

Supplementary Information for “GENOA v3: A Flexible Tool for Reduction and Exploration of Explicit Chemical Mechanisms”

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S1 Evaluation scenarios

S1.1 General simulation setup and input profiles

In addition to the scenario setups described in Sect. 4.2, solar positions for scenarios with dynamic photolysis are computed assuming a latitude of 45° and a longitude of 0° , with the simulation date set to 1 January 2015 (00:00 local time). Photolysis rates are prescribed using the `solarlight.phot` lookup table distributed with the GECKO-A box model Zenodo release (Aumont et al., 2025).

For all non-diurnal scenarios, initial concentration profiles are summarized in Table S1. For the diurnal scenario, hourly concentration profiles are prescribed, as listed in Table S2.

Table S1. Initial gas-phase species concentrations (molecules cm^{-3}) specified for non-diurnal scenarios.

Species	name ^a	urban ^b	remote	continental	poll-cont	remote-cont	simplified ^c
O ₃	GO3	1×10^{12}	1×10^{12}	1×10^{12}	1×10^{12}	1×10^{12}	1×10^{12}
NO	GNO	1.42×10^{11}	4.82×10^7	2.59×10^9	1.05×10^{10}	1.17×10^8	1.42×10^{11}
NO ₂	GNO2	3.58×10^{11}	2.02×10^8	9.91×10^9	3.95×10^{10}	5.08×10^8	3.58×10^{11}
HCHO	GCH2O	9.32×10^2	1.05×10^3	1.14×10^3	8.76×10^2	1.14×10^3	–
CO	GCO	1.11×10^5	1.33×10^5	1.47×10^5	1.01×10^5	1.48×10^5	–
CO ₂	GCO2	1.51×10^5	1.26×10^5	1.10×10^5	1.63×10^5	1.09×10^5	–
H ₂	GH2	8.61×10^4	9.21×10^4	9.59×10^4	8.35×10^4	9.61×10^4	–
H ₂ O	GH2O	5.33×10^{17}	5.33×10^{17}	5.33×10^{17}	5.33×10^{17}	5.33×10^{17}	–
H ₂ O ₂	GH2O2	2.22×10^9	8.29×10^{11}	1.81×10^{11}	1.56×10^{11}	6.65×10^{11}	–
HONO	GHNO2	3.54×10^9	8.84×10^5	3.67×10^7	3.03×10^8	1.66×10^6	–
HNO ₃	GHNO3	9.04×10^{11}	3.78×10^8	1.43×10^{10}	1.15×10^{11}	7.38×10^8	–
HNO ₄	GHNO4	3.41×10^8	3.45×10^6	7.50×10^7	3.29×10^8	7.36×10^6	–
OH	GHO	5.11×10^6	3.73×10^6	2.87×10^6	5.92×10^6	2.88×10^6	–
HO ₂	GHO2	8.41×10^7	1.51×10^9	6.68×10^8	7.35×10^8	1.28×10^9	–
CH ₃ ONO ₂	GN01001	1.04×10^5	1.07×10^5	1.08×10^5	1.02×10^5	1.08×10^5	–
N ₂ O ₅	GN2O5	3.49×10^7	2.10×10^2	3.78×10^5	3.58×10^6	1.30×10^3	–
NO ₃	GNO3	3.12×10^6	3.33×10^4	1.22×10^6	2.90×10^6	8.22×10^4	–
O ₂	GO2	4.87×10^{18}	4.87×10^{18}	4.87×10^{18}	4.87×10^{18}	4.87×10^{18}	–
O(³ P)	GO3P	4.68×10^4	6.18×10^3	7.29×10^3	1.06×10^4	6.22×10^3	–

^a Species name as used in GECKO-A mechanisms. For O₃ with fixed profiles, the initial concentration equals the fixed value. For NO_x (NO + NO₂), the total concentration is fixed, and the NO/NO₂ ratio is set by the initial concentrations.

^b Same values are applied to the urban-nophot and urban-highphot scenarios.

^c Same values are applied to the simpl-nophot and simpl-highphot scenarios.

Table S2. Hourly profiles (0–23 hour) of species concentrations (molecules cm^{-3}) and environmental parameters specified for the diurnal scenario. The diurnal constraints are derived from the 2013 Southern Oxidant and Aerosol Study (SOAS) field campaign compiled into a 24 h diurnal cycle at 1 h resolution and distributed with the F0AM box model framework. The corresponding data are provided in the F0AM example file `ExampleSetup_DielCycle.m`, archived in the F0AM Zenodo release (Wolfe and Haskins, 2023). Units are converted as needed to ensure consistency with the GECKO-A box model setup. Primary VOC (PVOC) concentrations adopt the corresponding α -pinene diurnal profile.

Hour	OH	NO	NO ₂	O ₃	PVOC	PRES ^a	RH (%)	SZA (°)	T (K)
0	1.71×10^5	1.13×10^8	1.63×10^{10}	5.21×10^{11}	1.16×10^{10}	2.44×10^{19}	85.2	90.0	296.91
1	1.78×10^5	1.67×10^8	1.92×10^{10}	4.60×10^{11}	1.29×10^{10}	2.45×10^{19}	88.7	90.0	296.18
2	1.40×10^5	1.16×10^8	2.13×10^{10}	4.29×10^{11}	1.30×10^{10}	2.45×10^{19}	90.8	90.0	295.61
3	9.21×10^3	6.95×10^7	2.08×10^{10}	4.22×10^{11}	1.53×10^{10}	2.46×10^{19}	91.9	90.0	295.20
4	8.42×10^4	2.52×10^8	3.10×10^{10}	4.04×10^{11}	1.49×10^{10}	2.46×10^{19}	92.1	90.0	294.91
5	1.70×10^5	4.63×10^8	2.50×10^{10}	3.27×10^{11}	1.47×10^{10}	2.46×10^{19}	94.8	90.0	294.32
6	1.10×10^4	1.46×10^9	2.57×10^{10}	3.05×10^{11}	1.37×10^{10}	2.47×10^{19}	95.7	87.1	294.08
7	2.36×10^5	6.89×10^9	2.35×10^{10}	2.79×10^{11}	1.60×10^{10}	2.47×10^{19}	94.8	76.2	294.50
8	4.34×10^5	8.23×10^9	2.24×10^{10}	3.82×10^{11}	9.37×10^9	2.45×10^{19}	89.8	63.6	296.18
9	7.80×10^5	5.63×10^9	1.76×10^{10}	5.36×10^{11}	7.76×10^9	2.44×10^{19}	83.2	51.2	297.88
10	1.08×10^6	3.46×10^9	1.38×10^{10}	6.39×10^{11}	5.38×10^9	2.43×10^{19}	79.6	39.1	298.84
11	1.17×10^6	1.89×10^9	9.57×10^9	7.35×10^{11}	4.68×10^9	2.42×10^{19}	74.2	26.2	299.76
12	1.53×10^6	1.22×10^9	6.91×10^9	8.34×10^{11}	3.72×10^9	2.42×10^{19}	69.4	14.8	300.68
13	1.64×10^6	1.00×10^9	5.85×10^9	8.65×10^{11}	3.73×10^9	2.41×10^{19}	65.5	9.8	301.30
14	1.49×10^6	9.64×10^8	4.92×10^9	9.03×10^{11}	3.53×10^9	2.40×10^{19}	61.2	17.9	302.05
15	1.47×10^6	8.93×10^8	5.34×10^9	9.56×10^{11}	3.17×10^9	2.40×10^{19}	58.7	29.8	302.64
16	1.24×10^6	9.01×10^8	5.57×10^9	9.58×10^{11}	3.60×10^9	2.40×10^{19}	59.1	41.8	302.61
17	9.92×10^5	1.02×10^9	7.14×10^9	9.72×10^{11}	3.72×10^9	2.39×10^{19}	57.6	54.9	302.76
18	5.41×10^5	6.82×10^8	8.16×10^9	9.93×10^{11}	3.79×10^9	2.40×10^{19}	59.5	67.2	302.41
19	3.11×10^5	3.33×10^8	8.51×10^9	9.18×10^{11}	5.18×10^9	2.40×10^{19}	62.2	78.7	301.73
20	2.46×10^5	5.72×10^7	1.17×10^{10}	8.68×10^{11}	5.94×10^9	2.41×10^{19}	66.6	89.6	300.75
21	2.45×10^5	0	1.40×10^{10}	7.60×10^{11}	6.47×10^9	2.42×10^{19}	72.0	90.0	299.65
22	1.52×10^5	1.31×10^8	1.32×10^{10}	6.25×10^{11}	1.79×10^{10}	2.43×10^{19}	78.6	90.0	298.52
23	2.17×10^5	8.63×10^7	1.14×10^{10}	5.68×10^{11}	8.06×10^9	2.43×10^{19}	80.2	90.0	298.02

^a Pressure (PRES) is expressed as air number density (molecules cm^{-3}). Hourly input settings for PRES, RH, SZA, and T are currently available only in the GENOA-coupled version of the GECKO-A box model.

S1.2 Time series of key oxidants and radicals

Figures S1–S6 present the time series of key oxidant and radical concentrations (O_3 , NO_x , HO_x , RO_2 , NO_3) simulated using the reference mechanisms for each VOC class (Cs, Us, MTs) under 11 evaluation scenarios. For readability, results are split into two scenario groups (“g1” with six scenarios: urban, remote, continental, poll-cont, remote-cont, diurnal; “g2” with five scenarios: simplified, simpl-nophot, simpl-highphot, urban-nophot, urban-highphot). In each panel, the blue line indicates the mean time series, and the gray shaded area denotes the simulated minimum-to-maximum range across all VOC in the corresponding group.

Mean (min-max range) across 12 Cs Ref mechanisms

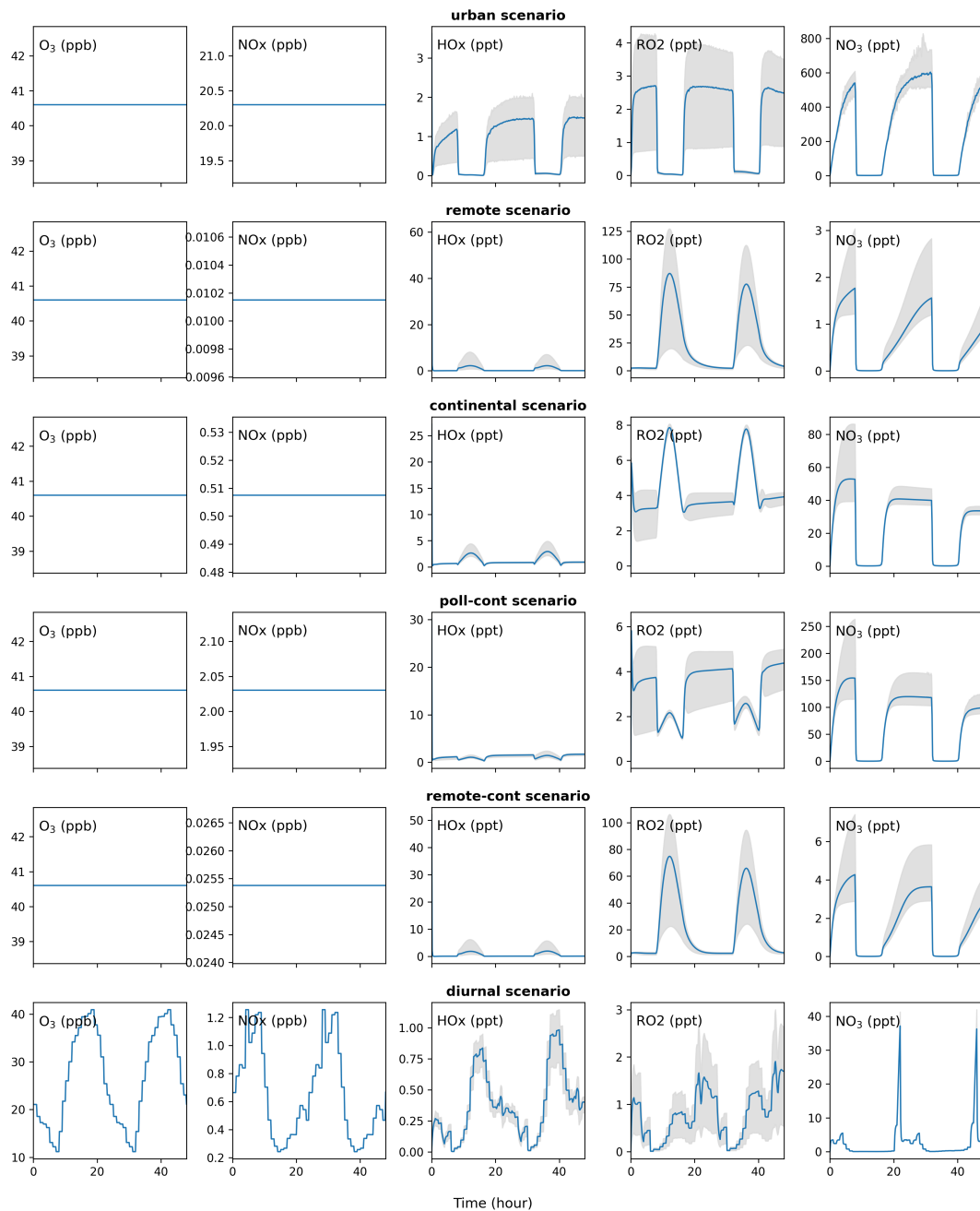


Figure S1. Time series of key oxidant and radical concentrations simulated using the reference Cs mechanisms (C5–C16) under scenario group g1.

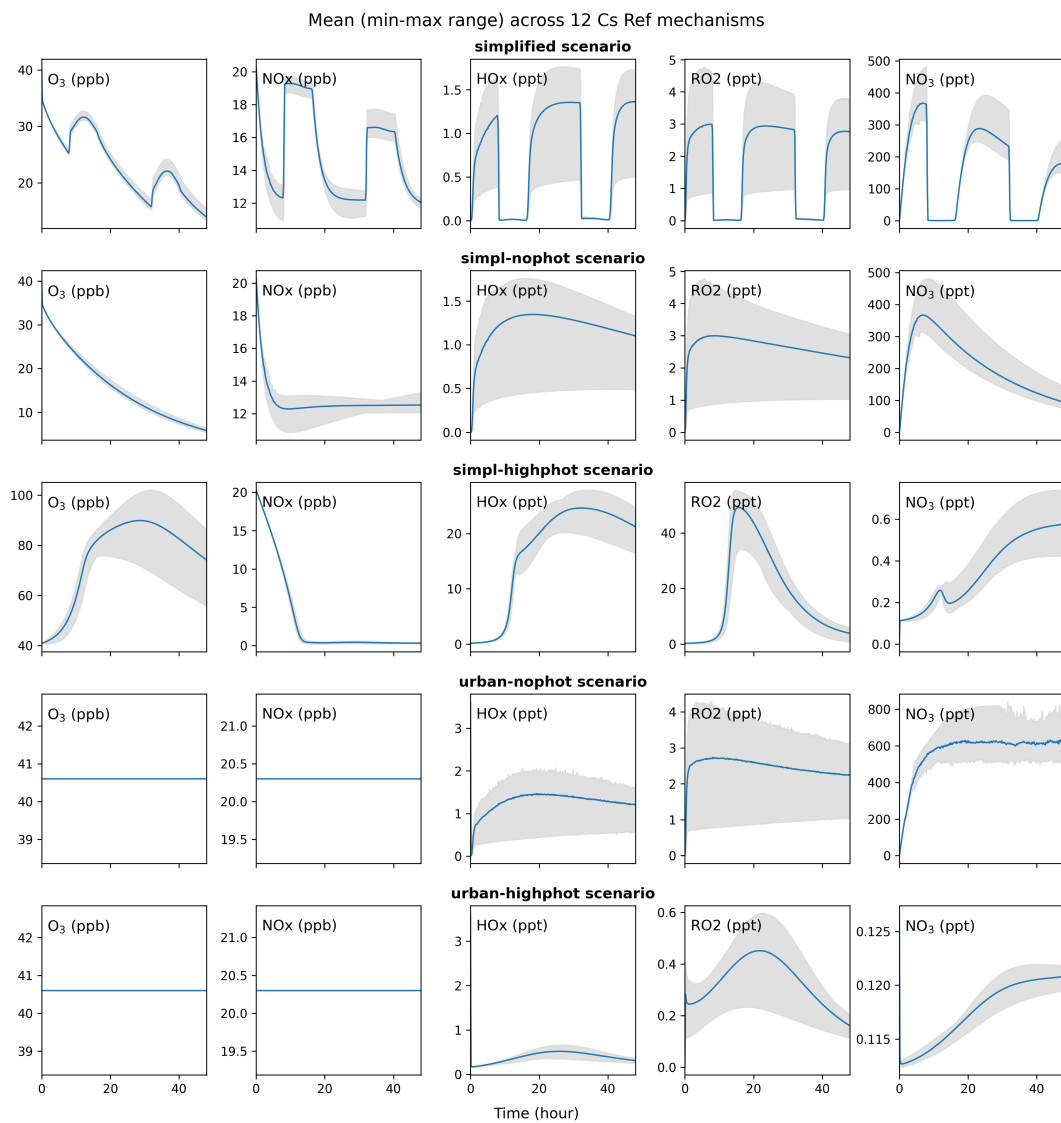


Figure S2. Time series of key oxidant and radical concentrations simulated using the reference Cs mechanisms (C5–C16) under scenario group g2.

Mean (min-max range) across 12 Us Ref mechanisms

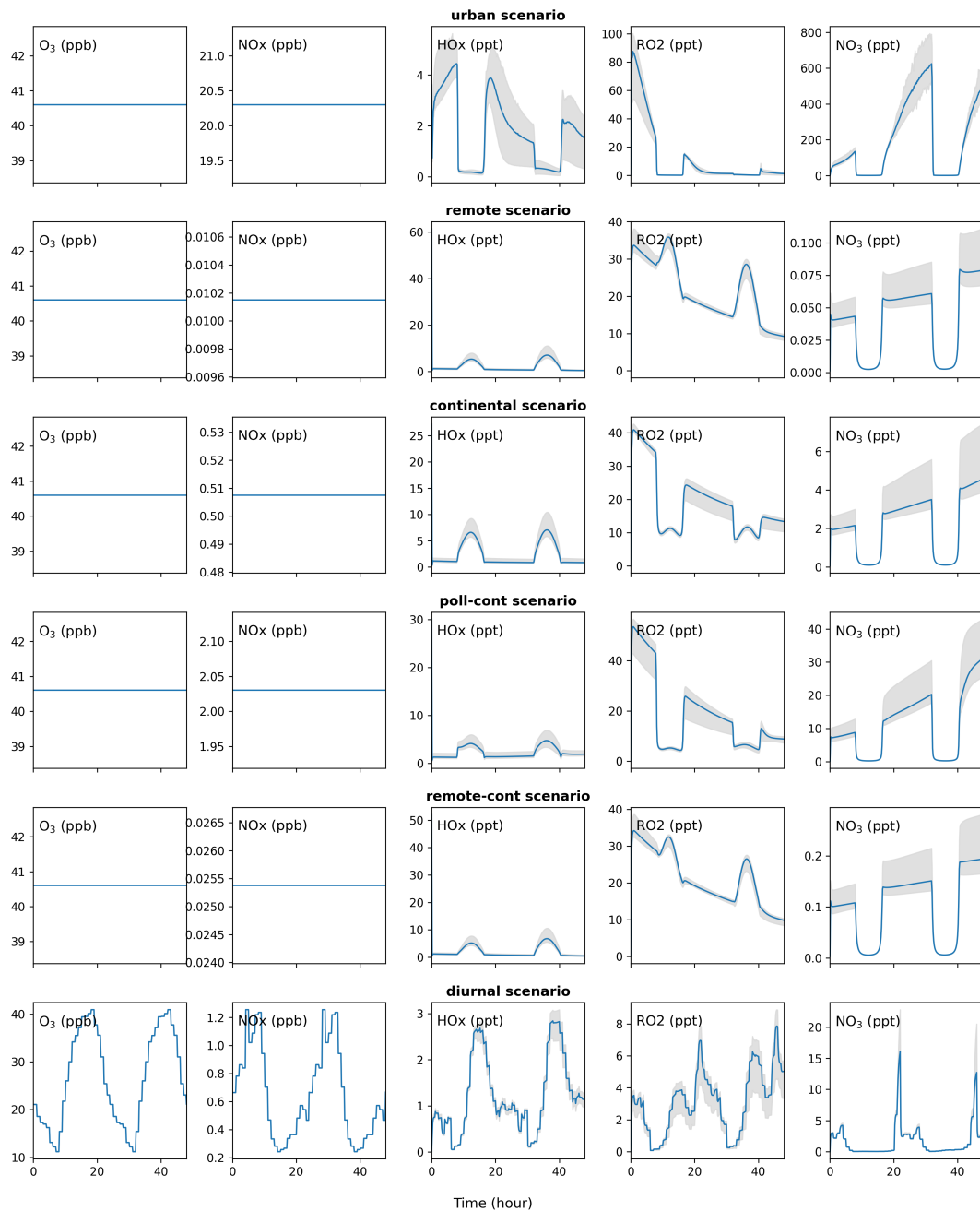


Figure S3. Time series of key oxidant and radical concentrations simulated using the reference Us mechanisms (U5–U16) under scenario group g1.

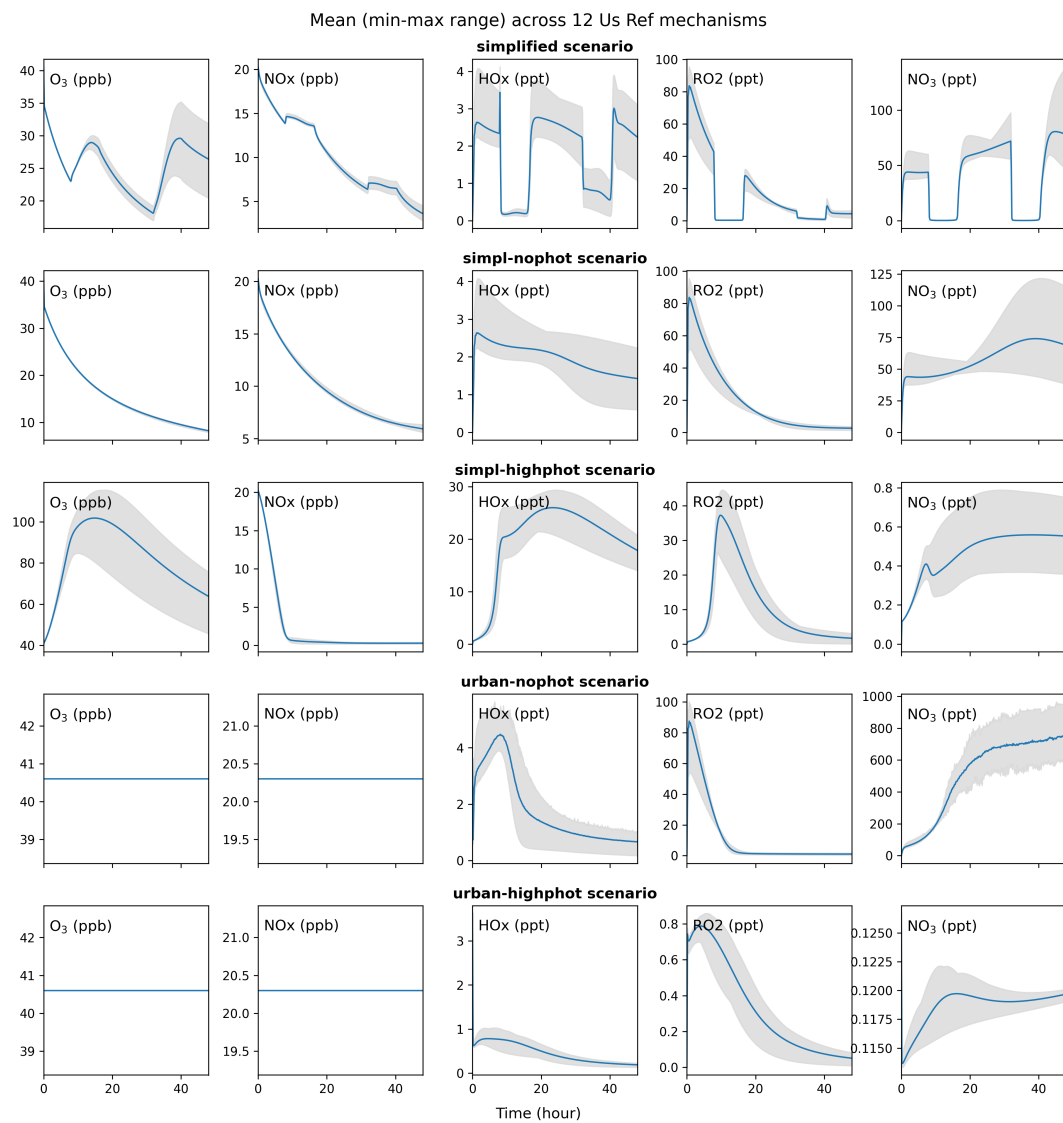


Figure S4. Time series of key oxidant and radical concentrations simulated using the reference Us mechanisms (U5–U16) under scenario group g2.

