Authors' Response to Anonymous Referee #2

GENOA v3: A flexible framework for reduction and exploration of highly detailed chemical mechanisms

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RC: Referee's Comment, AR: Authors' Response, ☐ Manuscript Text

General Comments

RC: Wang et al. present GENOA v3, a chemical mechanism reduction framework designed for the scalable reduction of highly detailed mechanisms containing millions of reactions and species. GENOA v3 combines two reduction approaches, beginning with a Threshold-Based Reduction (TBR) approach that uses predefined criteria to remove chemically less important reactions and species, followed by a Simulation-Based Reduction (SBR) approach that iteratively evaluates the impact of mechanism reduction on model performance while effectively preserving chemical accuracy. A graph-based representation of chemical mechanisms is employed, making the framework applicable to very large reaction networks. A wide range of scenarios has been used to evaluate the applicability of the GENOA v3 framework, demonstrating that it can successfully reduce highly detailed mechanisms while preserving SOA mass and gas-phase reactivity. Overall, the manuscript makes an important contribution to atmospheric chemistry modeling by providing a scalable strategy for translating highly detailed mechanisms into forms that can be used in large-scale regional and global simulations. The manuscript is well written, falls well within the scope of GMD, and could be published after addressing the following suggestions:

AR: The authors thank the referee for the positive assessment of the manuscript and for the helpful suggestions. We have considered each comment carefully and provide our responses below. Unless otherwise noted, the section and line numbers cited refer to the manuscript before revision.

Specific Comments

RC: 1. Section 3: It is scientifically sound, but it is overly technical and detail-oriented. The explanations would benefit by including practical examples. For example, the implementation of the SBR approach discussed in Appendix B5, together with the example provided there, is much more readable and easier to understand than the theoretical explanation presented in Section 3.3 and its subsections of the main manuscript. To avoid repetition and confusion, I suggest moving and integrating this content into the main manuscript. This would reduce redundancy, improve readability, and better highlight the importance of the SBR approach. It is also encouraged the authors to explain other parts of the manuscript in a similar manner.

AR: Thank you for this helpful suggestion. As this is the first paper describing GENOA v3, we would like to retain sufficient methodological detail for readers to understand the reduction workflow and key concepts. However, we agree that parts of Sect. 3 were overly technical and that the practical examples could be introduced more clearly. We have therefore streamlined the presentation and improved the links between the main text and the worked examples. To keep Sect. 3 focused, the more extensive TBR formulations and demonstration have been moved to the Supplement, while the supporting SBR methodology and demonstration are retained in Appendix B because they are more closely tied to the core SBR workflow described in Sect. 3.3.

The main changes were made to the TBR description. Technical material previously included in Sect. 3.2 and Appendix B1 has been moved to a new Sect. S2.1 of the Supplement. This section now contains the mathematical formulations of the TBR strategies, related calculations, their relation to GECKO-A mechanism generation, and a newly added worked example using a simple mechanism. Sect. 3.2 now provides a more concise description and directs readers to these supporting details:

> *Sect. 3.2, page 9, line 210*
>
> ~~Table B1 provides an overview~~ Additional TBR details are provided in Sect. S2.1, including mathematical formulations and related calculations for the available strategies ~~and their mathematical formulations.~~ (Table S3), the effects of prior GECKO-A generation settings on TBR, and a demonstration of TBR using a simple mechanism (Fig. S7).

For SBR, Sect. 3.3 is organized around the main workflow of species grouping and ordering, candidate identification, and candidate evaluation and selection. We prefer to retain this core description in the main text, while keeping the supporting mathematical descriptions and worked demonstration in Appendix B to avoid substantially increasing the length of Sect. 3. To make these materials easier to locate, we now introduce them explicitly at the beginning of Sect. 3.3:

> *Sect. 3.3, page 11, line 281*
>
> SBR, referred to as training in GENOA v1 and v2, ~~follows a hierarchical structure in which the concepts of stage, cycle, and step (explained in Sect. B1) support structured configuration and progressive reduction~~is organized hierarchically into stages, cycles, and steps, as defined in Appendix B1. This structure allows user-specified settings to be applied systematically as the mechanism is progressively reduced. Additional SBR methodology and illustrations are provided in Appendix B, including mathematical descriptions of species grouping and ordering and candidate identification (Appendices B2–B3), and a demonstration of SBR using a simple mechanism (Appendix B4).

