ other products	4.07E-11*exp(-400/T)
	IEPOX_B + OH $\rightarrow$ other products	5.79E-11*exp(-400/T)		

	IEPOX_D + OH → other products	3.20E-11*exp(-400/T)	
	IEPOX_A → IEPOX-SOA		
18	IEPOX_B → IEPOX-SOA		IEPOX → IEPOX-SOA
	IEPOX_D → IEPOX-SOA		
19	ISOPND + hv → other products		ISOPND + hv → other products
20	ISOPNB + hv → other products		ISOPNB + hv → other products
	ISOPOOH_A + hv → other products		
21	ISOPOOH_B + hv → other products		ISOPOOH + hv → other products
	ISOPOOH_D + hv → other products		
22	ISOPOOH(A,B,D) dry deposition		ISOPOOH dry deposition
23	IEPOX(A,B,D) dry deposition		IEPOX dry deposition

Table S2. Input parameter sets considered in this study for the evaluation of parameterizations using the box model.

#	Species	Values
1	NO [ppt]	1, 5, 10, 50, 100, 500, 1000, 5000, 10 ⁴ , 5x10 ⁴ , 10 ⁵ , 5x10 ⁵ , 10 ⁶
2	OH [molecules cm ⁻³]	10 ⁴ , 5x10 ⁴ , 10 ⁵ , 5x10 ⁵ , 10 ⁶ , 2x10 ⁶ , 3x10 ⁶ , 4x10 ⁶ , 5x10 ⁶
3	HO ₂ [ppt]	1, 2, 5, 10, 20, 50, 100
4	Aerosol pH [unitless]	-1,0,1,2,3,4
5	Aerosol surface area [um ² cm ⁻³]	10, 50, 100, 500, 1000, 5000, 10 ⁴
6	O ₃ [ppb]	10, 20, 30, 40, 50, 60, 70, 80, 90, 100
7	NO ₃ [ppt]	1, 2, 5, 10, 20, 30
8	Cl [molecules cm ⁻³]	10, 100, 500, 1000, 5000
9	CH ₃ O ₂ [ppt]	5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100
10	CH ₃ CO ₃ [ppt]	0.5, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10
11	Aerosol radius [nm]	50, 100, 150, 200, 250, 300, 500, 1000
12	Organic coating fraction [unitless]	0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9
13	Temperature [K]	288, 293, 298, 303, 308, 313, 318
14	Planetary boundary layer height [m]	100, 200, 500, 1000, 1500, 2000, 2500, 3000, 3500, 4000
15	Photolysis rate of ISOPOOH [s ⁻¹]	10 ⁻⁷ , 5x10 ⁻⁷ , 10 ⁻⁶ , 5x10 ⁻⁶ , 10 ⁻⁵ , 2x10 ⁻⁵

Table S3. Fitting constants for Eq. (12).

Constant [Unit]	Value (PAR1)	Value (PAR3)
C ₀ [s]	1.2766x10 ⁶	8.6804x10 ⁵
C ₁ [s]	-2.5853x10 ⁵	-6.8531x10 ⁵
C ₂	0.7812	0.8651
C ₃ [s ⁻¹]	1.1910x10 ⁻⁶	7.6927x10 ⁻⁷
C ₄ [s]	-2.2937x10 ⁵	-1.8233x10 ⁵
C ₅	1.1969	0.91796
C ₆ [s ⁻¹]	3.2483x10 ⁻⁶	1.4389x10 ⁻⁶
C ₇ [s]	-7.8766x10 ⁵	-1.8034x10 ⁵
C ₈	1.0760	1.3762
C ₉ [s ⁻¹]	1.5886x10 ⁻⁶	3.2078x10 ⁻⁶
C ₁₀ [s]	-2.2735x10 ⁵	
C ₁₁	1.3584	
C ₁₂ [s ⁻¹]	3.3567x10 ⁻⁶	
C ₁₃	-17.9610	-9.084
C ₁₄	1.4992	-2.004
C ₁₅	2.6901x10 ¹	2.8313x10 ¹
C ₁₆	1.8906x10 ¹	9.9961
C ₁₇	4.5583x10 ⁻²	1.0903x10 ⁻¹

Table S4. Computational time estimation using the Gprof performance analysis tool. Intel Fortran compiler 17.0.1 with ‘-p’ option was used for the compilation process for function profiling. Values were based on 7-days simulation using 32 cores (2.3-GHz Intel Xeon E5-2697V4 processors) on the NCAR Cheyenne supercomputer. More than 1,000 subroutines in GEOS-Chem were analyzed with the Gprof but we classified subroutines to 12 categories by keywords. For example, if ‘gckpp’ was included in Fortran filename or subroutine name, it was considered as chemistry calculation process.