Mean (min-max range) across 5 MTs Ref mechanisms

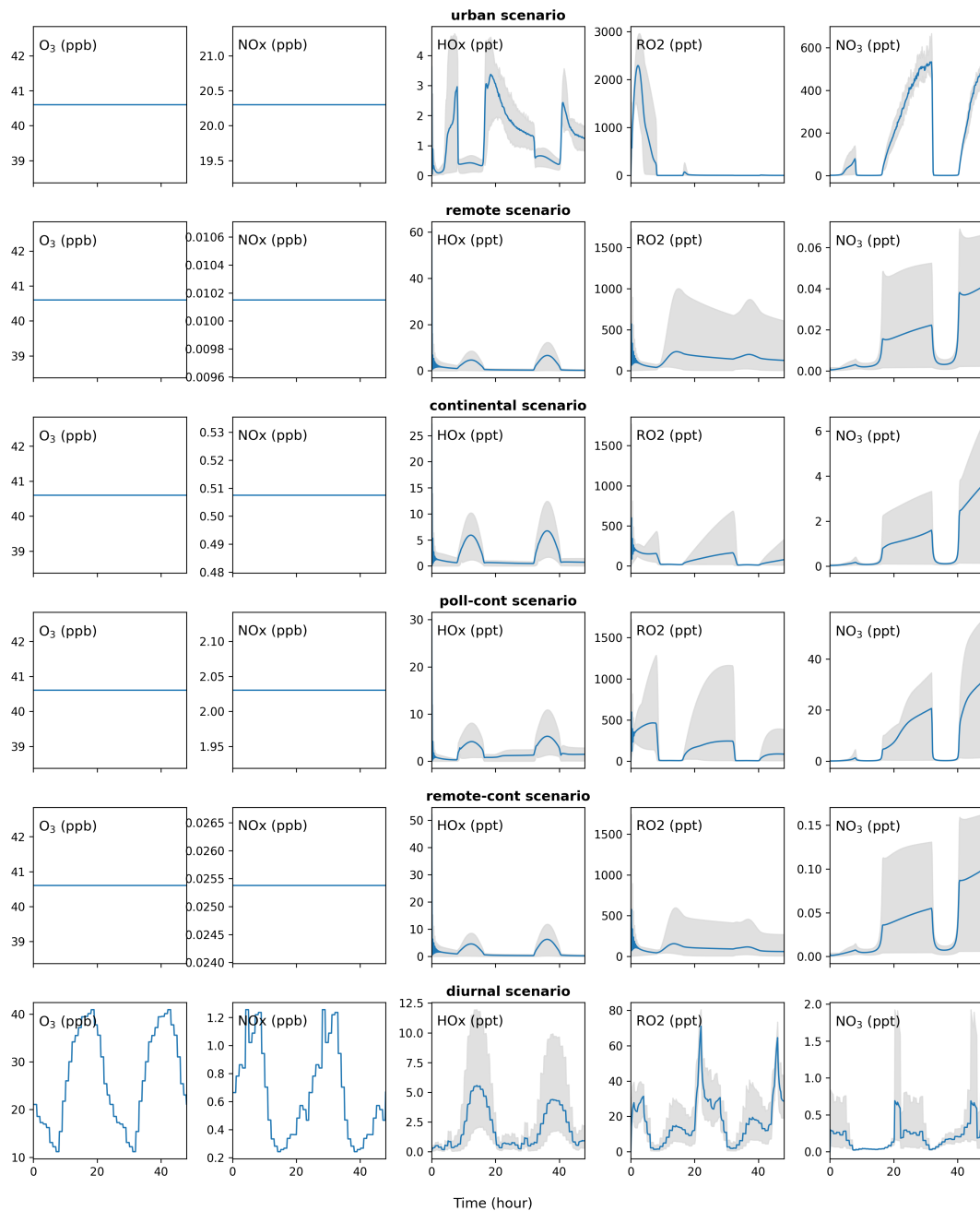


Figure S5. Time series of key oxidant and radical concentrations simulated using the reference MTs mechanisms (α -pinene, β -pinene, limonene, camphene, and carene) under scenario group g1.

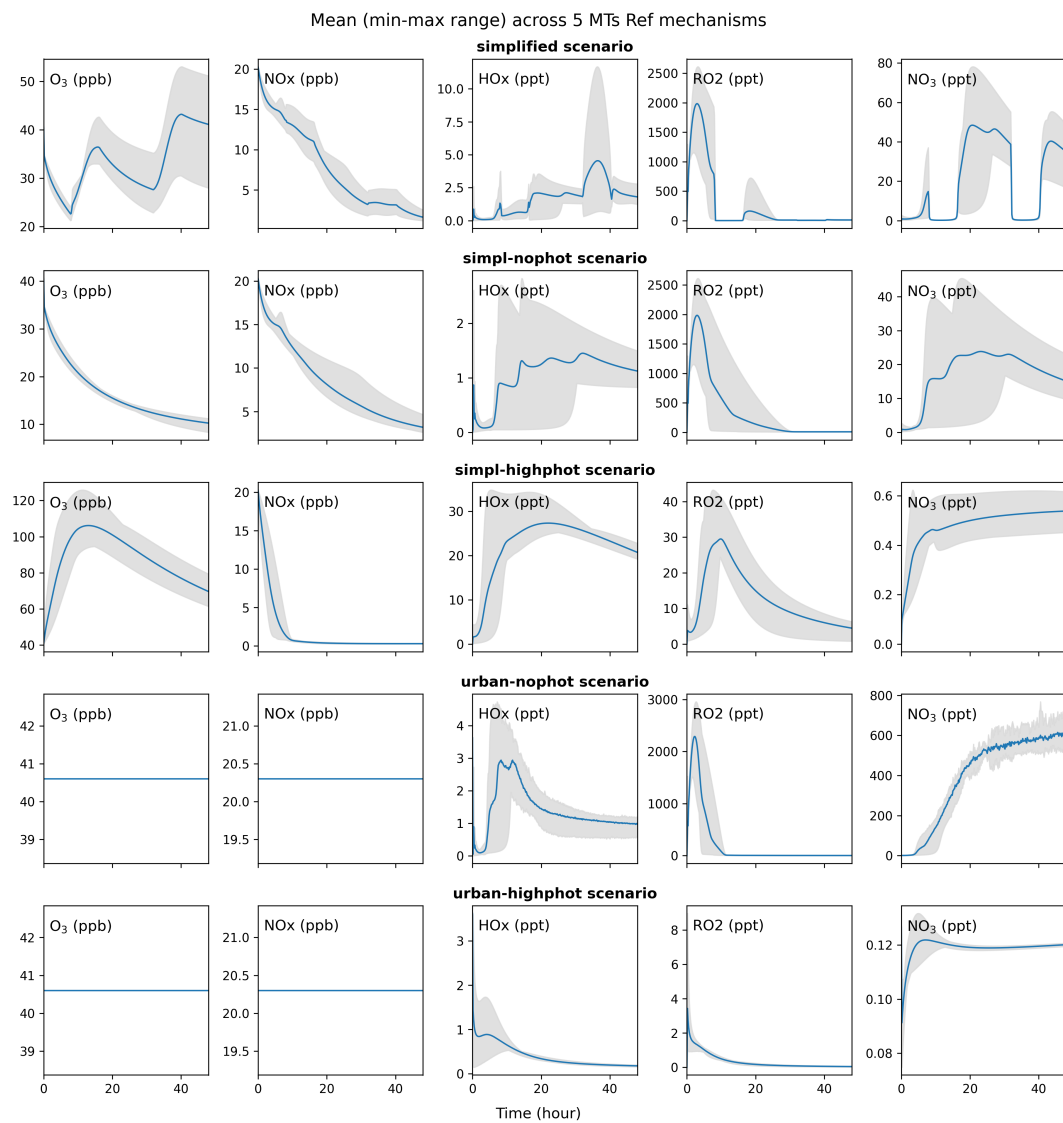


Figure S6. Time series of key oxidant and radical concentrations simulated using the reference MTs mechanisms (α -pinene, β -pinene, limonene, camphene, and carene) under scenario group g2.

S2 Additional TBR results

S2.1 Sensitivity analyses for TBR strategies

As described in Sect. 4.3, sensitivity analyses are performed for individual TBR strategies to identify suitable threshold ranges. Mechanism size reduction and reduction accuracy, quantified using reduction errors averaged across all simulation scenarios, are presented in Figs. S7–S15. In addition to tSOA and OH shown in the main paper, two additional evaluation targets are included here: IOH, the loss tracer for OH, and NO₃, representing nighttime chemistry. In all figures, marker shapes denote threshold values, and lines connect results from the same mechanism. For clarity, only one representative mechanism from each VOC class (U8, C12, and LIM) is shown.

The NVOC reclassification strategy is excluded from this sensitivity analysis because it does not affect GECKO-A simulations, in which non-volatile species are not treated explicitly or distinguished from other SVOCs. This strategy would become relevant only if NVOC species were handled differently in the chemical solver.

For the fast-degrading species jumping strategy, threshold scans over a wide lifetime range ($\tau^{\text{fast}} = 10^{-4}$ – 10^5 s) result in nearly identical size reduction and only minor variations in reduction error (Fig. S13). Under the evaluated scenarios, most species that allow jumping already have lifetimes shorter than 10^{-4} s. As a result, enlarging the threshold range adds very few additional species classified as fast-degrading, leading to nearly identical reduction outcomes and overlapping markers across thresholds. The upper bound of 10^5 s is intentionally chosen to extend well beyond what may normally be considered fast-degrading, in order to examine how size reduction and reduction error change across a wide range of thresholds. When selecting the threshold, 1 s is chosen as a representative value within the tested range (Table 4). Larger values are not adopted as they would include species whose lifetimes depend strongly on environmental conditions.

For the yield-to-depth ratio removal strategy, threshold values from 10^{-4} to 10 % are explored (Fig. S14). The smallest threshold (10^{-4}) leads to no reduction and is not shown. The largest threshold (10 %) results in excessive removal (size reduction $\sim 93\%$) and large errors (40–60 %), and is therefore omitted for clarity. This is consistent with the GECKO-A generation procedure, where relative yield cutoffs are already applied (Sects. 3.2.1 and 4.1). As a result, many low-yield branches have already been removed.

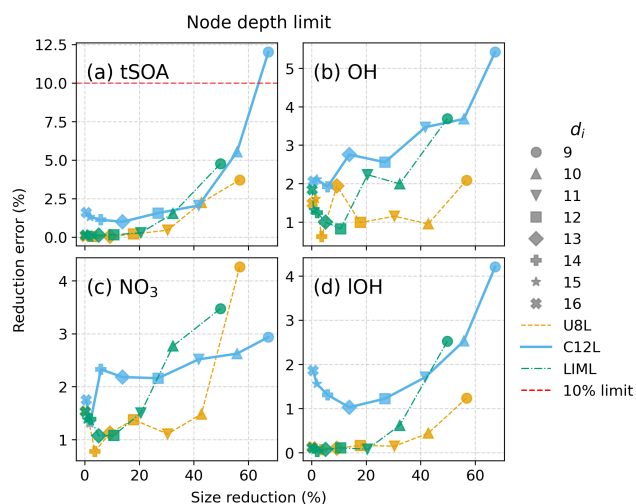


Figure S7. Sensitivity of mechanism size reduction and reduction error to threshold variation for the node depth limit (d_i), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

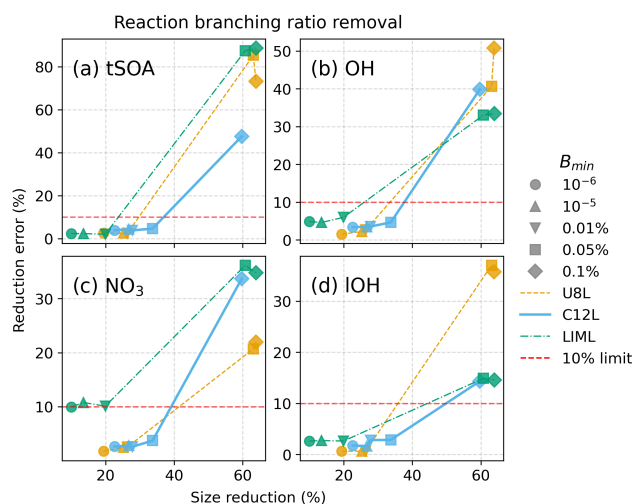


Figure S8. Sensitivity of mechanism size reduction and reduction error to threshold variation for the reaction branching ratio removal (B_{\min}), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

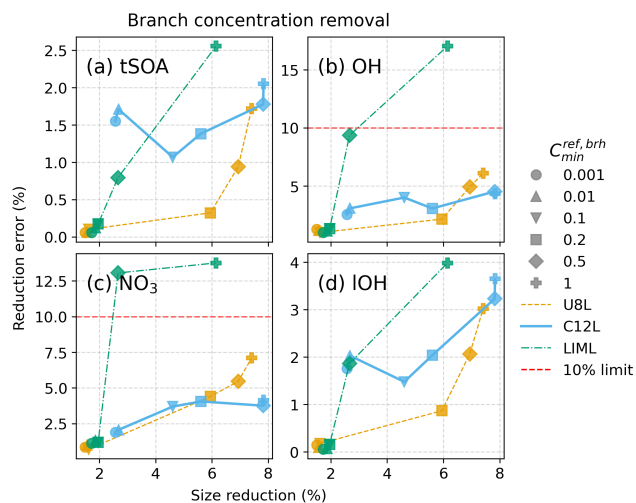


Figure S9. Sensitivity of mechanism size reduction and reduction error to threshold variation for the branch concentration removal ($C_{\min}^{\text{ref,brh}}$ in ppt), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

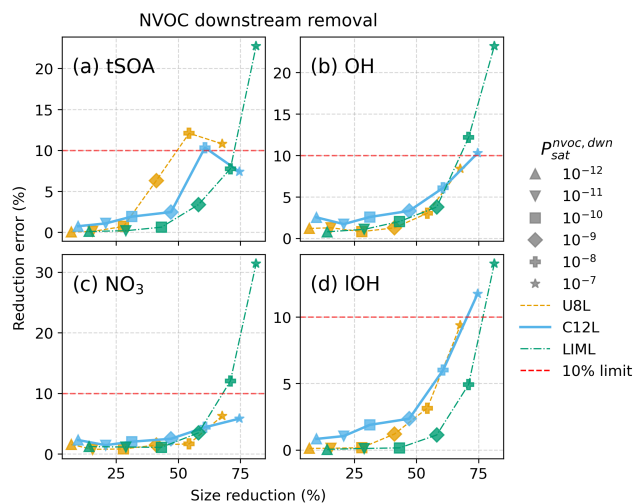


Figure S10. Sensitivity of mechanism size reduction and reduction error to threshold variation for the NVOC downstream removal ($P_{\text{sat}}^{\text{nvoc,dwn}}$ in atm), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

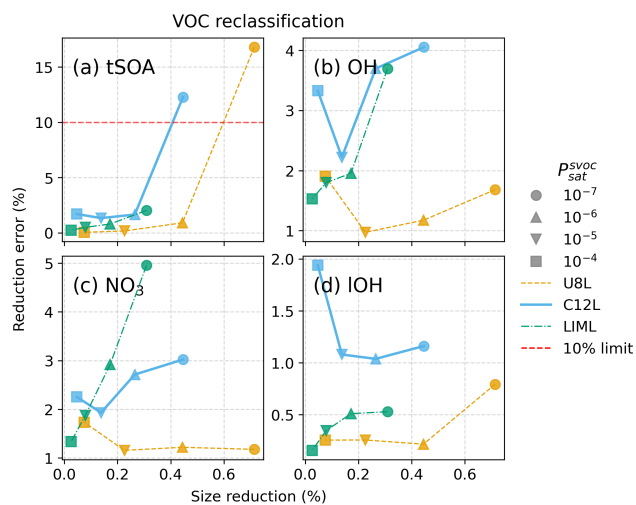


Figure S11. Sensitivity of mechanism size reduction and reduction error to threshold variation for the VOC reclassification ($P_{\text{sat}}^{\text{svoc}}$ in atm), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

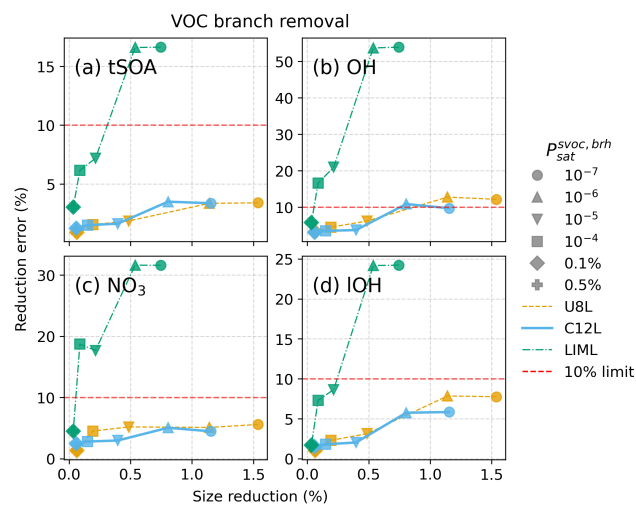


Figure S12. Sensitivity of mechanism size reduction and reduction error to threshold variation for the VOC branch removal ($P_{\text{sat}}^{\text{svoc,brh}}$ in atm), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

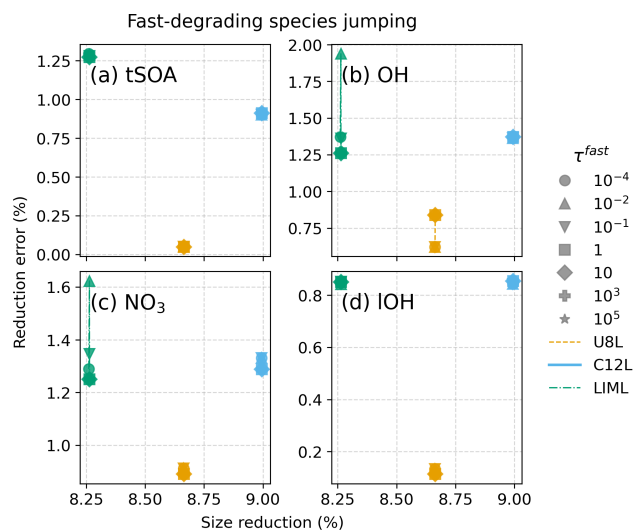


Figure S13. Sensitivity of mechanism size reduction and reduction error to threshold variation for the fast-degrading species jumping (τ^{fast} in s), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

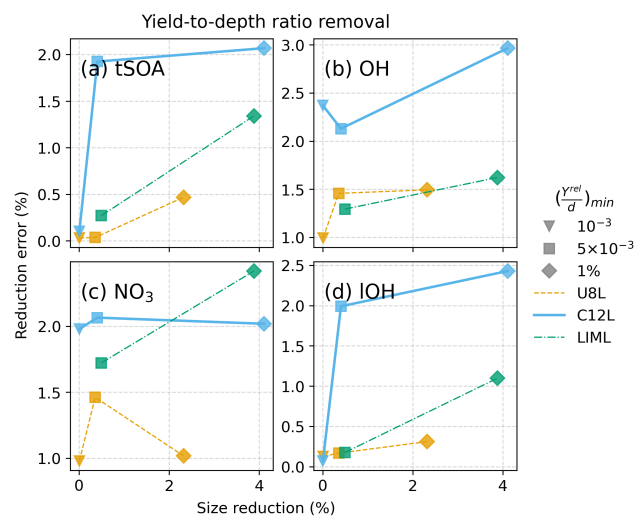


Figure S14. Sensitivity of mechanism size reduction and reduction error to threshold variation for the yield-to-depth ratio removal ($(\frac{Y^{\text{rel}}}{d})_{\text{min}}$), evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms. For LIM, the threshold ($\frac{Y^{\text{rel}}}{d})_{\text{min}}$ leads to no reduction.

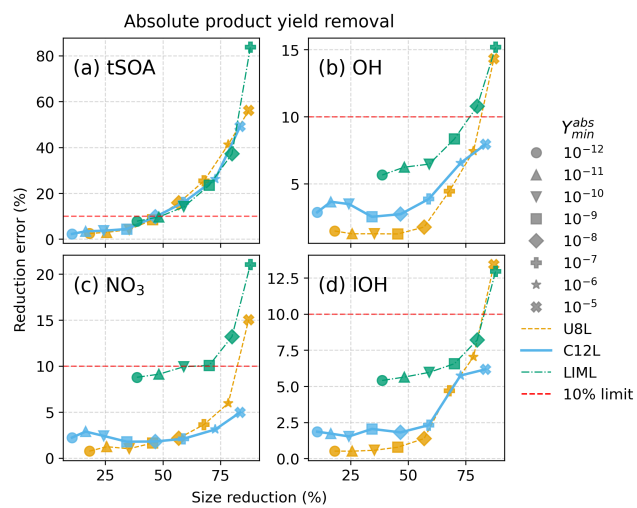


Figure S15. Sensitivity of mechanism size reduction and reduction error to threshold variation for the absolute product yield removal, evaluated using tSOA, OH, NO_3 , and IOH across the U8, C12, and LIM mechanisms.

Figure S16 further examines tracer–species response consistency using TBR sensitivity tests. Correlations of reduction errors across reduced mechanisms are used as a preliminary indicator of tracer representativeness. Strong correlations are found for OH and HO₂, while correlations for NO_x, NO₃, and O₃ are weaker and more variable across VOC classes.