We also revised the beginning of Sect. 3 to direct readers to both worked demonstrations before the detailed descriptions:

> *Sect 3, page 6, line 152*
>
> Table 2 provides a concise reference for key terminology used in GENOA v3, with more detailed explanations discussed throughout this section. ~~Appendix B5 provides an illustrative example using a schematic mechanism to support explanation and visualization of key concepts in reduction representation~~Worked demonstrations of TBR and SBR using simple example mechanisms are provided in Appendix B4 and Sect. S2.1 of the Supplement, respectively.

RC: 2. Section 3: Please mention a quantitative example showing how many reactions and species can be removed

during the TBR and SBR stages. This would help readers understand the practical significance of both reduction steps at this stage of manuscript.

AR: Thank you for this useful suggestion. We have revised Fig. 1 (Sect. 3, page 3; also shown below as Fig. 1) to provide a quantitative indication of the reduction scale in terms of reaction count. The updated figure shows that a starting mechanism with approximately 10^6 reactions can be reduced to approximately 10^5 reactions after TBR and to fewer than 100 reactions after SBR, providing readers with an early indication of the practical reduction achieved by the two processes.

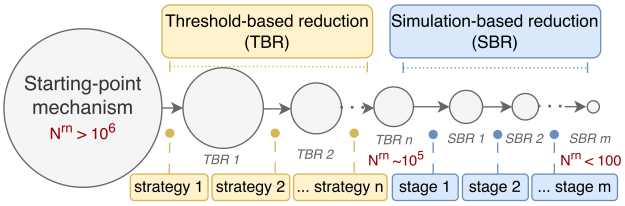

Figure 1: *Illustration of the sequential TBR–SBR workflow in this study. TBR n and SBR m represent mechanisms obtained after the nth threshold-based step or the mth simulation-based stage. Circle size and illustrative reaction counts (N^{rn}) indicate the progressive decrease in mechanism size through TBR and SBR.*

Detailed changes in both reaction and species counts are reported in Sects. 5–6. Worked demonstrations of TBR and SBR are also provided in Sect. S2.1 of the Supplement and Appendix B4, respectively.

RC: 3. Section 3.2: What is the importance of the TBR approach? Since it depends on user-defined protocols and predefined thresholds, could it potentially be a source of error? It would be helpful if the TBR strategy were also explained using a mechanism example, similar to the SBR approach presented in Appendix B5. Ideally, the authors could begin with a small example mechanism and then demonstrate both the TBR and SBR reduction processes using that mechanism. The technical details could then be moved to the appendix.

AR: TBR and SBR play complementary roles in the GENOA v3 workflow. TBR provides a rapid, mechanism-wide reduction before the more computationally intensive SBR, reducing the mechanism size and computational cost of subsequent SBR. In this work, T6 and T10 reduce mechanism size by approximately 46 % and 80 % on average, respectively. We revised the beginning of Sect. 3, where TBR and SBR are first introduced, to clarify their respective roles in the workflow:

Sect. 3, page 6, line 135

~~As illustrated in Fig. 1, reductions begin from a starting-point mechanism and are evaluated relative to a reference mechanism, which may be identical in some applications. The reduction framework consists of~~ The mechanism reduction framework supports sequential and iterative reduction through two main processes~~:~~ , described below, with mechanism performance evaluated against predefined reference mechanisms:

- Threshold-based reduction (TBR) performs system-level reduction using strategies and threshold values. In each TBR step, a single reduction strategy is applied consistently across the entire mechanism. This allows rapid reduction of reactions and species and produces a substantially smaller mechanism ~~that is suitable for further refinement~~for subsequent reduction or application.

- Simulation-based reduction (SBR) performs stepwise reduction guided by simulation feedback. ~~Starting from TBR-reduced mechanisms,~~ SBR proceeds through a sequence of stages with stage-specific accuracy constraints. Within each stage, reduction is applied iteratively to sub mechanisms, with multiple reduction candidates evaluated in parallel using metrics from 0-D simulations. This allows further accuracy-controlled size reduction and produces compact mechanisms manageable for ~~use in~~ large-scale ~~models such as 3-D chemical transport models.~~CTM applications.

~~These two processes are modular but typically used sequentially in GENOA v3, with TBR followed by SBR. This design allows computationally efficient pruning of large mechanisms at the system level before applying the more computationally demanding SBR for greater size reduction with user-controlled accuracy.~~ TBR and SBR are modular and can be applied independently. In the workflow used in this study and illustrated in Fig. 1, TBR is applied first to reduce the mechanism size efficiently and thereby lower the computational cost of the subsequent SBR, which provides further reduction under user-defined accuracy constraints.