Process	Estimated time [s]	Keywords for classification
Chemistry	10728	gckpp, flexchem, state_chm
Photolysis and non-tropospheric chemistry	630	strat_chem, fast_j
Emission	1214	hco
Transport	2978	transport, convection, tpcore
Dry deposition	410	drydep, mixing
Wet deposition	4808	wetscav
Unit conversion	2146	unitconv
VBS	23	soa, chem_nvoc, zeroin
PAR1	47	par1 ¹⁾
PAR2	13	par2 ¹⁾
PAR3	48	par3 ¹⁾
3%	1	pari1 ¹⁾
Others	2732	All others

1) Not included in the standard version of GEOS-Chem

Figure S1. (a) IEPOX reactive uptake coefficient (γ) and surface area (S_a) as a function of OA mass concentration. (b) IEPOX condensation rate (k_{18}) as a function of OA mass. Sulfate aerosol mass concentration was assumed as $10 \mu\text{g m}^{-3}$. Initial surface area of $3 \times 10^{-6} \text{ cm}^2 \text{ cm}^{-3}$ was assumed for organic aerosol mass = $0 \mu\text{g m}^{-3}$. Densities of sulfate and organic aerosols were set to be 1.7 and 1.3 g cm^{-3} , respectively, based on densities used by GEOS-Chem v11-02-rc.

Figure S2. Point to point comparison of IEPOX-SOA molar yields for the isomer-lumped (y-axis) versus isomer-resolved full GEOS-Chem (x-axis) mechanisms. Yields were calculated by the box model using 14,000 simulations by systematically varying the input parameters in Table S2.

Figure S3. Scatterplots of parameterized (PAR1 case) (y-axis) versus simulated (x-axis) results by the box model for (a) IEPOX-SOA molar yield and (b) formation timescale with randomly selected parameters in Table S1 of 14,000 simulations.

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Figure S4. Scatterplots of parameterized (y-axis) versus full chemistry IEPOX-SOA (x-axis) concentrations within the troposphere for July 2013 – June 2014 shown on a log scale with base of 10. Each point represents monthly averaged model grid value of IEPOX-SOA concentration. Colors represent the density of points, where densities were calculated by dividing x and y axis ranges into 100 by 100 grid cells.

Figure S5. Same as Fig. 4d but IEPOX-SOA concentrations were simulated without diurnal variation of chemical/meteorological fields. Fixed values used for this calculation are: $\text{OH} = 10^6 \text{ molecules cm}^{-3}$, $\text{HO}_2 = 100 \text{ ppt}$, $\text{O}_3 = 50 \text{ ppb}$, $\text{NO}_3 = 10 \text{ ppt}$, $\text{Cl} = 10^3 \text{ molecules cm}^{-3}$, $\text{NO} = 100 \text{ ppt}$, $\text{CH}_3\text{O}_2 = 10 \text{ ppt}$, $\text{CH}_3\text{CO}_3 = 10 \text{ ppt}$, IEPOX uptake rate = 10^{-5} s^{-1} , Dry deposition rate of ISOPOOH and IEPOX = 10^{-6} s^{-1} , ISOPOOH photolysis rate = 10^{-5} s^{-1} , temperature = 298.15 K.

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Figure S6. Diurnal variations of chemical/meteorological fields used in box model calculation (Fig. 5d). Values were extracted from GEOS-Chem global mean results for four major isoprene source regions [the Southeastern United States: 30°N – 40°N, 100°W – 80°W, Amazon: 10°S – 0°S, 70°W – 60°W, Central Africa: 5°N – 15°N, 10°E – 30°E, Borneo: 5°S – 5°N, 105°E – 120°E]. Figures represent annual mean diurnal variation profiles, which were calculated by using the first two days of each month model outputs at 30 minutes interval averaged within the PBL, averaging points of the same local time.

Figure S7. Timeseries of (a) regression slope and (b) R^2 for the full chemistry vs. parameterizations. Regression slope and R^2 are calculated for each month for concentrations within the troposphere.

Figure S8. Changes of chemical fields affecting the initial oxidation of isoprene and isoprene SOA concentrations simulated by the VBS. Ratios were computed as the 50% NO_x emission reduction case divided by the base case. All figures represent surface values for July – August 2013.