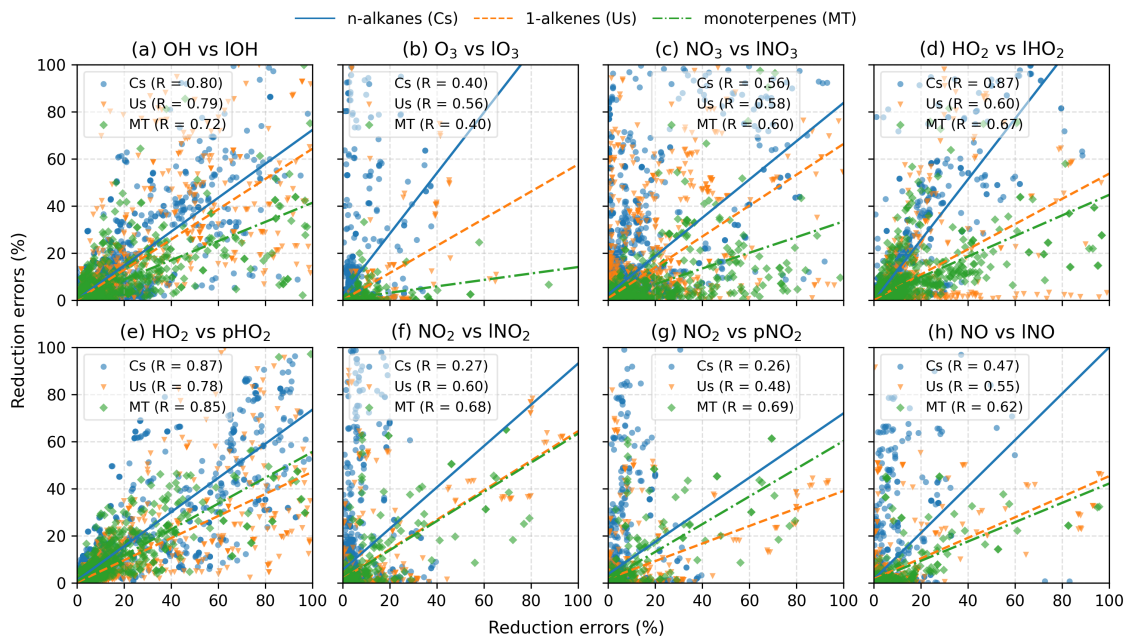


Figure S16. Correlation between reduction errors of tracer species and their corresponding explicit species (Sect. 4.4.1) across all reduced mechanisms and scenarios included in the TBR sensitivity tests (Sect. 4.3). Results are shown by VOC class, with correlation coefficients (R) indicated in each panel. Results for the pNO tracer are omitted due to concentrations that are too low (≈ 0) for reliable error estimation.

S2.2 Summary of size reduction and evaluation metrics

Detailed results of the TBR performance evaluation for the T6 and T10 strategy sets are presented. The achieved size reductions, together with the original mechanism sizes prior to TBR, are summarized in Table S3.

Tables S4–S5 report simulated values, reduction errors, and NMB for selected SOA and gas-phase metrics. These results focus on mean values across all PVOCs within each VOC class for individual scenarios (Table S4), as well as mean values across all scenarios for individual PVOCs (Table S5). For metrics that vary only in a subset of scenarios, deviations are computed using that subset. For example, mixing ratios of O_3 and NO_x are evaluated using three scenarios (simplified, simpl-nophot, and simpl-highphot), whereas PVOC loss ($\Delta PVOC$) is evaluated using ten scenarios, excluding the diurnal scenario in which the PVOC profile is prescribed hourly.

Table S3. Mechanism sizes before and after TBR. “ N^m ”, “ N^{sp} ”, and “ N^{cd} ” are the numbers of reactions, species, and condensable species, and “ Δ ” (%) denotes the reduction relative to the corresponding references.

PVOC	Reference mechanism			TBR mechanism with T6			TBR mechanism with T10		
	N^m	N^{sp}	N^{cd}	$N^m(\Delta)$	$N^{sp}(\Delta)$	$N^{cd}(\Delta)$	$N^m(\Delta)$	$N^{sp}(\Delta)$	$N^{cd}(\Delta)$
n-alkane mechanisms (Cs)									
C5	18 128	2 939	1 097	13 747 (24)	1 753 (40)	675 (38)	774 (96)	143 (95)	35 (97)
C6	34 841	5 543	1 797	26 012 (25)	3 135 (43)	1 124 (37)	8 931 (74)	1 578 (72)	461 (74)
C7	52 184	8 421	2 541	37 463 (28)	4 460 (47)	1 576 (38)	16 455 (68)	2 792 (67)	830 (67)
C8	65 766	10 617	3 088	45 362 (31)	5 308 (50)	1 819 (41)	20 551 (69)	3 348 (68)	976 (68)
C9	93 568	15 045	4 002	62 961 (33)	7 270 (52)	2 351 (41)	28 410 (70)	4 724 (69)	1 412 (65)
C10	127 464	20 336	5 038	79 111 (38)	9 172 (55)	2 902 (42)	34 740 (73)	5 975 (71)	1 783 (65)
C11	174 168	27 628	6 414	104 350 (40)	11 897 (57)	3 659 (43)	44 460 (74)	7 723 (72)	2 341 (64)
C12	219 743	34 865	7 775	124 327 (43)	14 208 (59)	4 380 (44)	51 078 (77)	9 006 (74)	2 779 (64)
C13	259 394	41385	8 762	129 010 (50)	15 116 (63)	4 878 (44)	51 242 (80)	9 626 (77)	3 041 (65)
C14	284 427	45 779	9 597	147 608 (48)	17 210 (62)	5 477 (43)	56 467 (80)	10 783 (76)	3 344 (65)
C15	330 077	53 087	10 427	154 247 (53)	18 229 (66)	5 877 (44)	53 900 (84)	10 740 (80)	3 373 (68)
C16	331 121	54 074	10 739	170 204 (49)	19 910 (63)	6 195 (42)	53 066 (84)	10 906 (80)	3 367 (69)
1-alkene mechanisms (Us)									
U5	27 634	4 571	1 586	22 045 (20)	2 903 (36)	1 216 (23)	5 492 (80)	1 015 (78)	388 (76)
U6	59 906	9 912	3 062	44 085 (26)	5 663 (43)	2 177 (29)	16 853 (72)	2 948 (70)	1 058 (65)
U7	103 852	16 806	4 601	68 945 (34)	8 652 (49)	3 183 (31)	30 442 (71)	5 199 (69)	1 756 (62)
U8	166 821	27 221	6 836	102 271 (39)	12 700 (53)	4 423 (35)	46 112 (72)	7 729 (72)	2 548 (63)
U9	241 632	39 073	9 122	136 763 (43)	16 703 (57)	5 677 (38)	59 820 (75)	10 037 (74)	3 271 (64)
U10	334 311	54 066	11 898	178 535 (47)	21 749 (60)	7 231 (39)	73 455 (78)	12 409 (77)	3 965 (67)
U11	418 116	67 674	13 994	216 360 (48)	26 226 (61)	8 556 (39)	85 401 (80)	14 719 (78)	4 611 (67)
U12	492 809	79 824	15 753	234 329 (52)	28 369 (64)	9 270 (41)	88 461 (82)	15 312 (81)	4 821 (69)
U13	556 551	90 808	17 395	260 543 (53)	31 568 (65)	10 255 (41)	94 345 (83)	16 430 (82)	5 048 (71)
U14	595 837	98 055	18 316	261 810 (56)	31 979 (67)	10 437 (43)	88 731 (85)	15 686 (84)	4 871 (73)
U15	618 232	102 744	19 129	260 208 (58)	31 776 (69)	10 308 (46)	71 416 (88)	13 262 (87)	4 023 (79)
U16	649 901	108 583	19 649	270 059 (58)	32 927 (70)	10 548 (46)	43 028 (93)	8 433 (92)	2 659 (86)
monoterpene mechanisms (MTs)									
API	993 317	160 696	40 985	403 882 (59)	51 655 (68)	18 847 (54)	116 530 (88)	17 720 (89)	5 727 (86)
BPI	791 937	125 226	30 408	285 660 (64)	36 292 (71)	13 280 (56)	108 186 (86)	17 963 (86)	5 811 (81)
LIM	762 747	125 314	29 071	391 072 (49)	51 924 (59)	18 398 (37)	107 658 (86)	15 667 (87)	5 468 (81)
CRN	657 399	105 052	27 657	283 221 (57)	35 577 (66)	12 878 (53)	86 572 (87)	13 136 (87)	4 271 (85)
CMP	656 220	103 821	26 062	238 973 (64)	29 552 (72)	11 021 (58)	84 040 (87)	13 128 (87)	4 309 (83)

Table S4: Metrics for SOA and gas-phase quantities in TBR-reduced mechanisms, summarized by VOC class (Cs, Us, MTs) across scenarios (“sc.”). Scenario labels: “U” (urban), “R” (remote), “C” (continental), “P” (poll-cont), “RC” (remote-cont), “S” (simplified), “U0” (urban-nophot), “UH” (urban-highphot), “S0” (simpl-nophot), “SH” (simpl-highphot), and “D” (diurnal). Group label “T” denotes totals across VOC classes. Values are omitted for scenarios with fixed evaluated quantities. Mean values are reported for all quantities, including the evaluated metric (“mean”), reduction error (“rdc”), and normalized mean bias (“NMB”). For errors and bias, values are shown for both T6 and T10 mechanisms, separated by “/”.

Item	sc.	Cs			Us			MTs			total		
		mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
tSOA	U	3.1	7/20	-4.6/-16	47	0.6/16	-0.3/-9	27	2.6/9	-2.2/-6	26	3.4/15	-2.4/-10
tSOA	R	2.9	0.8/6	-0.4/-5	10	0.2/1.5	-0.06/-1.2	13	1.7/15	-1.5/-13	9	0.9/8	-0.6/-7
tSOA	C	2.4	1.3/5	-0.8/-4.6	11	0.2/9	-0.01/-6	14	1.9/8	-1.8/-7	9	1.1/8	-0.9/-6
tSOA	P	3.3	1.6/8	-1.1/-7	19	0.2/14	-0.04/-8	18	2.9/9	-2.6/-8	13	1.6/10	-1.2/-7
tSOA	RC	2.7	0.8/4.7	-0.4/-4	10	0.2/1.9	-0.07/-1.5	13	1.6/11	-1.4/-10	9	0.9/6	-0.6/-5
tSOA	S	2.2	6/15	-3/-12	40	0.2/16	-0.04/-8	22	3/9	-2.5/-7	21	3.2/13	-1.8/-9
tSOA	U0	4.5	10/31	-4.7/-22	49	0.8/16	-0.2/-8	31	2.4/8	-2.1/-4.3	28	4.5/18	-2.3/-11
tSOA	UH	29	0.7/11	0.05/-9	30	1.3/10	-0.2/-8	18	4.1/13	-0.6/-11	26	2/11	-0.2/-9
tSOA	S0	2.8	6/17	-3.1/-13	45	0.2/15	0.02/-8	23	2.2/13	-0.5/-7	24	2.7/15	-1.2/-9
tSOA	SH	42	1.7/14	1.1/-11	47	3/19	1.7/-14	34	6/21	-2.9/-17	41	3.7/18	-0.04/-14
tSOA	D	0.4	2.4/10	-1.6/-8	1.8	0.3/15	-0.2/-9	6	1.5/8	-1.5/-7	2.6	1.4/11	-1.1/-8
tSOA	T	9	3.5/13	-1.7/-10	28	0.7/12	0.04/-7	20	2.7/11	-1.8/-9	19	2.1/12	-0.9/-9
OM:OC	U	1.7	1.6/1.5	1.2/0.9	2.1	0.06/0.6	-0.01/0.03	2.6	0.3/1.1	-0.2/-0.5	2.1	0.7/1	0.3/0.1
OM:OC	R	1.6	2.4/2.5	1.2/1.1	1.8	0.08/0.7	0.04/-0.5	1.8	0.06/1.1	-0.02/-0.9	1.7	0.9/1.4	0.4/-0.10
OM:OC	C	1.7	0.7/0.8	0.4/0.5	2	0.06/0.8	0.03/-0.5	2.1	0.1/0.6	0.03/-0.3	1.9	0.3/0.7	0.2/-0.1
OM:OC	P	1.8	0.6/0.7	0.4/0.5	2.1	0.04/0.5	0.01/0.1	2.3	0.3/0.9	-0.2/-0.6	2	0.3/0.7	0.07/-0.02
OM:OC	RC	1.6	2/2	1/0.9	1.8	0.08/0.8	0.04/-0.5	1.9	0.08/0.8	-0.01/-0.6	1.7	0.7/1.2	0.3/-0.07
OM:OC	S	1.6	1.6/1.5	1.2/0.8	2.1	0.05/0.6	-0.00/0.2	2.4	0.6/1.3	-0.4/-0.8	2.1	0.7/1.1	0.3/0.09
OM:OC	U0	1.7	1.6/1.8	0.9/0.04	2.1	0.06/0.5	0.01/-0.2	2.7	0.4/1.2	-0.05/-0.4	2.2	0.7/1.1	0.3/-0.2
OM:OC	UH	2.1	0.2/0.8	-0.01/-0.4	2.4	0.3/2.5	-0.2/-1.9	2.7	0.8/3	-0.6/-2.7	2.4	0.4/2.1	-0.3/-1.6
OM:OC	S0	1.6	1.5/1.7	0.9/0.6	2.1	0.03/0.3	0.02/0.2	2.3	0.1/2	0.01/-0.7	2	0.5/1.3	0.3/-0.01
OM:OC	SH	2.2	1.7/3	-0.9/-1.7	2.7	1.8/2.8	-1.3/-1.8	2.9	2.5/2.8	-1.9/-2.4	2.6	2/2.9	-1.4/-2
OM:OC	D	1.9	0.5/0.6	0.3/0.2	2.1	0.09/0.8	0.06/-0.4	2.3	0.3/0.6	0.2/-0.2	2.1	0.3/0.7	0.2/-0.1
OM:OC	T	1.8	1.3/1.5	0.6/0.3	2.1	0.2/1	-0.1/-0.5	2.4	0.5/1.4	-0.3/-0.9	2	0.7/1.3	0.1/-0.3
O:C	U	0.4	5/4.9	3.1/1.9	0.6	0.1/1.1	-0.01/0.02	1	0.6/2.2	-0.3/-1.1	0.6	2/2.7	0.9/0.3
O:C	R	0.3	14/14	7/6	0.4	0.3/1.6	0.2/-1	0.5	0.2/3.1	-0.03/-2.5	0.4	4.8/6	2.3/0.9

Item	sc.	Cs			Us			MTs			total		
		mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
O:C	C	0.4	3.5/3.6	1.9/1.8	0.5	0.2/1.2	0.1/-0.5	0.7	0.2/1.3	0.03/-0.8	0.5	1.3/2	0.7/0.1
O:C	P	0.4	2.2/2.2	1.3/1.1	0.6	0.1/1	0.03/0.2	0.8	0.6/1.8	-0.4/-1.4	0.6	1/1.7	0.3/-0.04
O:C	RC	0.3	11/12	6/5	0.4	0.3/1.6	0.2/-1	0.5	0.2/2.1	-0.03/-1.7	0.4	4/5	1.9/0.9
O:C	S	0.3	6/6	3.8/2.5	0.6	0.1/1	0.01/0.3	0.8	1/2.7	-0.7/-1.7	0.6	2.4/3.2	1/0.4
O:C	U0	0.4	5/6	2.8/-0.02	0.6	0.1/1.1	0.02/-0.3	1	0.6/2.1	-0.1/-0.8	0.7	2/3	0.9/-0.4
O:C	UH	0.6	0.5/1.9	-0.07/-1.1	0.8	0.6/4.5	-0.4/-3.5	1	1.3/4.9	-1/-4.4	0.8	0.8/3.7	-0.5/-3
O:C	S0	0.3	6/6	3.3/1.5	0.6	0.10/0.7	0.05/0.4	0.8	0.2/3.6	-0.01/-1.5	0.6	2/3.6	1.1/0.1
O:C	SH	0.7	3.4/7	-2/-4.2	1	3.2/6	-2.3/-4.2	1.2	4/5	-3.1/-4.3	0.9	3.6/6	-2.5/-4.3
O:C	D	0.5	1.8/2	0.8/0.5	0.6	0.3/1.6	0.2/-0.6	0.8	0.5/1.2	0.4/-0.7	0.6	0.9/1.6	0.5/-0.3
O:C	T	0.4	5/6	2.5/1.4	0.6	0.5/1.9	-0.2/-0.9	0.8	0.8/2.7	-0.5/-1.9	0.6	2.4/3.5	0.7/-0.3
N:C	U	0.04	10/11	6/7	0.1	0.1/1.1	-0.02/-0.4	0.2	0.8/2.1	-0.4/0.02	0.1	3.5/4.8	1.7/2.1
N:C	R	3.0e-03	1.6/4.2	0.4/3.4	3.1e-03	0.3/14	0.06/-4.9	2.8e-03	2.1/8	-0.6/6	2.9e-03	1.4/9	-0.06/1.4
N:C	C	0.04	1.4/2.3	0.9/1.8	0.07	0.2/6	0.09/-2.9	0.06	0.9/2.9	0.4/1.8	0.06	0.8/3.7	0.5/0.2
N:C	P	0.06	2/3.3	1.1/2.6	0.1	0.1/1.5	0.04/-0.07	0.1	0.8/2.8	-0.3/-0.6	0.09	1/2.5	0.3/0.6
N:C	RC	7.6e-03	1.6/3.6	0.7/3.1	7.4e-03	0.3/13	0.06/-5	7.0e-03	1.8/4.9	-0.3/3.9	7.3e-03	1.2/7	0.1/0.7
N:C	S	0.02	9/8	5/4.2	0.1	0.2/1.1	-0.01/0.2	0.1	1.1/2.9	-0.7/-0.2	0.09	3.6/4.2	1.5/1.4
N:C	U0	0.02	19/26	7/-1	0.1	0.1/2.2	0.03/-1.4	0.2	0.7/2.9	0.1/0.6	0.1	7/10	2.2/-0.6
N:C	UH	0.1	0.6/2.2	-0.08/0.2	0.2	0.7/4.3	-0.5/-3.4	0.2	2/7	-1.7/-6	0.2	1.1/4.3	-0.7/-3.1
N:C	S0	8.1e-03	30/41	11/0.6	0.1	0.08/0.9	0.04/-0.7	0.1	0.4/6	0.2/-0.3	0.08	10/16	3.8/-0.1
N:C	SH	0.1	4.6/4.9	-2.5/-2.4	0.2	5/6	-3.7/-1.1	0.2	5/5	-3.7/-2	0.2	4.9/5	-3.3/-1.8
N:C	D	0.10	1.7/2.6	0.6/1.7	0.1	0.4/3.6	0.2/-0.6	0.1	1.7/2.1	1.4/1.3	0.1	1.3/2.8	0.7/0.8
N:C	T	0.05	7/10	2.7/1.9	0.10	0.7/4.8	-0.3/-1.8	0.1	1.6/4.2	-0.5/0.4	0.09	3.3/7	0.7/-0.05
-OOH	U	0.03	10/15	8/12	0.08	0.2/4.8	0.03/5	0.07	2/5	-1.2/0.06	0.06	4.2/8	2.3/6
-OOH	R	0.1	18/19	9/10	0.1	0.5/0.7	0.3/-0.1	0.1	0.7/4.3	-0.5/1.6	0.1	6/8	3/3.7
-OOH	C	0.06	7/8	4.4/4.8	0.10	0.4/3.3	0.2/3.4	0.09	1.9/3.7	-1.4/-0.07	0.08	3.2/5	1/2.7
-OOH	P	0.04	4.8/6	3.1/3.8	0.08	0.3/4.1	0.05/4.5	0.07	2.5/6	-2/-1	0.06	2.6/5	0.4/2.4
-OOH	RC	0.10	16/16	8/8	0.1	0.5/0.8	0.3/0.07	0.1	0.9/3	-0.7/0.8	0.1	6/7	2.6/3.1
-OOH	S	0.05	10/13	7/10	0.07	0.2/4.7	0.07/5	0.07	1.7/6	-1.1/-1.8	0.06	4/8	2.1/4.5
-OOH	U0	0.04	12/21	9/15	0.08	0.3/5	0.05/6	0.07	3.1/5	-2.1/-0.6	0.06	5/10	2.4/7
-OOH	UH	5.7e-05	1.3/4.4	-0.2/-0.5	1.6e-03	3.9/9	3.1/7	9.9e-03	7/17	1.4/-6	3.8e-03	4.1/10	1.5/0.2
-OOH	S0	0.06	10/12	7/9	0.08	0.2/5	0.06/6	0.08	1.8/3.9	-1.3/0.5	0.07	3.8/7	1.8/5
-OOH	SH	0.05	2.3/3.8	0.5/-2	0.07	3.6/15	1.9/-10	0.06	10/27	-4/-17	0.06	5/15	-0.5/-10