As the referee notes, TBR can introduce larger errors when thresholds are too aggressive or not well suited to a particular mechanism or chemical regime. This size–accuracy trade-off is evaluated through the sensitivity analyses and performance evaluation in Sects. 4.3 and 5, while sources of reduction error are further discussed in Sect. 7.2. SBR then provides simulation-based accuracy control for further reduction.

As mentioned in the previous responses, we followed the suggestion and added a worked TBR demonstration using a simple mechanism in the new Sect. S2.1 of the Supplement, similar in purpose to the SBR demonstration in Appendix B5 (now Appendix B4 in the revision). We placed this demonstration in the Supplement rather than the Appendix to avoid making the main manuscript overly long and to keep the discussion focused. The detailed TBR formulations and related calculations have also been moved to Sect. S2.1 so that Sect. 3.2 remains concise and focused.

RC: 4. Section 4.1: mention the "MTs" in line 376 where it first appeared.

AR: Thank you for noting this omission. We have now defined MTs as monoterpenes at their first occurrence in Sect. 4.1:

Sect. 4.1, page 15, line 376

... and monoterpenes (MTs; $C_{10}H_{16}$: α-pinene, β-pinene, limonene, camphene, and carene).

RC: 5. Section 4.3: Since many similar thresholds have already been applied during GECKO-A mechanism generation, why is an additional TBR step necessary? Does this not make the mechanism reduction process more complex? Please clarify whether this step is essential and justify its inclusion.

AR: Thank you for raising this point. TBR and SBR are independent reduction processes in GENOA v3, and a mechanism can proceed directly to SBR without applying TBR. We agree that some TBR strategies are conceptually similar to cutoffs already applied during GECKO-A mechanism generation and may therefore provide limited additional reduction when comparable criteria have already been used during mechanism generation.

However, TBR remains an important reduction process in GENOA v3 because it provides a general post-generation framework for applying tighter or consistent reduction criteria across mechanisms. In addition, the environmentally sensitive TBR strategies use scenario-dependent information that is not considered by

the corresponding GECKO-A generation cutoffs. TBR is therefore not essential before SBR, but provides a practical and flexible pre-reduction step when further pruning or consistent post-generation treatment is desired. To clarify this point, we revised Sect. 3.2.3 as follows:

Sect. 3.2.3, page 11, line 275

~~As noted above, threshold cutoffs are also applied during the generationof explicit mechanisms, for example~~ Some TBR strategies are conceptually similar to cutoffs applied during explicit-mechanism generation, including in GECKO-A, to limit excessive growth of chemical schemes for large PVOCs ~~(Szopa et al., 2005; Aumont et al., 2005). These are conceptually similar to some TBR strategies, thus~~ (Szopa et al., 2005; Aumont et al., 2005, 2026). Consequently, additional reduction may be limited when comparable cutoffs have already been applied~~during mechanism generation, the additional reduction achievable by the corresponding TBR strategies may be limited.~~, but they remain useful when prior pruning is absent, tighter thresholds are required, or consistent criteria are applied across mechanisms. Further discussion of their application to the GECKO-A mechanisms evaluated here is provided in Sect. S2.1.3.

In this study, TBR is applied before SBR mainly for computational efficiency. Its additional reduction may be limited when comparable cutoffs have already been applied, but it remains useful when prior pruning is absent, tighter thresholds are needed, or consistent post-generation criteria are desired across mechanisms. As demonstrated by the additional SBR-only U8 test in the newly added Sect. S3.1.3, SBR can be initialized directly from the reference mechanism, but reaching Stage A1 required 21.93 kCPU-h compared with 3.59 kCPU-h when TBR was applied first. Thus, TBR is optional but provides a practical pre-reduction before the more computationally intensive SBR. We have further clarified this role and the associated computational benefit in Sect. 7:

Sect. 7.1, page 46, line 946

~~The presented examples illustrate these methodological differences~~Either TBR or SBR can be applied independently to any starting-point mechanism compatible with GENOA v3, although they are used sequentially in this study. These examples also demonstrate their different reduction capabilities and computational demands. For U8, TBR (U8StP) retained 20.7 % of the original size, while ~~the SBR decreased it further~~ subsequent SBR reduced the mechanism further to below 0.05 % (U8SOA-H and U8multi-H). Such reductions cannot be achieved by TBR alone while preserving reasonable accuracy. ~~However~~At the same time, the high computational demand for SBR limits its direct application to large VOC mechanisms. ~~As a result, a combined workflow that applies TBR first and then SBR provides a reasonable and scalable approach, enabling the preservation of accuracy while achieving extreme size reductions across diverse mechanisms and~~ Applying TBR before SBR therefore provides a practical and scalable workflow: TBR lowers the computational cost of SBR, while SBR enables substantial further reduction under user-defined ~~objectives~~accuracy constraints.