Item	sc.	Cs			Us			MTs			total		
		mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
-OOH	D	0.02	5/6	3.2/3.5	0.06	0.7/3.9	0.1/1.4	0.07	7/11	-5/-8	0.05	4.2/7	-0.6/-1.1
-OOH	T	0.05	9/11	5/7	0.08	1/5	0.6/2.5	0.07	3.5/8	-1.6/-2.8	0.07	4.4/8	2/3.1
-ONO2	U	0.03	12/14	8/10	0.1	0.1/0.8	0.02/-0.5	0.09	1/3	-0.2/2.1	0.08	4.4/6	2.7/3.8
-ONO2	R	2.5e-03	1.8/4.3	0.5/3.5	2.4e-03	0.4/13	0.1/-7	1.5e-03	5/10	-3.3/4.7	2.1e-03	2.5/9	-0.9/0.6
-ONO2	C	0.04	1.8/2.5	1.1/1.9	0.06	0.3/7	0.2/-3.6	0.04	1.3/5	0.3/4.2	0.04	1.1/5	0.5/0.8
-ONO2	P	0.05	2.5/3.7	1.5/2.8	0.09	0.2/2.2	0.1/-0.5	0.07	1/3.7	0.2/2	0.07	1.2/3.2	0.6/1.4
-ONO2	RC	6.4e-03	1.9/3.9	0.8/3.3	5.8e-03	0.4/13	0.1/-6	4.0e-03	4.5/7	-2.4/3.6	5.4e-03	2.3/8	-0.5/0.2
-ONO2	S	0.02	11/9	7/4.5	0.1	0.1/0.9	0.03/-0.02	0.10	0.6/3.3	0.06/2.5	0.07	4/4.6	2.3/2.3
-ONO2	U0	2.9e-03	31/41	31/38	0.1	0.1/2.2	0.06/-1.4	0.08	1.3/6	0.8/4.7	0.06	11/16	11/14
-ONO2	UH	0.1	0.6/2.1	0.1/1	0.2	0.7/2.8	-0.3/-2.1	0.2	1.4/6	-1.1/-6	0.1	0.9/3.6	-0.4/-2.2
-ONO2	S0	8.2e-04	58/59	45/48	0.1	0.10/1.3	0.05/-1	0.08	0.7/4.4	0.3/2.8	0.06	19/21	15/16
-ONO2	SH	0.1	2.7/3.3	-1.3/-0.7	0.1	4/5	-2.6/0.7	0.1	2.2/6	-0.6/1.5	0.1	2.9/4.6	-1.5/0.5
-ONO2	D	0.09	2.1/3.2	0.9/2.1	0.09	0.4/5	0.3/-1.2	0.09	1.8/2.2	1.4/1	0.09	1.4/3.5	0.9/0.7
-ONO2	T	0.04	11/13	9/10	0.09	0.6/4.8	-0.2/-2	0.08	1.9/5	-0.4/2.1	0.07	4.8/8	3/3.3
OHR	U	3.1	0.4/3.2	-0.1/-2	3.5	3.1/9	-1.3/-4	3.8	15/24	-6/-8	3.4	6/12	-2.4/-4.5
OHR	R	3	0.2/0.8	0.2/-0.3	8	0.2/0.9	0.08/-0.5	8	0.9/4.9	-0.7/-3.1	7	0.4/2.2	-0.1/-1.3
OHR	C	3	0.3/4.6	0.1/-2.7	8	0.3/1.5	-0.01/-0.8	8	1.3/4.3	-0.8/-2.8	6	0.6/3.5	-0.2/-2.1
OHR	P	3.1	0.4/6	-0.04/-3.5	7	0.7/3.3	-0.2/-1.6	6	2.2/4.6	-1/-2.6	5	1.1/4.5	-0.4/-2.6
OHR	RC	3	0.2/1.2	0.2/-0.6	9	0.2/1	0.05/-0.5	8	0.9/4.2	-0.7/-2.8	7	0.4/2.1	-0.1/-1.3
OHR	S	3	0.3/2.7	0.09/-1.6	4.7	1.4/6	-0.6/-2.7	5	5/10	-2.5/-3.5	4.3	2.4/6	-1/-2.6
OHR	U0	3	0.6/3.4	-0.3/-2.2	2.7	2.3/6	-1/-3.2	3	14/23	-6/-8	2.9	6/11	-2.4/-4.5
OHR	UH	2.6	1.3/12	-0.4/-8	2.8	2/16	-0.3/-4.9	2	7/17	0.02/-2.6	2.5	3.4/15	-0.2/-5
OHR	S0	3	0.3/2.6	0.00/-1.7	3.9	0.8/4.4	-0.4/-2.1	5	10/15	-2.8/-2.7	4.1	3.6/7	-1.1/-2.2
OHR	SH	1.4	9/30	-0.6/-7	1.4	30/66	-0.7/-3.2	1.2	13/97	1.2/-2.5	1.3	17/64	-0.03/-4.2
OHR	D	0.2	0.4/6	-0.3/-3.9	0.8	0.6/3.2	-0.5/-2.4	2.4	2.7/5	-2.1/-4.1	1.1	1.3/4.8	-1/-3.5
OHR	T	2.6	1.2/7	-0.1/-3	4.7	3.8/11	-0.4/-2.4	4.9	7/19	-1.9/-3.8	3.9	3.2/10	-0.6/-2.9
O ₃ R	U	2.7e-10	5/49	-1.1/6	3.0e-07	2.4/17	-0.3/-0.8	4.3e-07	9/69	0.08/2.4	2.4e-07	5/45	-0.4/2.4
O ₃ R	R	1.4e-10	0.8/28	0.5/-15	9.2e-07	0.3/0.9	0.2/-0.2	9.6e-07	0.4/5	0.00/-0.3	6.3e-07	0.5/11	0.2/-5
O ₃ R	C	1.0e-10	0.4/39	-0.05/-4.7	8.7e-07	0.3/1.2	0.2/-0.2	8.9e-07	3/5	0.2/-0.09	5.8e-07	1.3/15	0.1/-1.7
O ₃ R	P	1.8e-10	0.6/43	-0.3/1.1	6.6e-07	0.5/1.9	0.2/-0.2	7.6e-07	5/20	0.5/0.6	4.8e-07	2.1/22	0.1/0.5
O ₃ R	RC	1.1e-10	0.7/27	0.4/-15	9.3e-07	0.3/0.9	0.2/-0.2	9.6e-07	0.5/4.9	0.01/-0.3	6.3e-07	0.5/11	0.2/-5
O ₃ R	S	2.0e-10	4/47	0.7/11	4.9e-07	1/4.3	-0.03/-0.8	6.0e-07	10/35	0.6/3.5	3.6e-07	5/29	0.4/4.5
O ₃ R	U0	-	-	-	2.5e-07	1.2/24	-0.2/-0.8	4.3e-07	2.3/19	0.05/2.5	3.4e-07	1.8/21	-0.10/0.8

Item	sc.	Cs			Us			MTs			total		
		mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
O ₃ R	UH	5.1e-09	1.7/46	0.9/4.1	1.5e-07	7/27	1/2	3.3e-07	18/30	6/8	1.6e-07	9/34	2.6/4.7
O ₃ R	SO	-	-	-	4.4e-07	1.8/8	-0.2/-1.3	6.0e-07	1.4/50	0.2/6	5.2e-07	1.6/29	-0.02/2.4
O ₃ R	SH	1.1e-09	17/65	2/-1.7	1.3e-07	45/82	0.6/1.5	2.8e-07	89/136	4.4/6	1.4e-07	50/94	2.4/1.9
O ₃ R	D	4.8e-11	1.4/45	-1/6	9.2e-08	0.01/0.3	-0.01/-0.3	7.7e-07	0.03/0.2	-0.02/0.1	2.9e-07	0.5/15	-0.4/2
O ₃ R	T	8.1e-10	3.5/43	0.2/-1	4.7e-07	5/15	0.2/-0.1	6.4e-07	13/34	1.1/2.6	3.3e-07	6/29	0.4/0.08
NO ₃ R	U	2.2e-04	1.1/14	-0.5/-9	1.9e-03	4.2/19	-1.1/-4.9	0.06	11/17	0.2/8	0.02	5/17	-0.5/-2.1
NO ₃ R	R	1.5e-03	0.1/17	0.09/20	6.0e-03	0.4/2.9	-0.09/-1.6	0.1	1/10	0.2/1.4	0.05	0.5/10	0.07/7
NO ₃ R	C	3.7e-04	0.3/13	-0.07/-8	5.3e-03	0.6/3.8	-0.2/-1.9	0.1	2.3/7	0.3/-0.5	0.04	1/8	0.00/-3.4
NO ₃ R	P	3.4e-04	0.6/18	-0.3/-11	4.4e-03	1/8	-0.3/-3.5	0.1	2.3/9	0.7/1.3	0.04	1.3/12	0.00/-4.4
NO ₃ R	RC	1.3e-03	0.1/11	0.08/6	6.0e-03	0.4/2.5	-0.1/-1.4	0.1	0.8/7	0.2/-0.09	0.05	0.5/7	0.05/1.5
NO ₃ R	S	2.1e-04	0.9/12	0.2/-8	2.9e-03	2/14	-0.6/-4.8	0.08	4.7/18	0.8/8	0.03	2.5/15	0.1/-1.4
NO ₃ R	U0	2.5e-04	1.2/16	-0.7/-10	1.5e-03	4.3/17	-0.6/-3.4	0.06	11/22	0.2/8	0.02	5/18	-0.4/-1.7
NO ₃ R	UH	9.4e-04	5/43	-3.4/-26	2.4e-03	7/47	-3/-24	0.04	15/31	4.9/5	0.01	9/40	-0.5/-15
NO ₃ R	SO	2.6e-04	0.7/12	0.1/-8	2.5e-03	1.6/8	-0.4/-2.8	0.08	4/34	0.7/17	0.03	2.1/18	0.2/2
NO ₃ R	SH	1.3e-03	9/35	1.3/-5	1.6e-03	16/57	0.6/-15	0.03	8/73	4.4/4.1	0.01	11/55	2.1/-5
NO ₃ R	D	6.0e-05	0.5/15	-0.5/-10	6.4e-04	1.5/11	-1.1/-9	0.06	0.1/0.7	0.02/-0.5	0.02	0.7/9	-0.5/-7
NO ₃ R	T	6.2e-04	1.8/19	-0.3/-6	3.2e-03	3.5/17	-0.6/-7	0.08	5/21	1.1/4.7	0.02	3.1/19	-0.2/-4.5
OHR-r	U	0.8	3.1/16	-1.2/-10	1.8	2.8/8	-1.7/-5	2.5	14/16	-6/-7	1.7	7/14	-2.9/-7
OHR-r	R	0.6	0.2/2.1	0.08/-1.9	3.8	0.3/1.3	-0.04/-1	4.3	1.1/12	-0.9/-9	2.9	0.5/5	-0.3/-4.1
OHR-r	C	0.5	0.4/11	-0.3/-8	3.8	0.4/2.1	-0.2/-1.6	4.1	1.3/4.3	-1.1/-3.2	2.8	0.7/6	-0.5/-4.2
OHR-r	P	0.8	0.7/14	-0.5/-9	3.4	0.9/3.8	-0.5/-2.8	3.5	2/7	-1.4/-3.5	2.5	1.2/8	-0.8/-5
OHR-r	RC	0.5	0.3/3.3	0.1/-2.8	3.8	0.3/1.3	-0.09/-1	4.4	0.9/6	-0.8/-4.7	2.9	0.5/3.5	-0.3/-2.8
OHR-r	S	0.6	2.8/16	0.4/-10	2.2	1.4/6	-1/-4	3.5	4.3/12	-1.9/-3.8	2.1	2.8/11	-0.8/-6
OHR-r	U0	1.1	2.7/14	-0.7/-7	1.4	2.4/6	-1.5/-4.6	2	15/17	-8/-10	1.5	7/12	-3.4/-7
OHR-r	UH	1.8	1.2/17	-0.4/-10	1.8	1.3/13	0.1/-4.4	1.1	9/11	1/2.5	1.6	3.7/13	0.3/-4
OHR-r	SO	0.8	1.6/14	0.2/-9	1.7	0.8/4.7	-0.6/-3	3.9	10/16	-2.9/-4.6	2.1	4/12	-1.1/-5
OHR-r	SH	0.8	10/27	-0.7/-9	0.8	30/65	-1.2/-4.8	0.6	17/85	1/-2	0.7	19/59	-0.3/-5
OHR-r	D	0.05	1.1/16	-0.8/-11	0.3	1.1/5	-0.9/-4.6	1.4	2.6/4.7	-2.3/-4.2	0.6	1.6/9	-1.3/-7
OHR-r	T	0.8	2.2/14	-0.3/-8	2.3	3.8/11	-0.7/-3.4	2.8	7/17	-2.1/-4.5	1.7	3.7/13	-0.8/-5
O ₃ R-r	U	2.7e-10	5/49	-1.1/6	3.9e-09	1/22	-0.5/-9	4.8e-08	9/69	3.6/-9	1.7e-08	5/46	0.7/-4.3
O ₃ R-r	R	1.4e-10	0.8/28	0.5/-15	2.7e-08	0.2/9	0.01/-4.9	1.5e-07	1.3/25	-0.7/-15	5.9e-08	0.8/20	-0.06/-12
O ₃ R-r	C	1.0e-10	0.4/39	-0.05/-4.7	2.3e-08	0.3/14	-0.05/-7	1.3e-07	2/6	-0.2/-3.2	5.2e-08	0.9/20	-0.1/-5
O ₃ R-r	P	1.8e-10	0.6/43	-0.3/1.1	1.7e-08	0.4/19	-0.03/-9	1.0e-07	4.9/21	1.2/-2.1	4.0e-08	2/27	0.3/-3.4

Item	sc.	Cs			Us			MTs			total		
		mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
O ₃ R-r	RC	1.1e-10	0.7/27	0.4/-15	2.6e-08	0.2/9	-0.02/-5	1.5e-07	1/11	-0.5/-7	5.9e-08	0.6/16	-0.03/-9
O ₃ R-r	S	2.0e-10	4/47	0.7/11	7.6e-09	0.6/19	-0.2/-9	8.6e-08	10/32	4.3/1.4	3.1e-08	4.7/33	1.6/1.1
O ₃ R-r	U0	-	-	-	1.9e-09	1.2/24	-0.3/-8	8.2e-08	3.9/29	-1.4/-7	4.2e-08	2.5/26	-0.9/-7
O ₃ R-r	UH	5.1e-09	1.7/46	0.9/4.1	1.7e-08	7/39	3.1/-9	3.5e-08	18/32	15/26	1.9e-08	9/39	6/7
O ₃ R-r	S0	-	-	-	3.0e-09	0.4/8	-0.1/-2.2	1.6e-07	1.6/33	-1.5/-6	7.9e-08	1/21	-0.8/-3.9
O ₃ R-r	SH	1.1e-09	17/65	2/-1.7	7.0e-09	45/82	1.2/-12	2.5e-08	89/136	15/25	1.1e-08	50/94	6/3.9
O ₃ R-r	D	4.8e-11	1.4/45	-1/6	3.2e-09	0.2/18	-0.2/-11	1.0e-07	0.5/3.3	-0.1/-1.2	3.6e-08	0.7/22	-0.5/-2
O ₃ R-r	T	8.1e-10	3.5/43	0.2/-1	1.2e-08	5/24	0.3/-8	9.6e-08	14/37	3.6/0.7	2.3e-08	6/33	0.8/-3.8
NO ₃ R-r	U	1.7e-04	1.5/19	-0.8/-12	1.2e-03	4.2/20	-1.4/-7	0.02	10/25	0.3/20	5.7e-03	5/21	-0.6/0.4
NO ₃ R-r	R	1.5e-03	0.1/18	0.09/21	3.8e-03	0.5/3.4	-0.3/-2.4	0.02	2.5/22	1.2/10	8.8e-03	1/14	0.4/9
NO ₃ R-r	C	3.2e-04	0.3/13	-0.1/-8	3.3e-03	0.7/4.5	-0.4/-3	0.02	2.4/9	1.2/-0.3	6.2e-03	1.1/9	0.2/-3.8
NO ₃ R-r	P	2.9e-04	0.7/20	-0.4/-12	2.8e-03	1.1/9	-0.6/-5	0.02	3.4/14	2.2/7	6.6e-03	1.7/14	0.4/-3.2
NO ₃ R-r	RC	1.3e-03	0.1/11	0.08/6	3.8e-03	0.5/2.9	-0.3/-2	0.02	2.5/17	1.4/5	7.6e-03	1/10	0.4/3.1
NO ₃ R-r	S	1.6e-04	1.2/17	0.3/-10	1.8e-03	2.1/16	-1/-7	0.02	4.6/28	1.3/24	7.9e-03	2.6/20	0.2/2.3
NO ₃ R-r	U0	2.1e-04	1.3/19	-0.8/-12	8.8e-04	4.4/17	-0.8/-4.8	0.02	11/26	0.4/23	5.4e-03	6/21	-0.4/2
NO ₃ R-r	UH	9.1e-04	5/44	-3.5/-27	2.1e-03	7/49	-3.7/-30	3.6e-03	14/34	0.00/-3.1	2.2e-03	9/42	-2.4/-20
NO ₃ R-r	S0	2.1e-04	0.9/15	0.2/-10	1.5e-03	1.7/8	-0.5/-3.7	0.03	4.4/48	1.5/39	9.3e-03	2.3/24	0.4/9
NO ₃ R-r	SH	1.1e-03	9/35	0.7/-4.1	1.2e-03	17/57	-0.05/-19	2.5e-03	13/67	4.8/-9	1.6e-03	13/53	1.8/-11
NO ₃ R-r	D	5.8e-05	0.6/15	-0.5/-10	4.2e-04	2/16	-1.7/-13	7.9e-03	1.1/7	0.2/-4.3	2.8e-03	1.2/12	-0.6/-9
NO ₃ R-r	T	5.6e-04	2/21	-0.4/-7	2.1e-03	3.8/18	-1/-9	0.01	6/27	1.3/10	3.6e-03	3.5/21	-0.4/-4.8
NO _x	S	15	2/2.9	-0.7/0.7	10	0.4/1.7	0.2/0.4	8	5/13	1.6/5	11	2.5/6	0.4/2.2
NO _x	S0	13	2.2/4.1	-0.6/1.7	10	0.3/0.7	0.1/-0.3	8	1.5/14	0.6/8	10	1.3/6	0.04/3.2
NO _x	SH	3.3	14/17	-1/1.7	2.2	16/17	-2.2/0.5	1.7	20/27	1.3/4.6	2.4	17/20	-0.6/2.3
NO _x	T	10	6/8	-0.8/1.4	7	6/6	-0.6/0.2	6	9/18	1.2/6	8	6/9	-0.4/1.7
O ₃	S	23	0.9/1.3	0.2/-0.3	25	0.7/2.6	-0.4/-1.4	33	6/10	-3.9/-6	27	2.5/4.7	-1.3/-2.7
O ₃	S0	16	1.9/3.5	0.5/-0.4	16	0.09/0.6	-0.03/0.2	16	0.3/7	-0.1/-3	16	0.8/3.6	0.09/-1.1
O ₃	SH	75	4.9/14	-3.1/-10	83	8/13	-4.9/-9	88	11/23	-8/-16	82	8/17	-5/-12
O ₃	T	38	2.6/6	-0.8/-3.6	41	2.8/5	-1.8/-3.5	46	6/13	-4.1/-8	41	3.2/7	-1.8/-4.4
HO ₂	U	8.1e-04	2.5/10	-0.9/-5	1.7e-03	8/22	-3.3/-7	1.3e-03	40/58	-24/-34	1.3e-03	17/30	-9/-16
HO ₂	R	7.9e-04	0.1/9	-0.07/-2.9	2.2e-03	0.5/1.5	-0.3/0.8	2.0e-03	7/24	-3.6/-7	1.7e-03	2.5/11	-1.3/-3.1
HO ₂	C	1.2e-03	0.4/3.1	-0.2/-0.2	2.4e-03	0.8/2	-0.4/-0.3	2.1e-03	9/15	-6/-11	1.9e-03	3.4/7	-2.3/-3.9
HO ₂	P	1.3e-03	1/11	-0.6/-5	2.3e-03	2.3/6	-1.4/-3.1	2.1e-03	19/29	-13/-20	1.9e-03	7/15	-5/-10
HO ₂	RC	7.2e-04	0.1/6	-0.06/-0.7	2.1e-03	0.4/1.7	-0.2/0.8	1.9e-03	7/18	-4/-8	1.6e-03	2.7/9	-1.4/-2.5

Item	sc.	Cs			Us			MTs			total		
		mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
HO ₂	S	7.4e-04	1.4/8	0.03/-4.3	1.8e-03	3.6/11	-2/-4.1	1.7e-03	28/41	-22/-31	1.4e-03	11/20	-8/-13
HO ₂	U0	1.3e-03	2.8/13	-1.4/-7	1.8e-03	6/18	-1.7/-4.1	1.4e-03	40/68	-24/-35	1.5e-03	16/33	-9/-16
HO ₂	UH	2.9e-04	3.2/26	-2/-15	3.5e-04	7/35	-4.4/-18	2.9e-04	25/62	-18/-36	3.1e-04	12/41	-8/-23
HO ₂	S0	1.2e-03	1.1/8	-0.00/-4.9	2.0e-03	0.8/4.4	-0.2/0.7	1.1e-03	18/45	-14/-28	1.4e-03	7/19	-4.7/-11
HO ₂	SH	0.02	3.4/32	-2.9/-19	0.02	6/21	-4.9/-15	0.02	15/37	-9/-27	0.02	8/30	-6/-20
HO ₂	D	3.5e-04	0.4/3.5	-0.3/-2.6	1.2e-03	1.4/6	-1.1/-4.3	1.9e-03	14/22	-11/-17	1.2e-03	5/10	-4.3/-8
HO ₂	T	2.2e-03	1.5/12	-0.8/-6	3.3e-03	3.4/12	-1.8/-4.8	3.3e-03	20/38	-14/-23	2.8e-03	6/16	-3.4/-9

Table S5: Metrics for SOA and gas-phase quantities in TBR-reduced mechanisms, reported for individual PVOCs. The same metrics and reporting format as in Table S4 are used.

PVOC	Evaluation target								
	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
	tSOA			OM:OC			O:C		
C7L	0.3	9/53	-6/-39	2.3	2.4/3	1.4/1.5	0.8	5/6	3/2.8
C8L	0.8	9/15	-6/-12	2.1	1.8/1.8	1/0.3	0.6	4.4/4.2	2.6/0.8
C9L	1.7	5/10	-3.1/-9	2	1.3/1.5	0.7/-0.07	0.5	3.6/3.9	2.1/0.04
C10L	3.2	1.8/19	0.05/-15	1.8	0.3/0.8	-0.04/-0.2	0.5	0.6/2.3	-0.03/-1.4
C11L	5	0.9/12	-0.2/-10	1.7	1.1/1.2	0.4/0.2	0.4	4.2/4.8	1.7/0.7
C12L	8	1/6	0.08/-5	1.7	1.1/1.2	0.4/0.2	0.3	4.8/5	1.9/1
C13L	11	1.1/5	-0.4/-4.7	1.6	1.2/1.3	0.4/0.1	0.3	6/6	2.2/1
C14L	14	1.5/3.3	0.4/-2.9	1.5	1.2/1.3	0.5/0.2	0.3	7/7	3/1.7
C15L	18	1.8/2.1	-0.6/-1.2	1.5	1.4/1.5	0.5/0.3	0.2	8/9	3.4/2.7
C16L	24	2.9/3	-1.1/-1.6	1.4	1.4/1.6	0.6/0.5	0.2	11/11	5/4.5
U5L	1.1	1.6/113	-0.4/-63	3.2	0.2/5	0.1/-1.2	1.3	0.4/8	0.2/-1.1
U6L	2.1	1.4/8	0.4/-5	2.8	0.3/1.3	-0.2/-0.8	1.1	0.3/2.3	-0.2/-1.7
U7L	4.3	1.4/6	0.4/-4.8	2.5	0.3/0.9	-0.2/-0.8	0.9	0.5/1.9	-0.3/-1.5
U8L	7	0.7/3.5	0.01/-3.1	2.3	0.2/0.6	-0.1/-0.5	0.8	0.3/1.3	-0.2/-1.1
U9L	12	0.5/2.1	0.00/-1.2	2.1	0.2/0.7	-0.1/-0.5	0.6	0.3/1.3	-0.2/-1
U10L	19	0.4/2.3	-0.1/-1.8	2	0.2/0.6	-0.2/-0.5	0.6	0.4/1.4	-0.3/-1
U11L	29	0.3/1.7	-0.07/-1.4	1.9	0.2/0.4	-0.1/-0.3	0.5	0.4/0.9	-0.3/-0.7
U12L	38	0.3/1.7	-0.2/-1.4	1.8	0.2/0.4	-0.2/-0.3	0.4	0.5/0.9	-0.3/-0.7

PVOC	Evaluation target								
	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
U13L	46	0.3/1.9	-0.2/-1.5	1.8	0.2/0.4	-0.1/-0.2	0.4	0.5/0.9	-0.2/-0.6
U14L	53	0.2/1.5	0.09/-1.1	1.7	0.2/0.3	-0.10/-0.2	0.4	0.5/0.9	-0.2/-0.5
U15L	60	0.4/1.7	0.2/-1.3	1.7	0.3/0.4	-0.08/-0.2	0.3	0.8/1.3	-0.1/-0.6
U16L	66	0.5/1.2	0.4/-0.6	1.6	0.4/0.6	-0.02/-0.2	0.3	1.3/2.1	0.09/-0.5
APIL	16	1.6/11	-1.2/-9	2.3	0.3/0.8	-0.2/-0.5	0.8	0.5/1.5	-0.4/-1
BPIL	23	4.2/7	-3.3/-3.6	2.3	0.7/1.2	-0.4/-0.6	0.8	1.2/2.2	-0.7/-1.2
CMPL	21	2.9/11	-1.6/-8	2.5	0.7/1.9	-0.3/-1.2	0.9	1.1/3.6	-0.6/-2.4
LIML	33	3.3/9	-1.3/-8	2.4	0.3/1.4	-0.2/-1.1	0.9	0.5/2.7	-0.3/-2.1
CRNL	7	1.8/18	-1.5/-15	2.3	0.5/1.6	-0.3/-1.3	0.8	0.8/3.6	-0.4/-2.9
	N:C			-OOH			-ONO2		
C7L	0.1	6/11	2.2/7	0.1	14/15	12/13	0.08	12/18	11/16
C8L	0.09	6/6	2.5/0.1	0.09	12/12	9/9	0.07	10/10	8/8
C9L	0.07	5/10	2.5/-3.9	0.08	8/9	6/7	0.06	8/7	6/6
C10L	0.05	1.5/7	-0.3/3.1	0.06	1.3/14	0.4/10	0.05	1.4/12	-0.6/6
C11L	0.04	7/10	2.5/4.3	0.05	5/12	2.5/8	0.04	12/15	10/14
C12L	0.04	8/10	2.9/2	0.04	6/7	2.4/4.7	0.03	12/13	9/11
C13L	0.03	8/10	2.8/1.8	0.03	7/8	3.4/2.1	0.03	12/12	9/10
C14L	0.03	8/9	3.3/1.3	0.02	9/10	4.3/2	0.03	12/13	8/9
C15L	0.02	10/11	3.1/1.2	0.02	12/12	6/3.5	0.02	15/15	10/10
C16L	0.02	14/15	5/2.2	0.01	15/15	8/7	0.02	19/19	15/14
U5L	0.2	0.6/41	0.2/-20	0.2	2.3/38	2/34	0.2	0.6/46	0.3/-24
U6L	0.2	0.8/3.6	-0.5/0.6	0.2	1.2/9	1/-1.6	0.2	0.8/3.4	-0.3/1.1
U7L	0.1	1/2.2	-0.5/0.1	0.1	1/1.6	0.7/0.5	0.1	1/2.2	-0.4/1
U8L	0.1	0.6/1.3	-0.4/-0.3	0.10	0.6/1.1	0.5/0.1	0.1	0.5/1	-0.3/0.2
U9L	0.1	0.6/1.5	-0.4/-0.8	0.08	0.8/1.6	0.5/-0.4	0.09	0.5/0.9	-0.3/-0.6
U10L	0.09	0.7/1.2	-0.5/-0.7	0.06	0.5/1	0.2/-0.2	0.08	0.5/0.6	-0.3/-0.5
U11L	0.08	0.6/0.9	-0.4/-0.4	0.05	0.5/0.9	0.3/-0.2	0.07	0.4/0.6	-0.2/-0.4
U12L	0.07	0.6/1	-0.4/-0.2	0.05	0.4/1	0.1/-0.4	0.06	0.4/0.5	-0.2/-0.3
U13L	0.06	0.6/1	-0.3/0.04	0.04	0.6/1.2	0.2/-0.5	0.05	0.4/0.4	-0.1/-0.2
U14L	0.05	0.6/1	-0.4/-0.07	0.04	0.6/1	0.3/-0.2	0.05	0.5/0.7	-0.2/-0.4
U15L	0.05	0.7/1.2	-0.3/-0.08	0.03	0.9/2.3	0.3/-0.3	0.04	0.6/0.7	-0.1/-0.1
U16L	0.05	1/1.6	-0.1/-0.04	0.03	2.4/3.8	0.6/-0.3	0.04	1.1/1.3	-0.00/-0.2
APIL	0.1	1/4.6	-0.5/2.7	0.09	1/2.9	0.2/2.5	0.05	1.1/4.6	-0.4/2.6

PVOC	Evaluation target								
	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
BPIL	0.1	2/3.4	-0.06/-0.3	0.04	9/12	-4.4/-8	0.08	1.7/3.1	0.9/0.5
CMPL	0.1	1.9/6	-0.4/0.4	0.04	6/14	-3.6/-8	0.1	1.3/5	0.4/2.3
LIML	0.1	1.8/2.6	-1.2/-0.9	0.09	1.4/6	-0.6/2.2	0.07	3.9/5	-3/0.6
CRNL	0.1	1.2/3.9	-0.4/0.05	0.10	0.5/7	0.3/-3.4	0.06	1.7/7	0.01/4.6
	OHR			O ₃ R			NO ₃ R		
C5L	1	0.5/39	-0.3/-22	5.4e-12	3.3/200	0.3/-100	2.9e-04	1.7/97	-0.5/-57
C6L	1.4	0.5/18	-0.2/-10	8.6e-11	2.8/178	0.5/-93	3.7e-04	1.8/48	-0.3/-25
C7L	1.6	0.5/2.8	-0.2/-1.8	1.2e-10	3.8/90	1.4/177	4.5e-04	1.8/29	-0.06/12
C8L	1.9	0.6/1.1	-0.2/-0.5	2.9e-10	2.9/7	-0.4/-0.04	5.3e-04	1.6/6	-0.5/-0.9
C9L	2.4	0.5/1.2	-0.1/-0.4	7.8e-10	3.8/6	0.7/1.3	6.3e-04	1.7/7	-0.2/-0.8
C10L	2.7	0.8/1.4	-0.2/-0.5	1.2e-09	3.3/7	-0.1/-0.3	7.1e-04	1.7/7	-0.3/-1.6
C11L	2.9	0.7/1.1	-0.2/-0.2	1.3e-09	2.6/6	0.1/1	7.3e-04	1.4/7	-0.2/-1.2
C12L	3	0.8/1	-0.3/-0.2	1.3e-09	2.4/4.2	0.1/0.5	7.4e-04	1.6/5	-0.3/-0.1
C13L	3.3	1.6/1.8	-0.3/-0.4	1.1e-09	2.1/3.2	-0.2/0.04	7.5e-04	1.7/4.3	-0.6/-0.4
C14L	3.5	1.2/1.4	0.04/-0.01	1.2e-09	2.3/2.2	0.4/0.7	7.5e-04	1.3/3.6	0.08/0.03
C15L	3.6	4.5/6	0.2/-0.01	1.2e-09	9/9	0.1/0.7	7.4e-04	4/6	-0.7/-0.7
C16L	3.6	2.7/4.1	0.3/0.00	1.1e-09	4.7/5	-0.3/0.04	7.1e-04	2/4.3	-0.3/-0.7
U5L	3.9	3/42	-1/-13	4.9e-07	2.3/55	0.02/-1.7	2.1e-03	4.5/57	-1.3/-22
U6L	4.5	3.5/24	-0.5/-7	4.6e-07	2.2/42	0.1/-1.5	2.8e-03	3/43	-0.4/-17
U7L	4.9	4.2/4.9	-0.6/-1.3	5.0e-07	2.7/6	0.08/0.08	3.1e-03	3.7/16	-0.8/-7
U8L	5	2.9/3.6	-0.5/-0.7	4.9e-07	2.7/3.5	0.07/0.1	3.3e-03	2.9/11	-0.7/-4.6
U9L	5	2.5/3.3	-0.4/-0.6	4.7e-07	3.2/5	0.05/0.04	3.3e-03	2.7/9	-0.6/-3.9
U10L	5	3.9/4.3	-0.7/-0.8	5.0e-07	4.6/6	0.04/0.08	3.5e-03	3.3/9	-0.8/-3.4
U11L	5	3.1/3.8	-0.5/-0.6	4.7e-07	4.3/5	0.08/0.1	3.5e-03	2.9/6	-0.6/-2.4
U12L	4.9	3.9/5	-0.6/-0.7	4.7e-07	7/7	0.05/0.07	3.5e-03	3.3/7	-0.7/-2.5
U13L	4.8	4/6	-0.7/-0.9	4.7e-07	7/8	-0.09/-0.1	3.4e-03	3.8/8	-0.9/-2.7
U14L	4.6	3.2/4.9	-0.01/-0.10	4.6e-07	3.9/4.3	0.3/0.2	3.4e-03	2.6/7	-0.2/-2
U15L	4.4	4.2/8	0.06/-1	4.6e-07	14/20	0.4/0.6	3.3e-03	3.2/8	-0.2/-1.9
U16L	4.3	7/17	0.3/-2.4	4.6e-07	11/20	0.7/0.7	3.2e-03	6/28	-0.3/-9
APIL	3.4	4.4/7	-1.9/-3.8	7.7e-07	14/29	0.03/0.3	0.06	3.4/8	-0.00/1.6
BPIL	4.3	12/27	-3.4/-5	4.8e-07	17/25	3.2/5	0.07	8/22	3.7/9
CMPL	6	6/23	-0.09/-1.2	4.0e-08	13/49	1.7/5	0.08	7/36	1.5/11
LIML	7	8/12	-2.6/-6	1.3e-06	15/21	0.6/0.8	0.08	8/20	0.5/-1.6

PVOC	Evaluation target								
	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
CRNL	4.5	3.8/26	-1.5/-2.8	5.7e-07	3.8/46	-0.06/1.5	0.1	1.2/19	-0.03/3.4
	OHR-r			O ₃ R-r			NO ₃ R-r		
C5L	0.3	1.5/102	-0.6/-62	5.4e-12	3.3/200	0.3/-100	2.6e-04	1.8/110	-0.6/-63
C6L	0.4	1.4/31	-0.6/-25	8.6e-11	2.8/178	0.5/-93	3.3e-04	1.9/51	-0.5/-27
C7L	0.5	2.4/6	0.4/-4.5	1.2e-10	3.8/90	1.4/177	4.1e-04	1.9/31	-0.09/11
C8L	0.6	1.6/2.8	-1/-1.6	2.9e-10	2.9/7	-0.4/-0.04	4.8e-04	1.6/7	-0.7/-1
C9L	0.8	1.9/2.7	-0.08/-0.3	7.8e-10	3.8/6	0.7/1.3	5.7e-04	1.8/7	-0.3/-0.8
C10L	0.9	1.8/2.8	-0.3/-1.1	1.2e-09	3.3/7	-0.1/-0.3	6.4e-04	1.8/8	-0.4/-1.9
C11L	0.9	1.1/2.1	-0.2/-0.05	1.3e-09	2.6/6	0.1/1	6.8e-04	1.4/7	-0.3/-1.3
C12L	1	1.2/1.7	-0.2/-0.2	1.3e-09	2.4/4.2	0.1/0.5	6.8e-04	1.5/5	-0.4/-0.2
C13L	1	2.1/2.4	-0.5/-0.6	1.1e-09	2.1/3.2	-0.2/0.04	6.9e-04	1.9/4.5	-0.7/-0.4
C14L	1	2.1/1.7	0.3/0.1	1.2e-09	2.3/2.2	0.4/0.7	6.9e-04	1.4/3.8	0.09/0.04
C15L	0.9	6/7	-0.6/0.00	1.2e-09	9/9	0.1/0.7	6.8e-04	4.3/6	-0.8/-0.6
C16L	0.7	3.5/4.3	-0.6/-0.8	1.1e-09	4.7/5	-0.3/0.04	6.5e-04	2.2/4.5	-0.4/-0.8
U5L	2	2.9/42	-1.3/-18	4.8e-09	1.2/89	0.3/-36	1.4e-03	4.9/59	-2/-30
U6L	2.3	3.3/22	-0.7/-9	1.2e-08	2.2/111	0.4/-59	1.9e-03	3.4/45	-0.7/-22
U7L	2.6	4.2/5	-0.8/-1.5	1.4e-08	2.5/6	0.2/0.8	2.1e-03	4.2/18	-1.2/-9
U8L	2.7	2.8/3.7	-0.6/-0.8	1.5e-08	2.6/3.1	0.2/0.5	2.2e-03	3.1/12	-1/-6
U9L	2.8	2.4/3.5	-0.5/-0.5	9.4e-09	3.2/4.8	0.1/0.6	2.2e-03	2.8/10	-0.9/-5
U10L	2.7	4/4.7	-0.9/-1	8.5e-09	4.4/6	0.4/1	2.3e-03	3.6/9	-1.1/-4.4
U11L	2.4	3.3/4	-0.8/-0.8	1.5e-08	3.9/5	0.3/0.7	2.3e-03	3.2/7	-0.9/-3.3
U12L	2.2	4.1/6	-1/-1.1	1.6e-08	6/7	0.2/0.4	2.2e-03	3.7/8	-1/-3.4
U13L	2.1	4.1/6	-1.3/-1.4	1.6e-08	6/8	-0.1/0.02	2.1e-03	4/9	-1.2/-3.7
U14L	1.9	3.2/4.7	-0.2/-0.2	1.4e-08	3.7/4.3	0.03/0.2	2.0e-03	2.8/7	-0.4/-2.9
U15L	1.8	4.4/8	-0.4/-1.7	1.3e-08	14/20	0.5/-0.2	1.9e-03	3.3/9	-0.5/-2.7
U16L	1.7	7/17	-0.10/-4.5	1.2e-08	11/21	0.6/-2.6	1.8e-03	6/29	-0.7/-12
APIL	2.7	5/7	-2.3/-3.4	2.1e-08	14/30	-0.3/-7	7.7e-03	3.7/15	-0.5/3.4
BPIL	1.9	11/22	-3.9/-7	2.5e-10	21/30	15/19	0.01	9/30	5/11
CMPL	1.3	5/25	0.8/-8	3.9e-10	16/57	6/-11	0.02	8/42	1.8/21
LIML	5	10/14	-3.1/-6	4.0e-07	15/22	1/6	0.03	9/21	0.7/-3
CRNL	3.3	4.2/19	-2/0.9	2.6e-08	4.4/46	-1.7/-1.1	9.6e-03	1.4/27	-0.5/18
	NO _x			O ₃			HO ₂		
C5L	10	3.2/21	0.3/18	38	1.3/29	-0.8/-17	2.2e-03	2/62	-1.3/-31

PVOC	Evaluation target								
	mean	rdc	NMB	mean	rdc	NMB	mean	rdc	NMB
C6L	10	4.6/8	-0.8/6	39	2/14	-1/-10	2.2e-03	1.6/38	-1/-20
C7L	10	7/8	-1.7/-1.9	39	3/4.5	-0.7/-1.2	2.3e-03	1.5/12	-0.4/-7
C8L	10	9/9	2.3/1.2	40	4.1/4.5	-2.3/-2.8	2.3e-03	1.2/3.2	-0.9/-2.1
C9L	10	7/8	-1.3/-1.8	41	2.6/4	-0.7/-1.4	2.4e-03	1.4/3.8	-0.5/-1.7
C10L	10	9/8	-2.8/-0.6	40	4/3.1	-0.3/-2.1	2.4e-03	1.5/3.7	-0.7/-2.1
C11L	10	8/7	-1.9/-1.2	39	3.1/3	-0.5/-1.4	2.3e-03	1.4/3.3	-0.8/-1.8
C12L	10	7/8	-0.1/-0.8	38	2/2.7	-1.1/-1.5	2.2e-03	1.5/3.2	-0.9/-1.8
C13L	10	4.7/5	-0.2/-0.8	38	1.6/2.5	-1/-1.3	2.2e-03	1.4/3.2	-0.9/-1.9
C14L	11	8/6	-3/-1.6	36	3.7/2.9	0.4/-0.6	2.1e-03	1.4/2.9	-0.4/-1.5
C15L	10	3/2.9	-0.5/-0.8	35	2/2.9	-0.7/-1.1	2.1e-03	1.4/3.1	-0.7/-1.5
C16L	10	4.1/4.7	0.6/0.9	34	1.8/3.1	-1/-1.7	1.9e-03	1.4/2.9	-0.6/-1.5
U5L	7	1.5/11	0.02/4.8	42	1.5/16	-1/-9	3.9e-03	4.2/44	-2/-13
U6L	7	6/6	-1/3	44	3.4/13	-2.3/-9	3.8e-03	4.1/27	-2.1/-12
U7L	7	7/7	-1.1/-0.7	45	3.7/4	-2.4/-2.9	3.8e-03	4.2/7	-2.3/-2.5
U8L	7	7/7	-1/-1	46	3.5/3.8	-2.3/-2.7	3.8e-03	3.5/4.8	-2.1/-2.5
U9L	7	8/8	-1/-1.1	45	3.6/4.1	-2.3/-2.8	3.7e-03	3.5/5	-2.1/-2.7
U10L	7	8/8	-0.8/-0.9	44	3.6/4	-2.3/-2.7	3.5e-03	3.6/5	-2.2/-3
U11L	7	8/8	-0.7/-0.8	42	3.2/3.7	-2/-2.4	3.3e-03	3.4/5	-1.9/-2.8
U12L	7	7/7	-0.5/-0.6	41	2.9/3.5	-1.8/-2.3	3.1e-03	3.4/6	-1.9/-2.8
U13L	7	6/6	-0.4/-0.4	39	2.6/3.2	-1.6/-2	2.9e-03	3.5/6	-1.8/-2.8
U14L	7	4.9/4.8	-0.5/-0.4	37	2/2.6	-1.2/-1.6	2.7e-03	2.7/5	-1.3/-2.3
U15L	7	3/3.7	-0.4/0.2	36	1.7/3.9	-1/-2.5	2.6e-03	2.4/11	-1.2/-6
U16L	7	1.8/1.2	-0.4/0.2	34	1.7/4.3	-1/-2.8	2.5e-03	2.3/15	-0.9/-6
APIL	5	9/13	-1.4/1	47	4.9/8	-3.5/-6	3.3e-03	13/17	-9/-12
BPIL	6	10/19	5/11	43	9/18	-7/-11	2.9e-03	36/53	-26/-34
CMPL	7	10/22	2.7/7	41	6/15	-4.2/-8	2.1e-03	26/60	-15/-28
LIML	5	9/12	-0.2/0.4	51	5/7	-3.9/-5	4.8e-03	17/22	-14/-18
CRNL	6	7/24	-0.6/10	48	3.2/19	-2.3/-12	3.4e-03	9/38	-5/-24

S2.3 Additional NMB distributions for evaluation metrics

Additional distributions of mean values and NMB are presented for metrics used to evaluate the preservation of SOA formation and gas-phase reactivity in TBR mechanisms. These figures complement the discussion in Sect. 5 of the main paper and provide extended results across a broader range of metrics and simulation scenarios.

Additional size reduction versus reduction error relationships for tSOA, corresponding to Fig. 7 in the main paper, are shown in Fig. S17 for nine simulation scenarios. These scenarios include continental, polluted continental, remote continental, simplified, urban, and diurnal conditions. As in the main paper, mechanisms C5–C7 and U5 are excluded from the discussion due to their negligible contribution to SOA formation.

In addition to Fig. 8 in the main paper, Fig. S18 presents aerosol elemental ratios and selected functional group distributions for all three VOC classes. Elemental ratios OM:OC and H:C are shown together with functional groups that contribute significantly to aerosol composition, specifically >CO and -OH.

Additional gas-phase evaluation metrics are shown in Fig. S19, including bulk reactivities of reducible species (OHR-r, O₃R-r, and NO₃R-r) and concentrations of key oxidants and radicals (NO_x, O₃, NO₃, HO₂, OH, and RO₂).

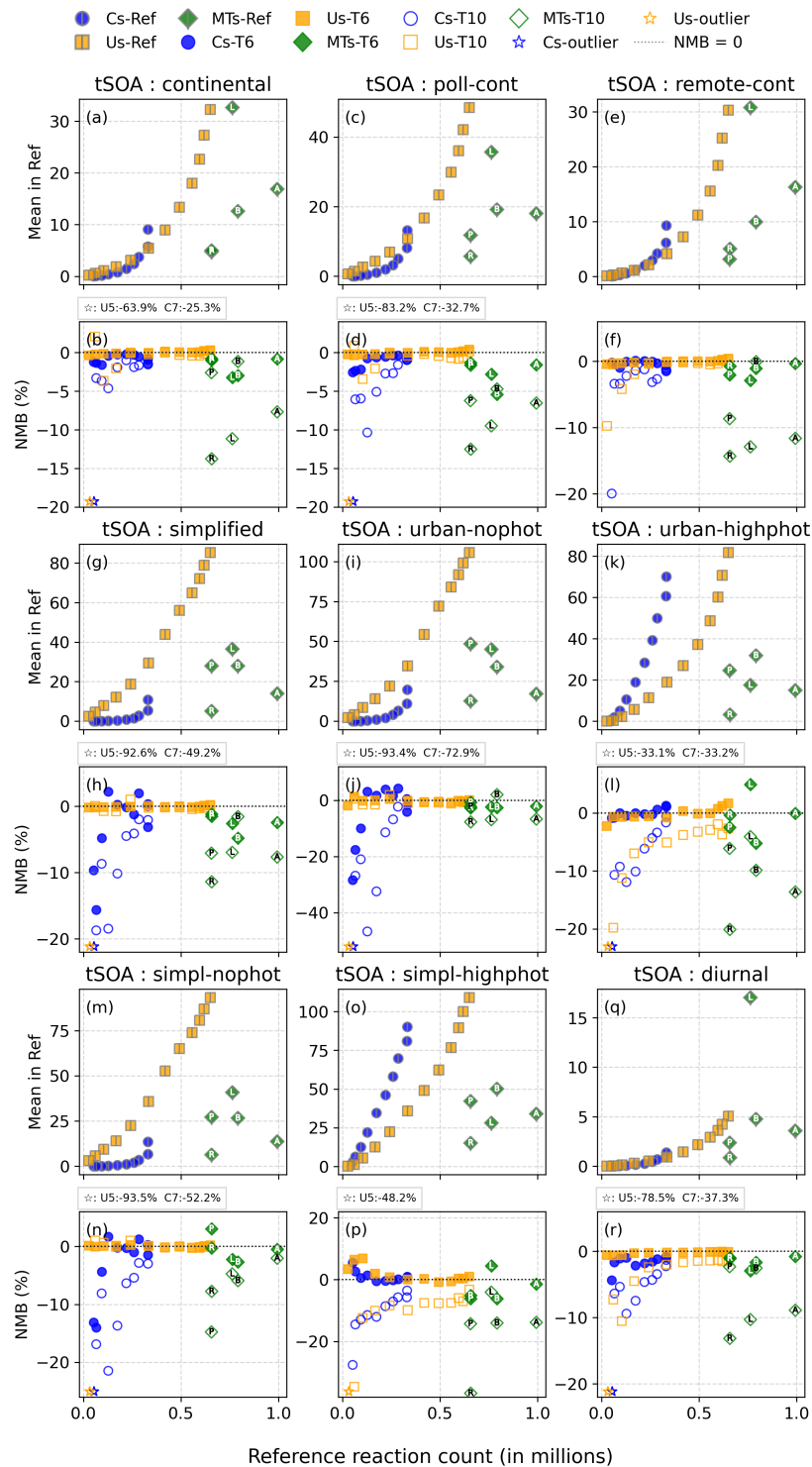


Figure S17. TBR-induced deviations in tSOA for additional evaluation scenarios beyond those shown in Fig. 7; symbols and notation are consistent.