Sect. 7.2.3, page 48, line 1000

~~More aggressive TBR prior to SBR, or the introduction of an~~ An additional U8 comparison in Sect. S3.1.3 of the Supplement shows that, using the same Stage A1 settings, SBR initialized directly from Ref required 21.93 kCPU-h to reach the end of Stage A1, whereas the TBR–SBR workflow required 3.59 kCPU-h. Prior TBR, or a similar intermediate reduction stage, may ~~help address this limitation~~ therefore help reduce the computational cost of SBR for very large mechanisms.

RC: 6. In Figures 5–10 and the corresponding discussion sections, the trends are reported, but the underlying

mechanisms are not discussed. For example, the authors mention that reduction performance improves with increasing carbon number because larger VOCs produce lower-volatility products that dominate SOA formation; however, this is not qualitatively discussed. The authors may strengthen this argument by presenting cumulative SOA contributions by generation, volatility bin, and dominant species for C7, C12, C16, U8, U16, and LIM systems. Such an analysis would help highlighting that a limited number of dominant species control SOA formation in larger systems.

AR: We appreciate this suggestion. To provide additional chemical context for the carbon-number and precursor-class trends observed during TBR, we added Sect. S2.5 to the Supplement. Following the reviewer's suggestion, this section compares the number of condensable species across volatility bins (Fig. S21), particle-phase mass fractions by volatility bin (Fig. S22), and cumulative particle-phase mass contributions of leading condensable species (Fig. S23) for the Ref, T6, and T10 mechanisms of selected PVOCs (C7, C12, and C16 for Cs; U5, U8, U12, and U16 for Us; and all five MTs).

The analysis shows that TBR substantially reduces the number of condensable species while generally preserving the volatility distribution and the distribution of particle-phase mass among leading species. However, the proposed interpretation that SOA formation becomes progressively dominated by fewer species as carbon number increases is not supported by the results. In the reference mechanisms, the ten leading species contribute approximately 44 % of particle-phase mass for selected Cs and 60–77 % for the selected Us, without a monotonic dependence on carbon number. Thus, the improved TBR performance for higher-carbon-number Cs and Us is more consistently associated with the lower volatility of their oxidation products and preservation of the overall SOA-forming product distribution than with a universal increase in species-level dominance. We therefore revised Sect. 5.2.1 to provide a more qualified interpretation:

Sect. 5.2.1, page 25, line 559

As ~~the~~ carbon number increases, ~~early-generation oxidation products form lower-volatility species with larger SOA contributions. Consequently, SOA formation becomes increasingly dominated by early-generation products and a smaller number of high-contribution species, which are more readily retained during reduction for~~ oxidation products generally have lower volatility and contribute more readily to SOA. An additional analysis of condensable species in the Supplement (Sect. S2.5; Figs. S21–S23) further shows that TBR substantially reduces their number while generally preserving the volatility distribution and SOA mass distribution among the leading SOA-forming species. However, no monotonic carbon-number dependence is observed in the contributions of the leading species. Thus, the improved TBR performance for larger Cs and Us is consistent with preservation of their aggregate SOA-forming product distributions rather than a universal increase in species-level dominance. In contrast, MTs show weaker and less systematic scaling with mechanism size, consistent with ~~structural isomerism and more diverse oxidation pathways.~~their precursor-dependent SOA product and oxidation-initiation distributions (Sects. S2.3 and S2.5).

Generation-resolved contributions were not included because TBR can remove or bypass intermediate products and modify pathway connectivity, making generation-based comparisons less consistent between the reference and reduced mechanisms. We therefore focus on volatility- and species-resolved diagnostics, which provide a more direct initial assessment of the particle-phase material preserved during reduction. More detailed pathway-level chemical analyses will be pursued in future work when developing application-ready mechanisms and evaluating them in 3-D chemical transport models.

RC: 7. Sections 5.2.1 and 5.3.1: It is interesting that small-VOC systems (C5–C7 and U5–U6) behave differently from larger systems and appear to be more prone to over-reduction. The authors suggest that this is due to

the exclusion of short-chain oxidation pathways, including C2–C3 chemistry. It would be valuable to perform a pathway attribution analysis to identify which removed pathways (e.g., HOx recycling, PAN formation, formaldehyde/acetaldehyde chemistry, etc.) are primarily responsible for the observed errors.