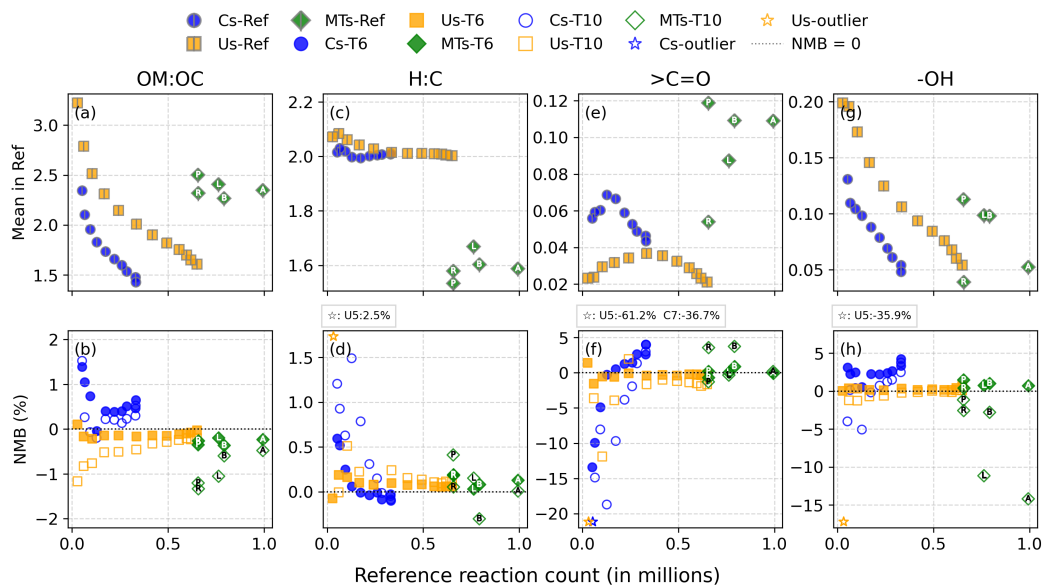


Figure S18. TBR-induced deviations in selected elemental SOA ratios and carbon-normalized functional group fractions beyond those shown in Fig. 8, including OM:OC and H:C ratio, ketone (>CO) and alcohol (-OH) functional groups across all VOC classes. Symbols and notation are consistent with Fig. 7.

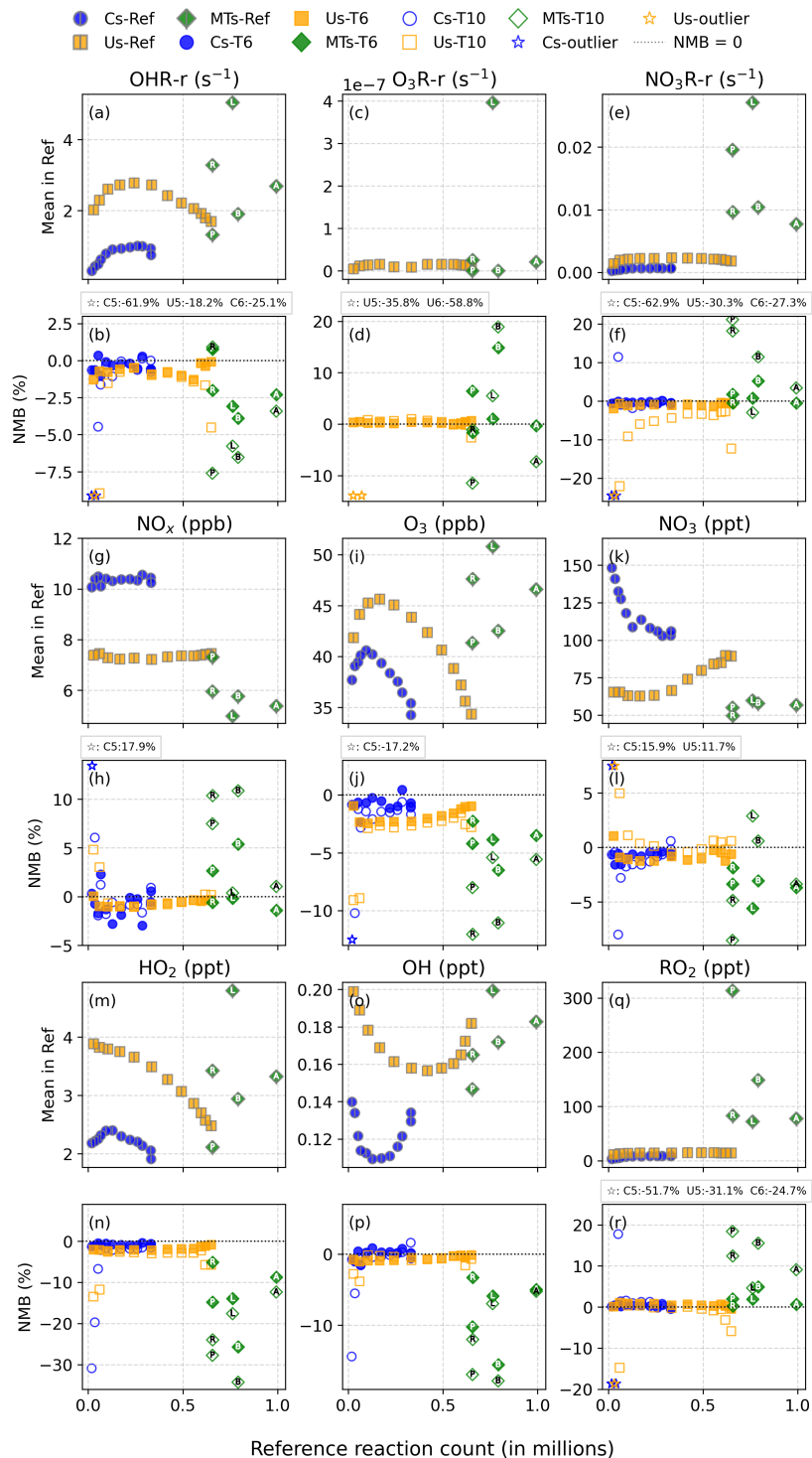


Figure S19. TBR-induced deviations in selected elemental SOA ratios and carbon-normalized functional group fractions beyond those shown in Fig. 10, including OHR-r, O₃R-r, NO₃R-r, NO_x, O₃, NO₃, HO₂, OH, and RO₂. Symbols and notation are consistent with Fig. 7.

S3 Additional SBR results

S3.1 Additional stage settings and U8A3d reduction trajectory

As a continuation of Sect. 4.4.2, additional SBR treatments not described in the main paper are summarized here. In early stages (A1 and B1), treatments are configured for efficient reduction of large mechanisms:

- species are grouped and ranked using predefined rules (Sect. 4.2) to identify reduction candidates;
- only base reduction candidates are considered (variant candidate generation is disabled);
- each reduction cycle stops under the current error tolerance when fewer than five valid candidates remain, after which the procedure proceeds to the next tolerance setting or stage, if applicable.

This cutoff of five candidates is an empirical threshold used to avoid restarting SBR cycles under strict error tolerances, where additional cycles are computationally expensive and typically yield only limited or no further reduction.

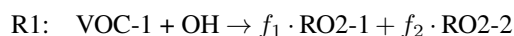
In later stages (A2, A3, and B2), as the mechanism size decreases, treatments are adjusted to explore additional reduction candidates:

- species grouping is performed per species, and species are ranked using the GENOA v2 method based on removal importance (species inducing larger errors are evaluated later);
- variant candidates are enabled to test combinations of reduction options for each targeted species;
- reduction cycles proceed under each tolerance setting until no valid candidates remain.

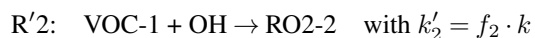
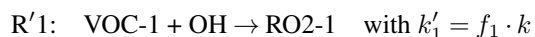
S3.1.1 Elementary-like treatment

The elementary-like treatment is applied during Stages A3 and B2 to expose additional reduction candidates. It is conceptually opposite to reaction merging. In this treatment, reactions producing multiple reducible products are temporarily separated into reactions with a single reducible product, and reduction is performed on this modified reaction list. This increases the number of reactions but preserves the overall chemical budget and expands the set of candidates for removal. When removal of merged reactions does not satisfy the error tolerance settings, individual product channels enabled by this treatment may be removed if they contribute negligibly to the target quantities.

For example, in reaction R1 with rate constant k , species VOC-1 reacts with OH to form RO2-1 and RO2-2:



After applying the elementary-like treatment, it is separated into two reactions (R'1 and R'2):



This treatment is applied after all candidates under the same error settings are explored. It allows independent removal of product channels and may introduce additional reductions under the same tolerances. At the end of the cycle, reactions are merged to restore a compact mechanism (deactivating the elementary-like treatment).

S3.1.2 U8A3d reduction trajectory

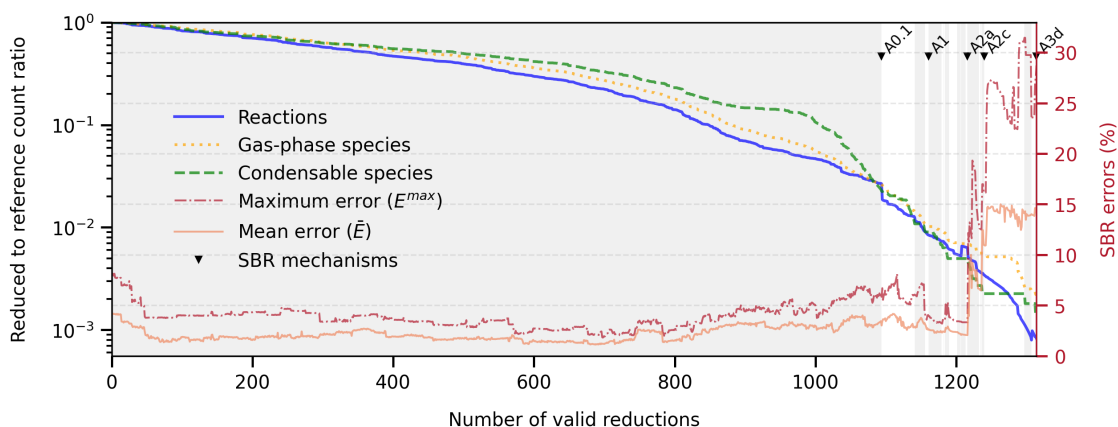


Figure S20. Reduction trajectory from U8StP to U8A3d as a function of the number of valid reduction steps. The evolution of the numbers of reactions, gas-phase species, and condensable species is shown together with the corresponding maximum and mean errors across evaluation scenarios. Gray and white intervals denote successive reduction cycles.

Figure S20 is included as an example to illustrate the evolution of mechanism size and errors during SBR for U8 reduction. The trajectory spans from the starting-point mechanism (StP) to the final reduced mechanism A3d. Representative mechanisms from Table 4 generated along this trajectory are marked, including A0.1, A1, A2a, A2c, and A3d.

Most valid reduction steps (1094 out of 1314) occur during the first reduction cycle in Stage A1. During this stage, all mechanism size metrics decrease steadily. Error levels initially decrease slightly relative to StP, then remain stable, followed by a gradual increase toward the end of the cycle under relatively strict error tolerances. This results in smooth and continuous changes in both mechanism size and accuracy, consistent with early-stage reduction, where many candidates are available and their influence on the evaluation targets is limited.

As the reduction proceeds, the number of valid reduction steps decreases as the mechanism becomes smaller and approaches the error tolerances. The cumulative numbers of accepted reductions reach 1161 at the end of Stage A1, and 1216, 1240, and 1314 for mechanisms A2a, A2c, and A3d, respectively. The decrease in condensable species is more pronounced than that of gas-phase species between A2a and A2c, consistent with the application of the elementary-like treatment.

In later stages (A2–A3), reduction continues under relaxed constraints with additional candidate exploration. This leads to faster decreases in relative mechanism size, accompanied by increased variability in errors. Occasional increases in error

occur when more aggressive reductions are accepted under looser tolerance settings, and small structural changes can induce relatively large error variations. These late-stage reductions exhibit clearer trade-offs between mechanism size and error.

S3.2 NMB distribution and time variation preservation

The U8 reduction is used as an illustrative example in the main paper to demonstrate SBR performance, with preservation of key SOA-related and gas-phase metrics evaluated in Sect. 6.2 and time-variation behavior examined in Sect. 6.3. To extend this analysis and assess the robustness of SBR across different VOC classes, corresponding results for C12 and LIM reductions are presented here. These include NMB distributions of key metrics (Figs. S21–S22) and time series of tSOA and OHR-r (Figs. S23–S24). All figures follow the same format, symbols, and notation as those used for U8 to facilitate direct comparison. In addition, scenario-specific time variations for U8 that are not shown in Fig. 14 are provided in Fig. S25.

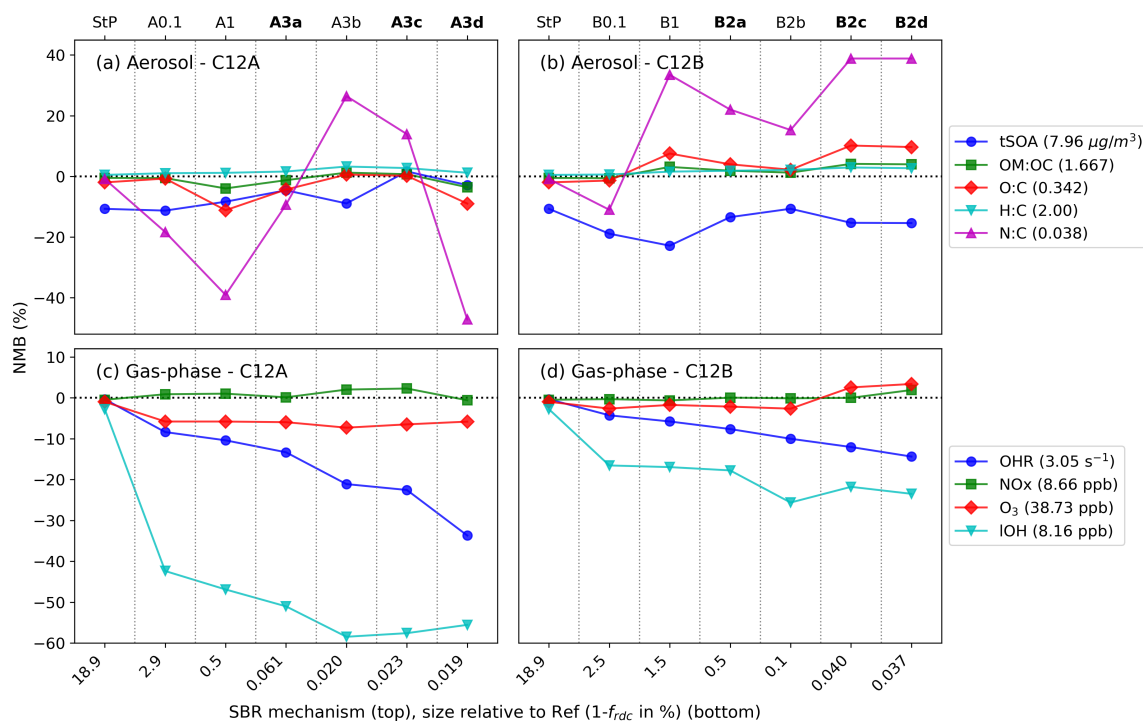


Figure S21. NMB distributions of key SOA-related and gas-phase metrics simulated with C12 reduced mechanisms. Symbols and notation are consistent with Fig. 12.

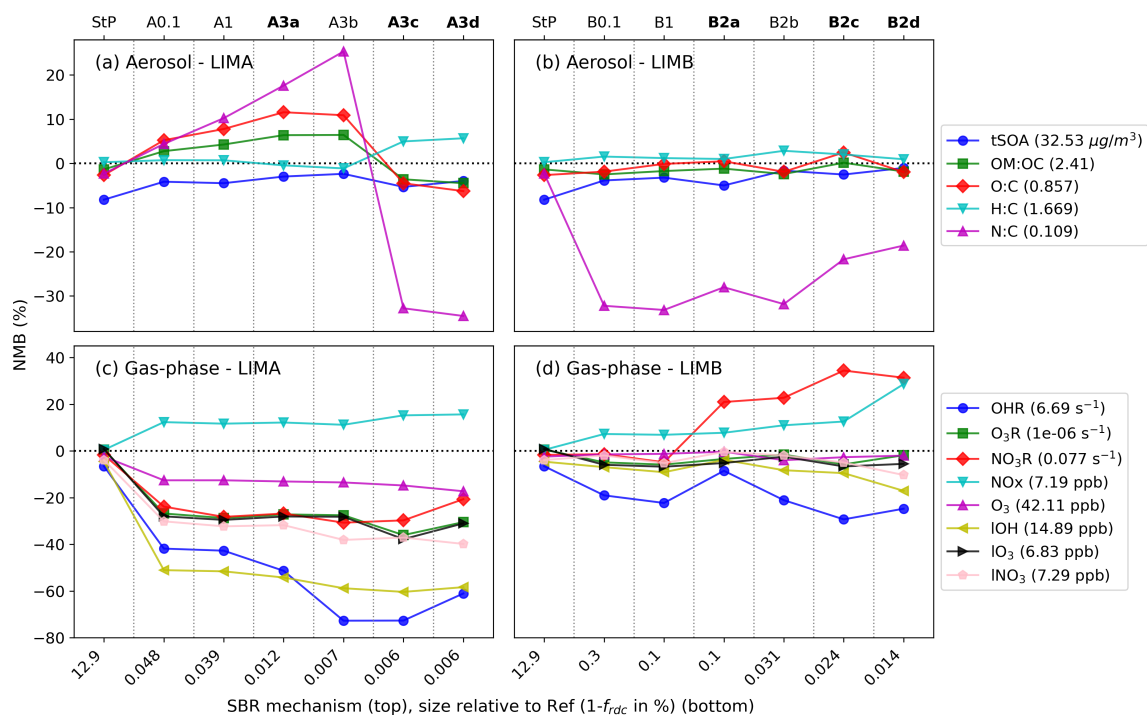


Figure S22. NMB distributions of key SOA-related and gas-phase metrics simulated with LIM reduced mechanisms. Symbols and notation are consistent with Fig. 12.

S3.2.1 Scenario-dependent chemical behavior (U8 example)

The chemistry-driven differences across scenarios of the U8 reduction (Fig. 14) summarized in Sect. 6.3 are expanded here with quantitative detail and process-level interpretation.

In high- NO_x regimes such as the urban scenario (Fig. 14(c)), elevated and fixed NO_x and O_3 concentrations produce rapid nighttime oxidation, resulting in fast increases in both tSOA and OHR-r. By 8 h, tSOA reaches approximately $13.5 \mu\text{g m}^{-3}$ and OHR-r reaches about 3.0 s^{-1} . In contrast, the remote scenario (Fig. 14(e)), characterized by extremely low NO_x (0.01 ppb), exhibits weak nighttime oxidation, with tSOA remaining below $0.2 \mu\text{g m}^{-3}$ during the same period, while OHR-r increases more gradually to 2.1 s^{-1} . Following sunrise, enhanced OH production accelerates daytime oxidation, with RO_2 chemistry shifting toward HO_2 -dominated pathways and peroxide formation, leading to increases in tSOA to $1.2 \mu\text{g m}^{-3}$ and OHR-r to 4.2 s^{-1} by 16 h. For scenarios with diurnally varying photolysis, diurnal variability is explicitly reflected in the time series. As simulations are initialized under winter conditions (January 1), daylight periods are short (gray shaded regions), limiting photolysis-driven daytime oxidation and leaving nighttime chemistry dominant for much of the simulation.

Conversely, under fixed photolysis conditions, scenarios such as urban-nophot, urban-highphot, simpl-nophot, and simpl-highphot prescribe constant photolysis settings and rely on specified O_3 and NO_x levels. Under these scenarios, both tSOA and OHR-r evolve smoothly, with generally rapid increases during the initial oxidation period followed by slower temporal changes. For the U8 mechanism under the simpl-nophot scenario shown in Fig. 14(k), tSOA reaches $16.6 \mu\text{g m}^{-3}$ by the end of the simulation, while OHR-r peaks 4.0 s^{-1} at 40 h before decreasing slightly to 3.4 s^{-1} , reflecting gradual shifts in dominant reaction pathways during multi-generation oxidation.

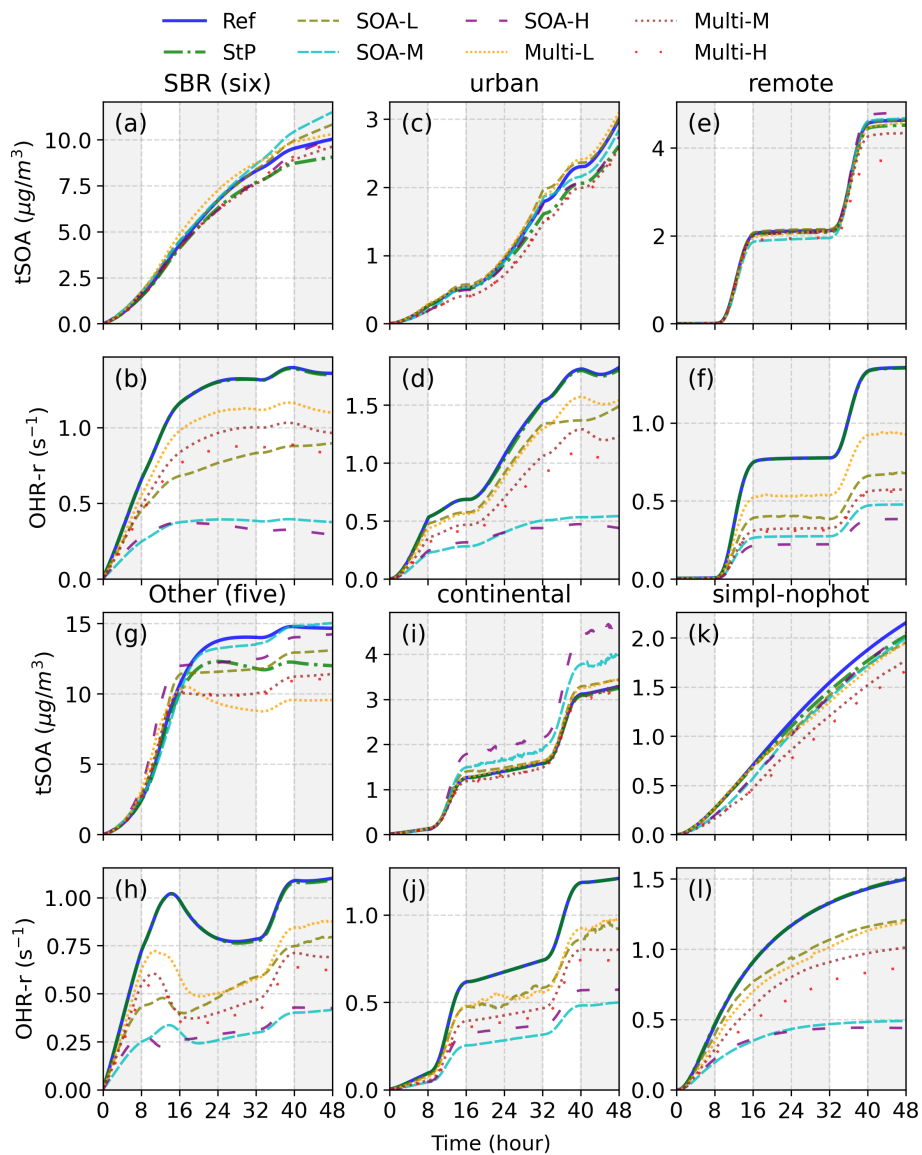


Figure S23. Time evolution of tSOA and OHR-r simulated with C12 mechanisms for the same set of scenarios in Fig. 14; Symbols and notation are consistent.

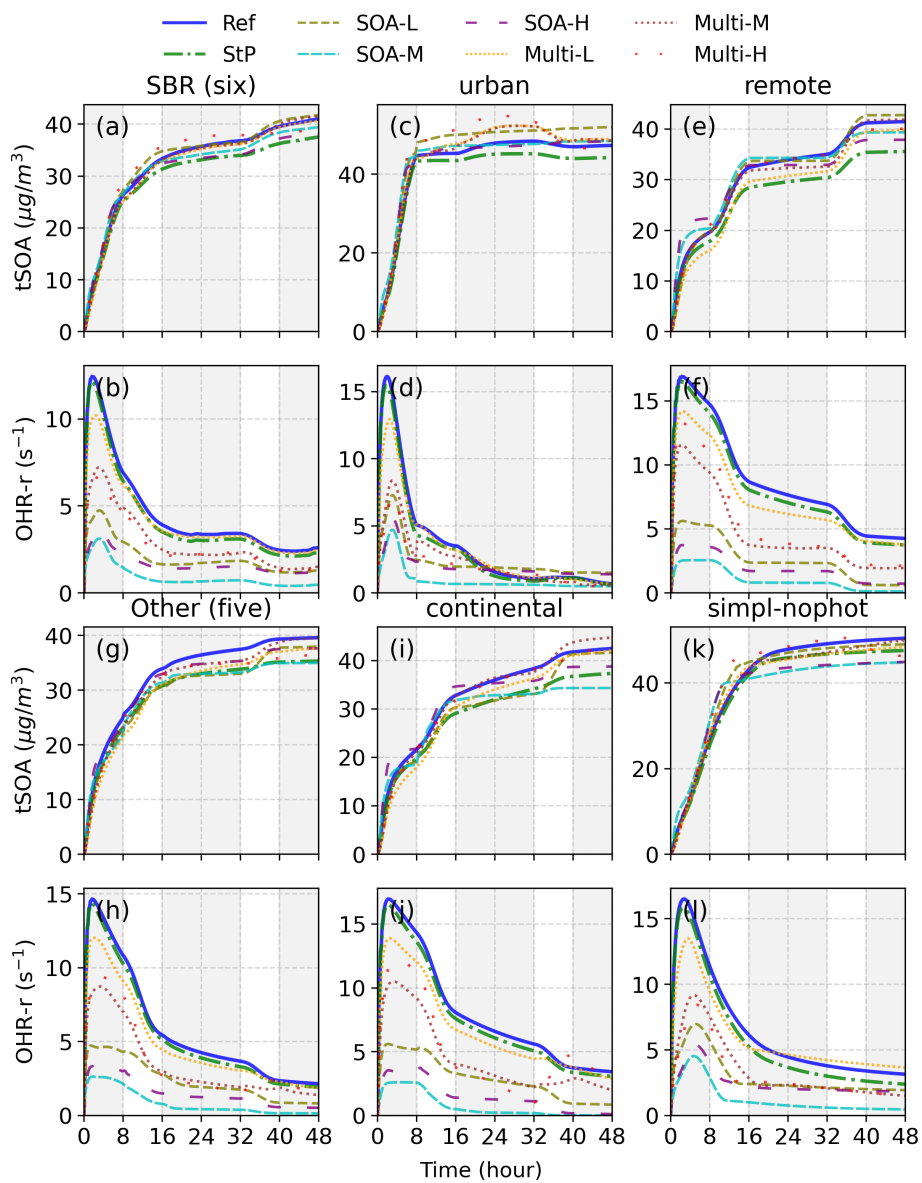


Figure S24. Time evolution of tSOA and OHR-r simulated with LIM reduced mechanisms for the same set of scenarios shown in Fig. 14, with symbols and notation consistent.

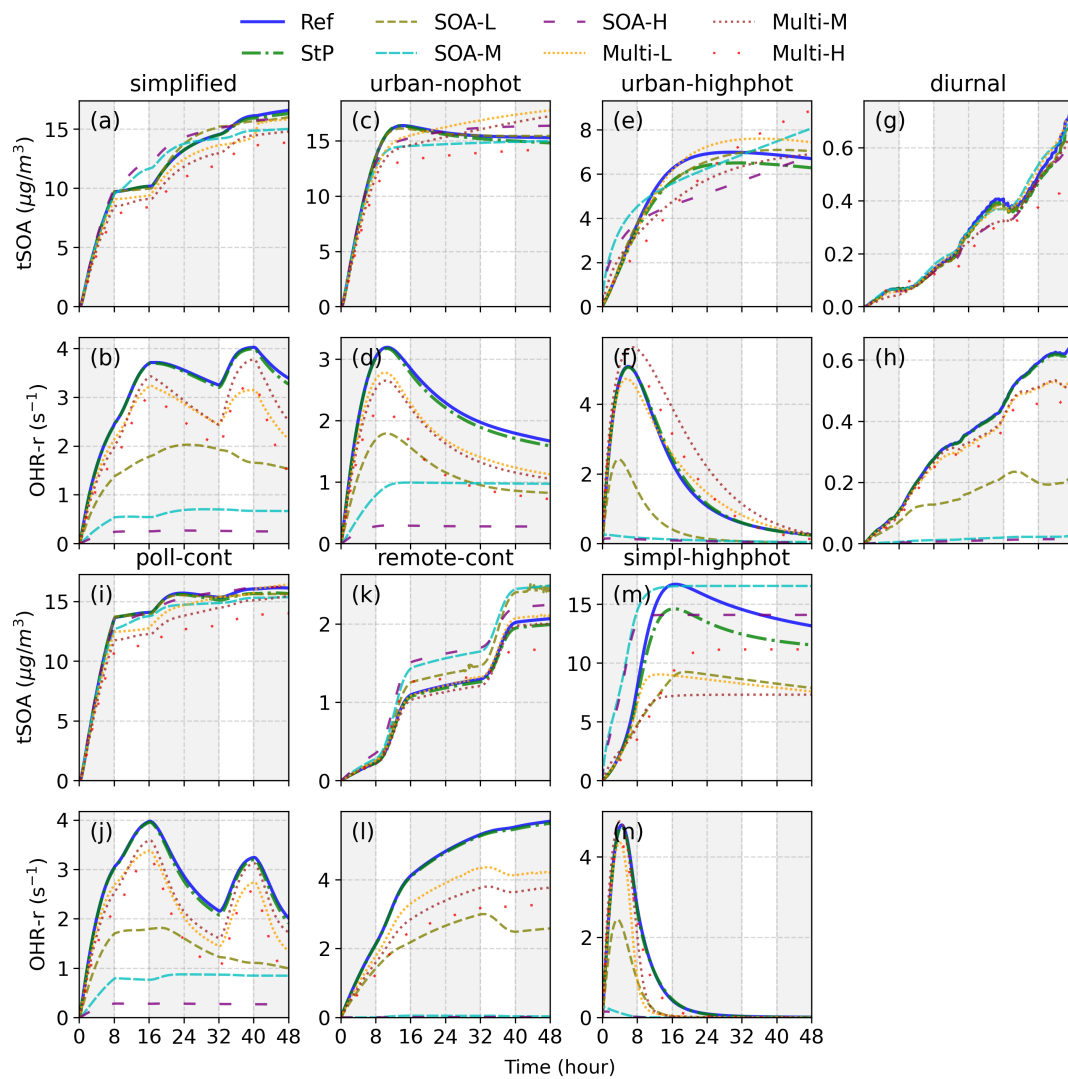


Figure S25. Time evolution of tSOA and OHR-r simulated with U8 reduced mechanisms for evaluation scenarios not included in Fig. 14.

S3.3 Reaction pathway visualization for SBR mechanisms

Reaction pathways (Figs. S26–S31) are presented for the final reduced SBR mechanisms derived from the C12 and LIM reference mechanisms, using the same tolerance settings as the U8 SBR mechanism discussed in Sect. 6.4. These comparisons illustrate how differences in chemical complexity across mechanisms influence the resulting reduced mechanism structure and retained reaction pathways.

In all reaction graphs presented, the same legends as in Fig.15 are applied, consistent with those used in the main paper. Species are represented as nodes labeled by chemical name and molecular structure. PVOCs, basic non-reducible species, and other reducible species are indicated by red, blue, and black text, respectively. Reducible condensable species are shown as boxes, with SVOCs ($P_{\text{sat}} > 10^{-9}$ atm at 298 K) in light gray and lower-volatility species in black. Reactions are shown as edges with colors and symbols indicating reaction types: OH oxidation (red line with open diamond), O_3 oxidation (blue filled V-shaped arrow), NO_3 oxidation (green open triangle), reactions with HO_2 (cyan open circle), reactions with NO (orange filled circle), RO_2 reactions (gray filled diamond), unimolecular reactions (“uni”, black filled tee), photolysis reactions (“ $h\nu$ ”, brown open square), and isomerization reactions (“isom”, darkcyan inverted triangle). Terminal species (i.e., species that do not lead to the formation of other reducible species) that undergo further atmospheric processing not explicitly shown are connected to a gray dot.

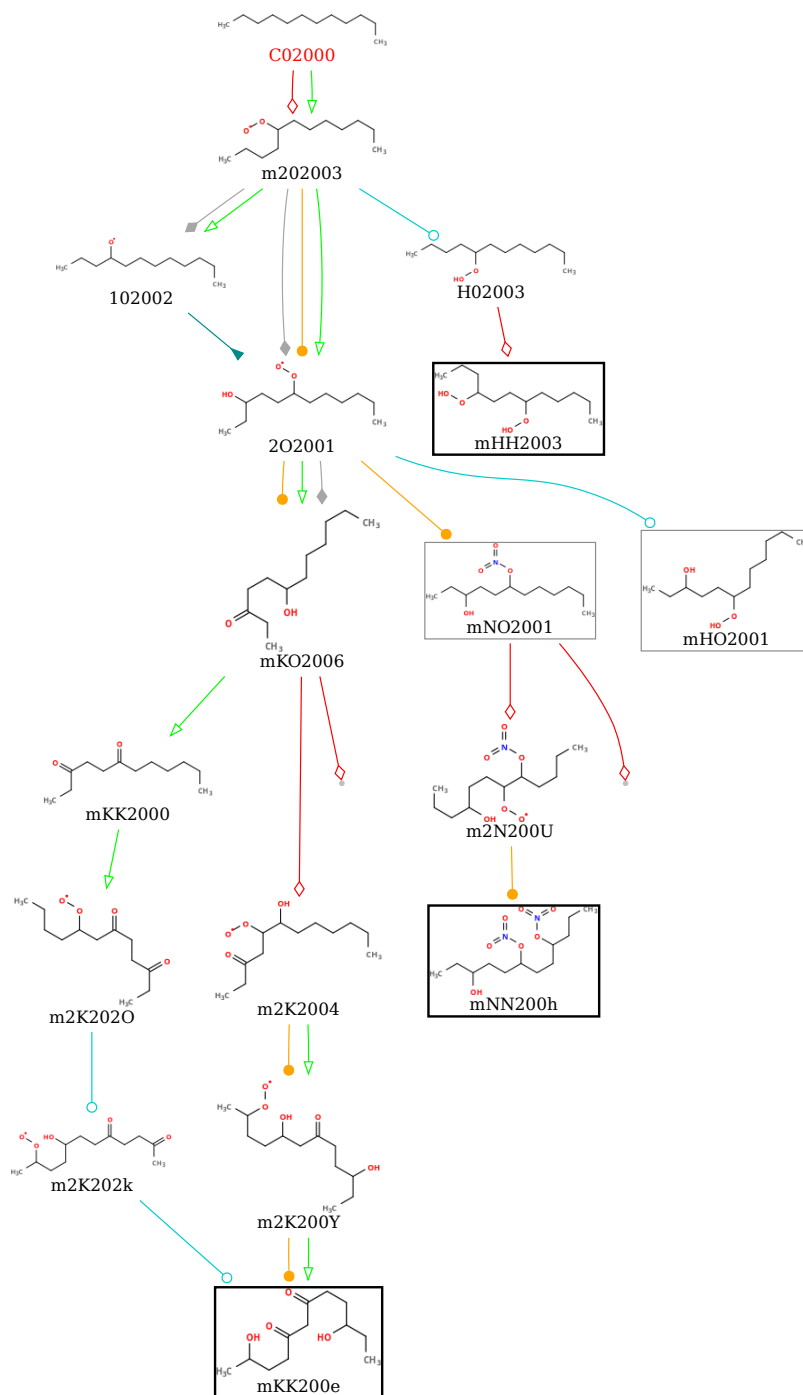


Figure S26. Reaction pathways of C12SOA-H (C12A3d) mechanism.

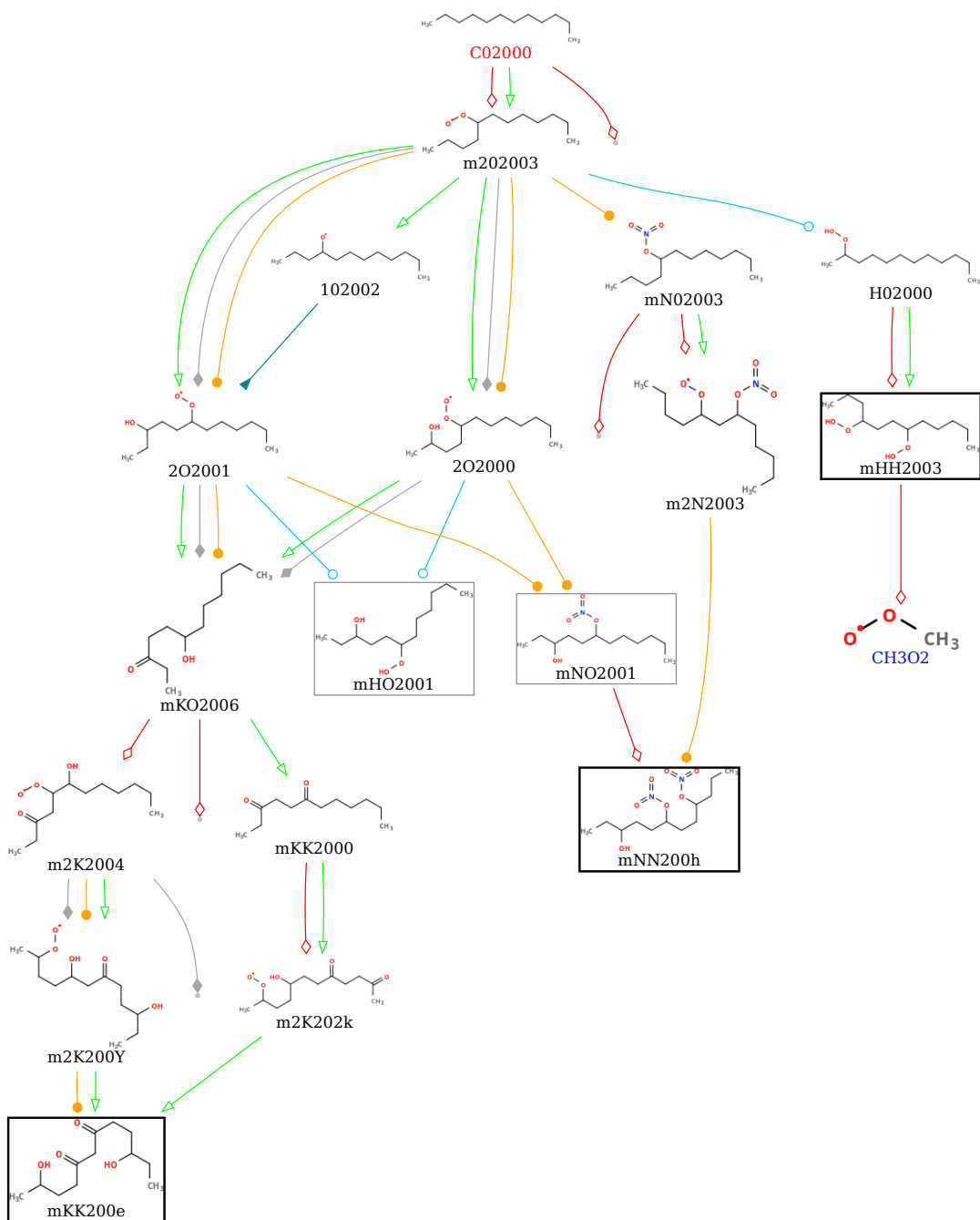


Figure S27. Reaction pathways of C12SOA-M (C12A3c) mechanism.

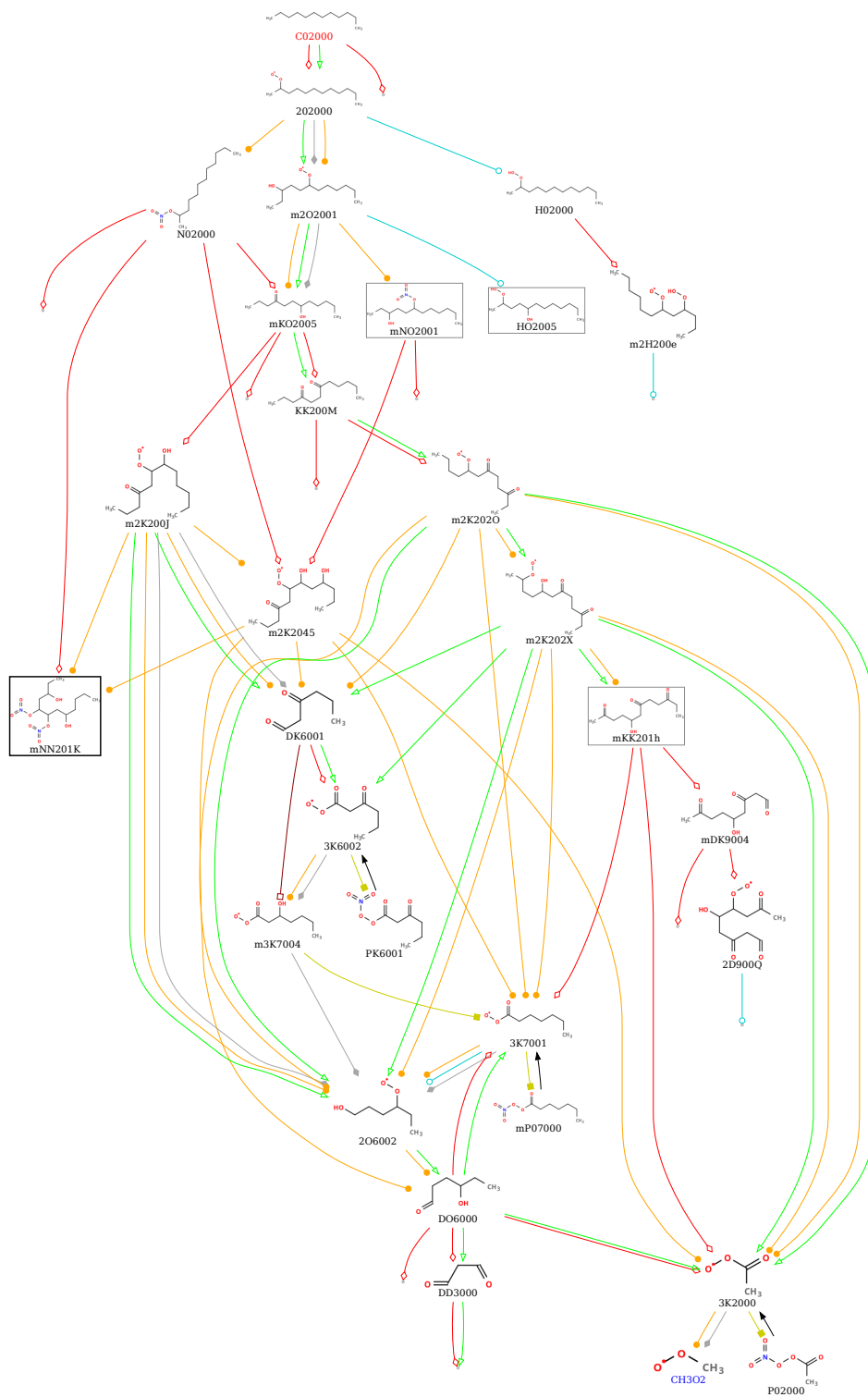


Figure S28. Reaction pathways of C12Multi-H (C12B2d) mechanism.

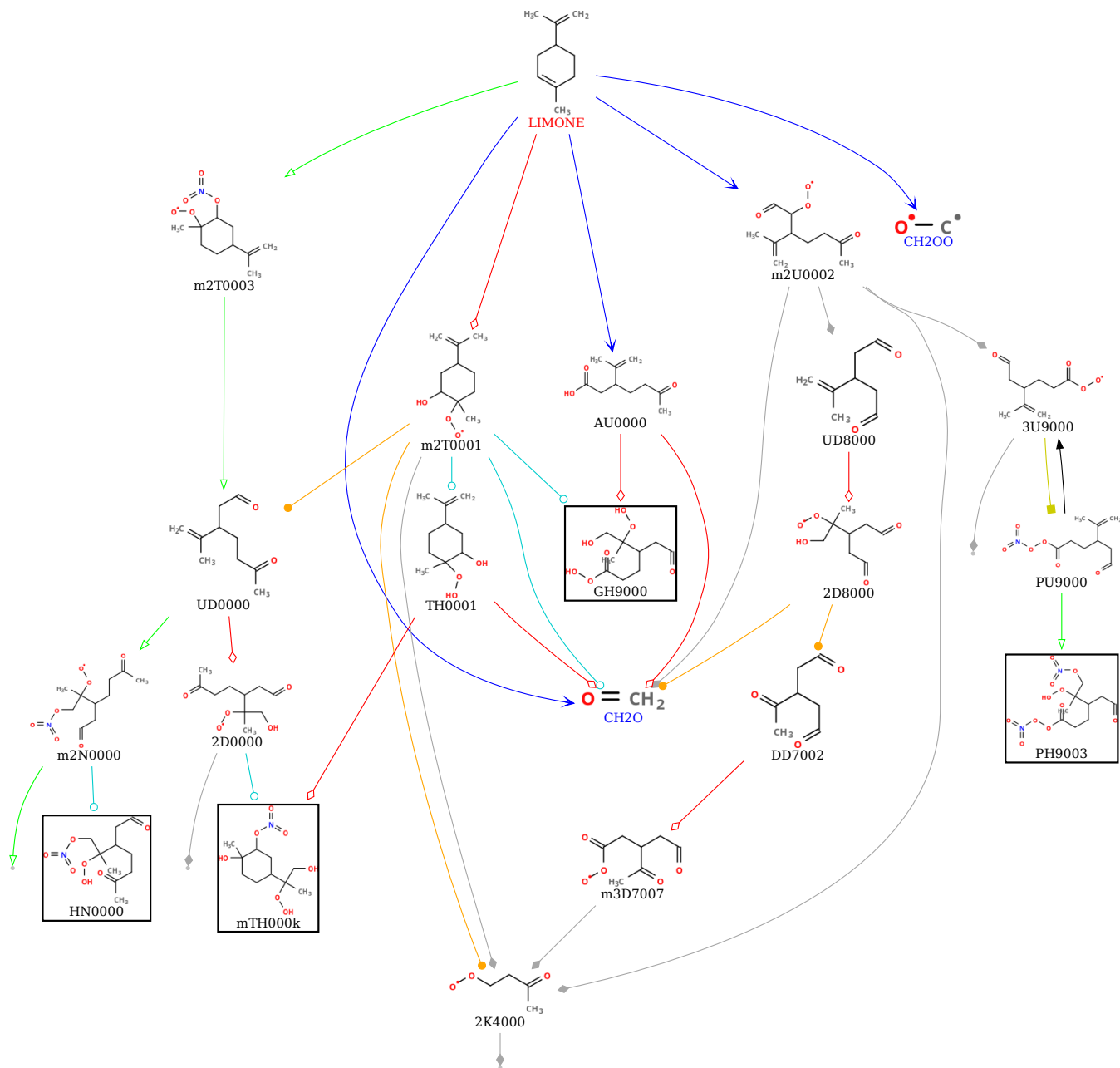


Figure S29. Reaction pathways of LIMSOA-H (LIMA3d) mechanism.

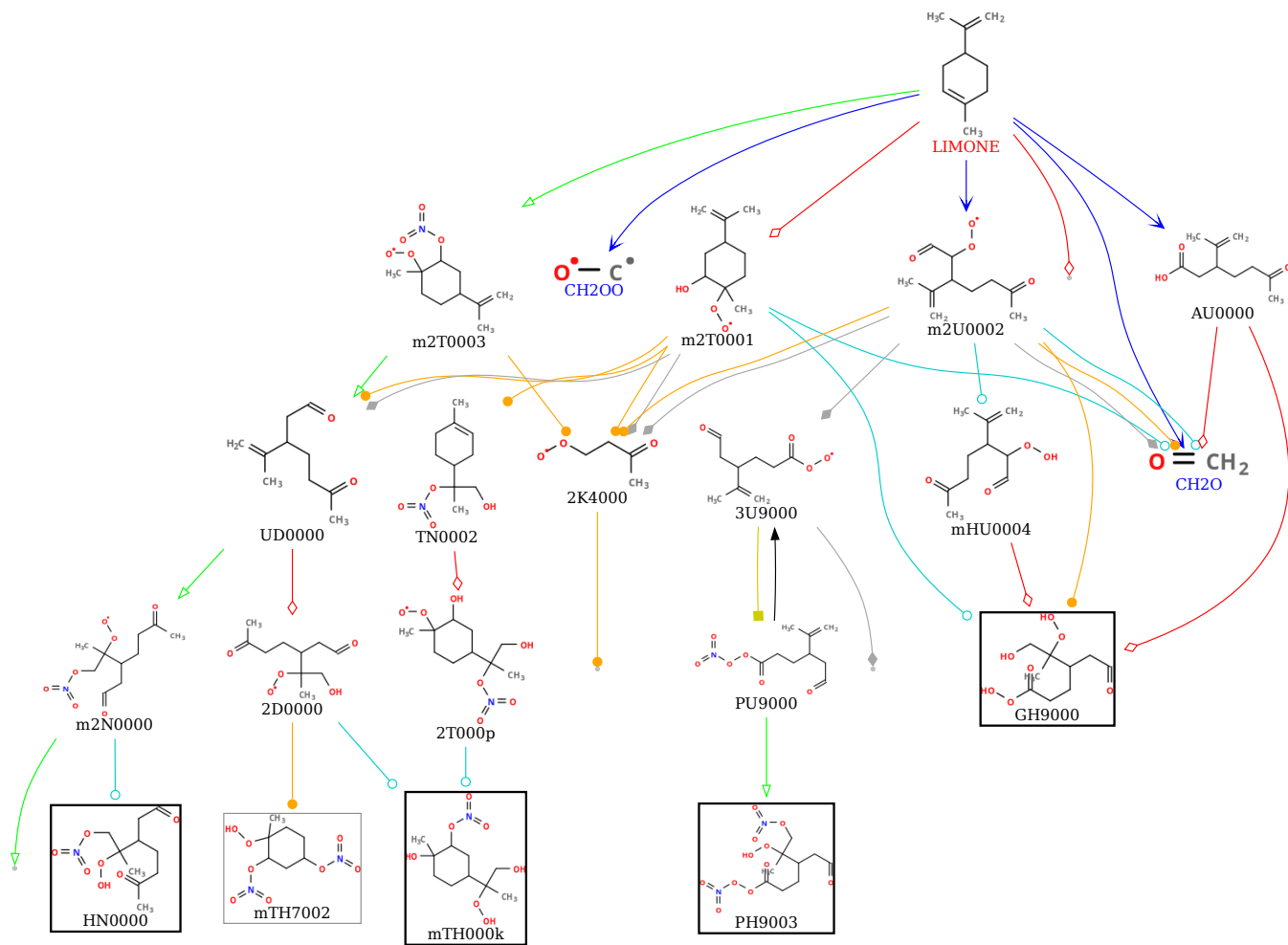


Figure S30. Reaction pathways of LIMSOA-M (LIMA3c) mechanism.

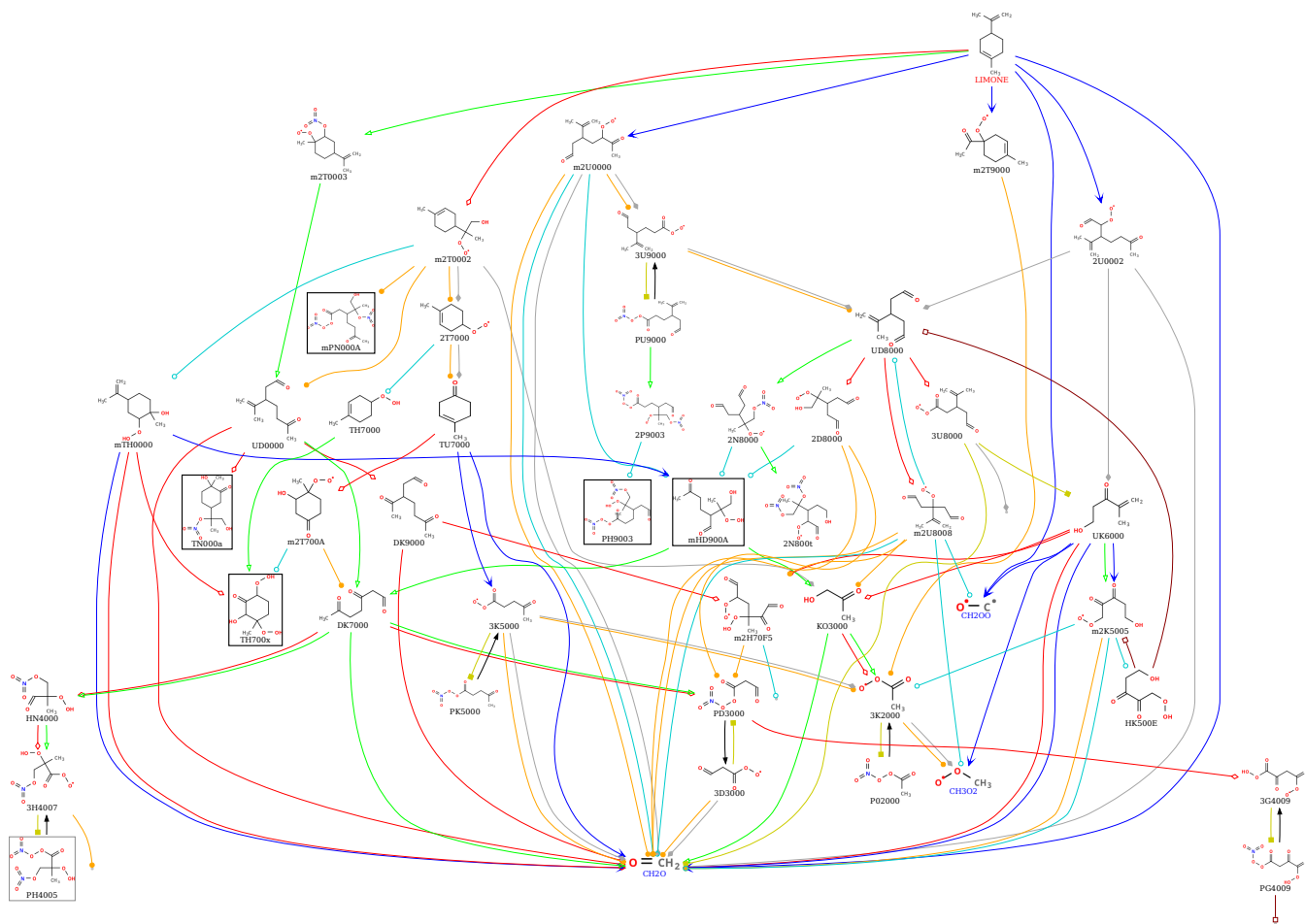
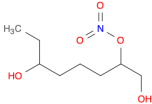
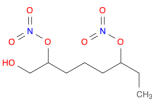
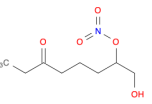
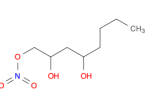
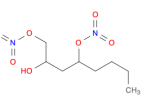
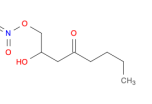

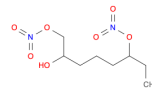
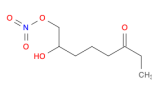
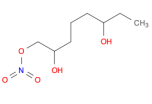
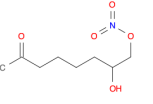
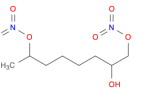
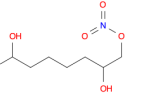
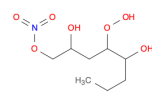
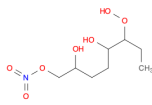
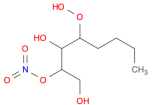
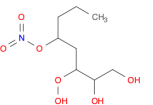
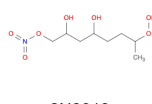
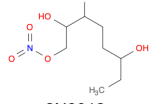
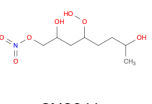
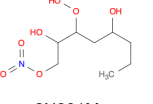
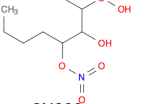
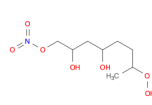
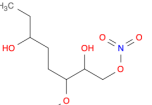
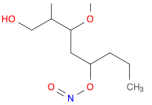
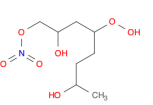
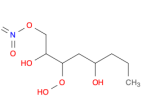
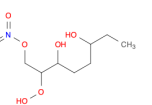

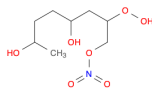
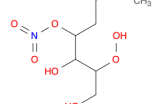
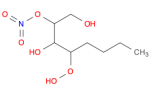
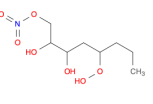


Figure S31. Reaction pathways of LIMMulti-H (LIMB2d) mechanism.

S3.4 Reduction mechanism details

S3.4.1 Species mapping for surrogates from lumping

Table S6: Newly introduced surrogate species in U8SOA-H (U8A3d) and their associated reduced species, generated through lumping (“lp”) and, where applicable, replacement (“rp”). Molecular drawings are shown for all species. The dominant GECKO-A species defining each surrogate (“m” + species name) is listed in the first column, consistent with the reaction graph in Fig. 15(a), and is implicitly included in the lumped group but not duplicated in the associated species column.

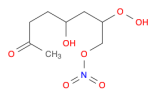
Surrogate	Sgy.	Merged species (U8SOA-H)						
		 NO8006	 NN800h	 NK800A	 NO800G	 NN801Q	 NK800z	
	rp	 m2N800L	 NN801P	 NK800y	 NO800F	 NK800x	 NN801O	 NO800E
		 2N801L	 2N801K	 2N8017	 2N800P			
	lp	 2N8013	 2N8012	 2N8011	 2N801M	 2N800q		
		 HN8022	 HN8021	 HN801Y	 HN801z	 HN802N	 HN800S	
	lp	 mHN800n	 HN800P	 HN801K	 HN800w	 HN8007		

Surrogate

Sgy.

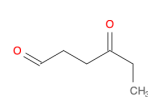
Merged species (U8SOA-H, continued)

rp

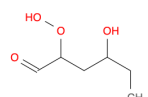


HN800U

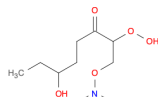
rp



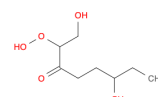
DK6003



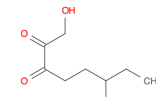
2D6005



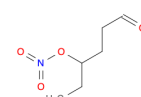
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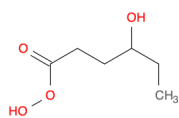
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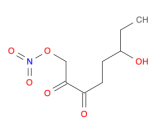
KK8003



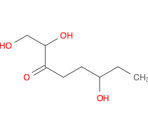
ND6006



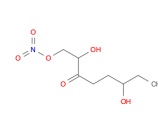
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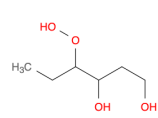
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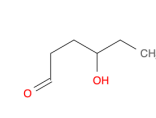
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NK800I

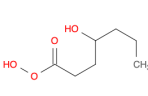


HO6002

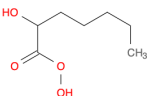


DO6000

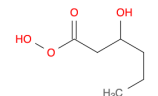
lp



3K7000

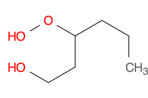


3K7002

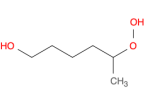


3K6002

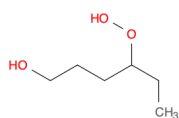
lp



2O6004

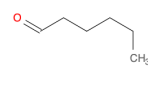


2O6003



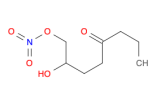
m2O6000

rp

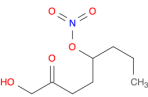


D06000

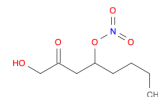
lp



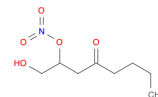
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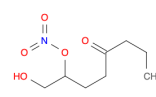
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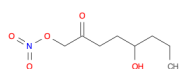
NK800s



NK8008

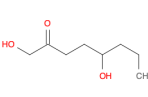


NK800B

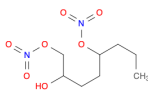


mNK8002

rp



KO8002



NN8001

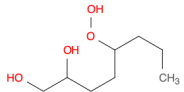
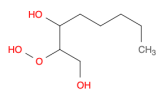
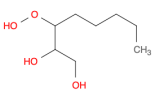
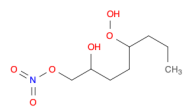
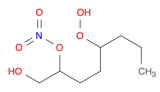
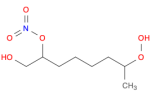
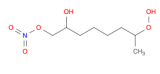
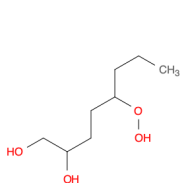
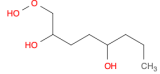
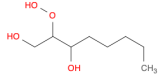
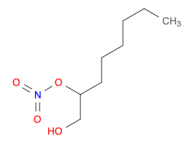
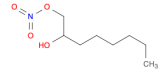
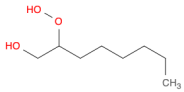
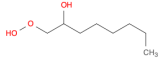
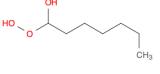
Surrogate	Sgy.	Merged species (U8SOA-H, continued)	
 m2O8002	lp	 2O8005	 2O8006
 m2N8001	rp	 2N800J	 2N800H
	lp	 2N800w	
 mHO8002	lp	 HO8004	
	rp	 HO800G	
 mNO8001	lp	 NO8000	
 m2O8001	lp	 2O8000	 2O7000

Table S7: New surrogate species and associated reduced species in U8SOA-M (U8A3c). The table follows the layout of Table S6. For clarity, only surrogate species and associated reduced species differing from Table S6 are shown. Surrogate species identical to those in Table S6 include m2N800L, mHN800n, m3K6001, m2O6000, mNK8002, m2O8002, m2N8001, mHO8002, mNO8001, and m2O8001. The corresponding reaction graph is presented in Fig. 15(b) of the main paper.

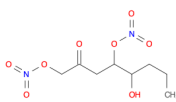
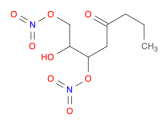
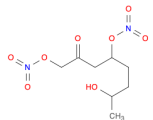
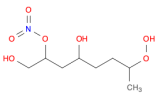
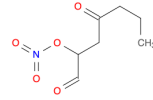
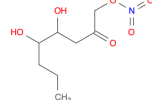
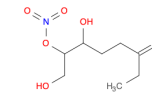
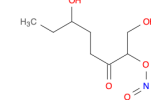
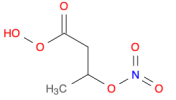
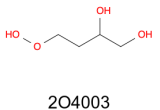
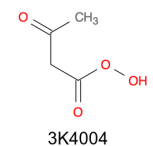
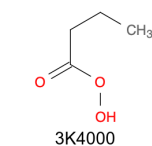
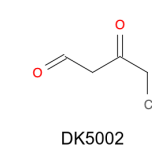
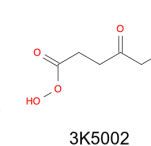
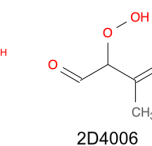
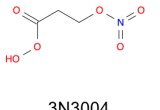
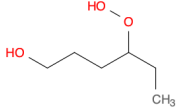
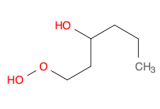
Surrogate	Sgy.	Merged species (U8SOA-M)				
 mNN8003	lp	 NN800q	 NN800w			
	rp	 1H803c	 ND700F	 NK8007	 NK800F	 NK800D

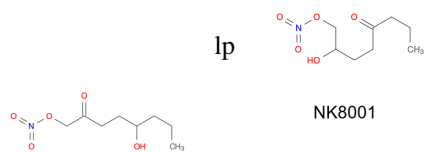
Table S8: New surrogate species and associated reduced mechanisms in U8Multi-H (U8B2d). The table layout is shown in Table S6, with the corresponding reaction graph shown in Fig. 16 of the main paper.

Surrogate	Sgy.	Merged species (U8Multi-H)					
 m3N4002	rp	 2O4003	 3K4004	 3K4000	 DK5002	 3K5002	 2D4006
	lp	 3N3004					
 m2O6000	lp	 2O6001					

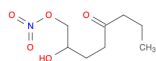
Surrogate

Sgy.

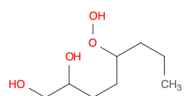
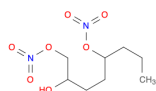
Merged species (U8Multi-H, continued)



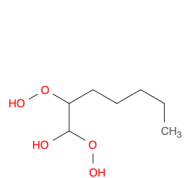
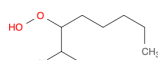
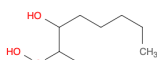
lp



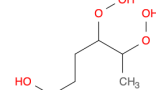
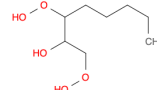
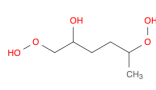
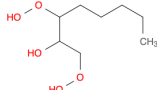
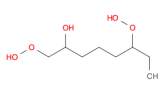
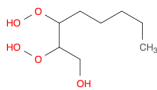
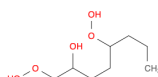
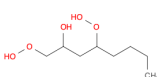
rp



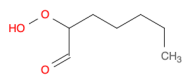
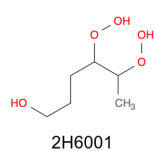
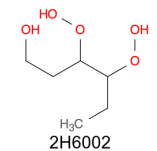
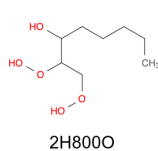
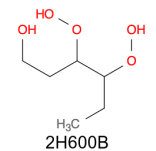
lp



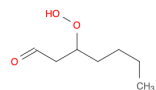
rp

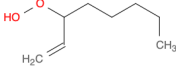
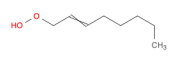
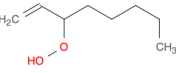
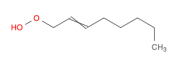
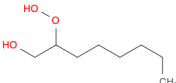
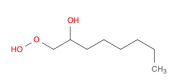
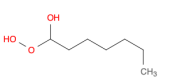
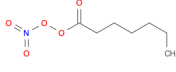
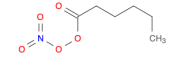
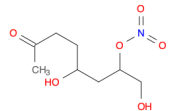
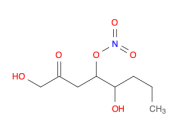
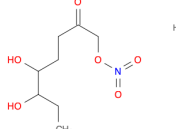
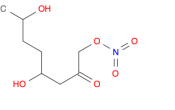
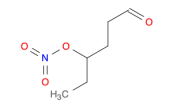
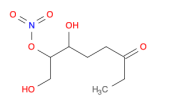


lp



lp



Surrogate	Sgy.	Merged species (U8Multi-H, continued)
	lp	
m2U8000		2U8001
	lp	
mHU8000		HU8001
	lp	
m2O8001		2O8000
		
		2O7000
	lp	
mP07000		P06000
	lp	
mNK800E		NK800H
		
		NK8005
		
		NK800g
	rp	
		ND6006
		
		NK800F

S3.5 Carbon propagation and conservation

To diagnose how different reduction configurations affect carbon representation, a carbon propagation analysis was performed for reduced mechanisms derived from the U8, C12, and LIM reductions. The carbon loss fraction (C_{loss}) measures the fraction of PVOC carbon not propagated into explicitly represented downstream products. This metric reflects the extent to which

downstream reaction pathways remain represented in a reduced mechanism and does not imply a lack of stoichiometric consistency within individual reactions. This diagnostic is intended to characterize configuration sensitivity rather than to serve as a performance metric.

As shown in Table S9, reference mechanisms (Ref) show negligible carbon loss across all PVOCs ($C_{\text{loss}} < 0.03$), while the TBR mechanisms used as starting points for SBR (StP) show carbon loss in the range of 0.23–0.31, reflecting pruning induced in TBR. SOA-focused reductions exhibit substantially higher carbon loss at early SBR stages, with C_{loss} reaching 0.77–0.87 for U8 and LIM and 0.56–0.85 for C12 during Stage 1. This behavior is expected, as SOA-focused reduction prioritizes compact mechanisms by truncating downstream oxidation pathways that are weakly relevant for SOA formation. At Stage 3, carbon loss decreases for some configurations, with C_{loss} ranging from 0.48–0.61 for U8, 0.28–0.86 for C12, and 0.56–0.62 for LIM.

Multi-target reductions retain a larger fraction of carbon than SOA-focused reductions, with the final reduced mechanisms (B2a–B2d) exhibiting $C_{\text{loss}} = 0.56$ –0.60 for U8, 0.60–0.73 for C12, and 0.35–0.54 for LIM. This reflects the additional constraints imposed by gas-phase evaluation targets, which limit pathway truncation and preserve greater propagation depth.

These results are consistent with the reduction philosophy described in the main text. The reduction workflow prioritizes removal-based strategies to produce compact mechanisms optimized for selected targets, rather than enforcing carbon conservation across all generations. Reduction therefore proceeds primarily through branch truncation, with downstream chemistry excluded once it no longer influences the specified targets. That said, elevated C_{loss} values quantify the resulting pathway truncation and do not indicate numerical or chemical inconsistency.

Table S9. Fraction of carbon not propagated into explicitly represented downstream species (C_{loss}) for SOA-focused (A) and multi-target (B) reduction configurations across the U8, C12, and LIM reductions.

SOA-focused (A)				Multi-target (B)			
Mech.	U8	C12	LIM	Mech.	U8	C12	LIM
Ref	0.003	0.030	0.001	Ref	0.003	0.030	0.001
StP	0.232	0.310	0.251	StP	0.232	0.310	0.251
A0.1	0.774	0.563	0.859	B0.1	0.566	0.715	0.389
A1	0.826	0.846	0.871	B1	0.604	0.770	0.391
A2a	0.819	0.792	0.736	–	–	–	–
A2b	0.774	0.751	0.740	–	–	–	–
A2c	0.776	0.752	0.692	–	–	–	–
A3a	0.478	0.864	0.619	B2a	0.591	0.734	0.349
A3b	0.511	0.371	0.559	B2b	0.600	0.671	0.346
A3c	0.612	0.638	0.608	B2c	0.556	0.604	0.412
A3d	0.556	0.278	0.597	B2d	0.591	0.680	0.535

References

- Aumont, B., Camredon, M., Lee-Taylor, J., and Valorso, R.: GECKO-A: Generator for Explicit Chemistry and Kinetics of Organics in the Atmosphere, <https://doi.org/10.5281/zenodo.15309905>, 2025.
- Wolfe, G. and Haskins, D. J.: F0AM v4.3.0.1, <https://doi.org/10.5281/zenodo.10069985>, 2023.