AR: Motivated by this comment, we added two complementary analyses to provide a broader characterization of the chemistry and condensable species retained across all TBR mechanisms, including the small-VOC mechanisms highlighted here.

The newly added Sect. S2.3 reports RO_2 species counts and selected organic oxidation and RO_2 reaction classes for all Ref, T6, and T10 mechanisms. T10 removes substantially greater fractions of these classes than T6, with particularly low retention for some small mechanisms. For example, U5 retains approximately 35 % of the selected organic oxidation reactions, 34 % of its RO_2 species, and 20 % of the total reactions. However, C7 retains approximately 48, 55, and 32 %, respectively, comparable to or greater than several mechanisms with much smaller tSOA errors. Thus, structural retention alone does not consistently explain the observed errors. We added the corresponding discussion to the paper:

> *Sect. 5.3.1, page 29, line 641*
>
> In particular, the current T10 configuration may exclude short-chain oxidation pathways, including C2 and C3 chemistry, that are weakly relevant for SOA formation but ~~substantially~~ can contribute to VOC–NO_x–HO_x gas-phase chemistry. ~~The exclusion of these pathways reduces chemical representation in mechanisms dominated by C5–C6 precursors and~~ Consistently, the structural analysis in Sect. S2.3 shows substantial removal of selected organic oxidation and RO_2 reaction classes under T10, particularly for some small mechanisms. Although these counts do not identify the responsible pathways without flux-resolved analysis, their reduced representation is consistent with the larger errors observed, suggesting that further refinement of the T10 strategy is needed ~~for these mechanisms when~~ when these mechanisms are targeted.

As also discussed in our response to Specific Comment 6, the newly added Sect. S2.5 examines condensable-species numbers, particle-phase mass distributions across volatility bins, and cumulative contributions of leading species across the TBR mechanisms. This analysis provides additional compositional context and helps distinguish the two largest-error cases discussed here. The large C7 tSOA error occurs with little change in its normalized volatility distribution, indicating that the error primarily reflects a change in total particle-phase mass, whereas U5 shows changes in both tSOA and its volatility distribution. Thus, these outliers do not exhibit a single structural or compositional response to TBR.

The analyses indicate that the larger errors for some small mechanisms cannot be attributed to a single structural or compositional change. More detailed attribution to HO_x recycling, PAN formation, small-carbonyl chemistry, and other individual pathways would require reaction-flux or controlled pathway-perturbation analyses, which are beyond the scope of the present study and may be considered in future work.

RC: 8. Section 4.4.1: The authors note that tracer-species correlations vary across species and VOC classes, and Figure S16 shows that NOx, NO3, and O3 tracers exhibit weaker correlations than OH and HO2. However, these tracers are still included as optimization targets within the SBR framework. This raises the question of whether preserving tracer concentrations necessarily implies preservation of the underlying chemistry. It would be useful to quantitatively relate tracer errors to actual species or pathway errors during the reduction process, particularly for NOx-, NO3-, and O3-related chemistry.

AR: We appreciate this important point. As discussed in Sects. 4.4.1 and 6.2.2, preserving a tracer does not necessarily ensure preservation of the corresponding species, reactivity, or individual pathways. The pro-

duction and loss tracers are used as efficient integrated constraints on chemical budgets associated with the reducible mechanism, particularly when the corresponding species follow fixed profiles and therefore cannot be constrained directly by their concentrations, or when radical concentrations are too low for reliable error evaluation. Unlike reaction-resolved fluxes, however, tracers aggregate production or loss across multiple reactions and do not identify the contributions of individual pathways.

Sect. 6.2.2 quantitatively compares tracer biases with the corresponding reactivity and species biases. NO_3 reactivity and lNO_3 show weak correspondence for U8B2c–U8B2d, whereas O_3 reactivity and lO_3 show closely aligned biases; comparisons with the corresponding species also show clearer correspondence for HO_2 than for NO_2. These results demonstrate that tracer effectiveness depends on its coupling to the targeted chemistry.

As complementary structural information, we also added Sect. S3.3.4 and Tables S14–S15 to quantify RO_2 species and selected organic oxidation and RO_2 reaction classes during SBR. The results show that multi-target mechanisms generally retain more RO_2 species and reactions than the corresponding SOA-focused mechanisms, consistent with their broader representation of gas-phase chemistry. This analysis is now referenced throughout Sect. 6:

Sect. 6.1, page 34, line 703

To complement the overall size analysis, Sect. S3.3.4 of the Supplement provides RO_2 species counts and the numbers and relative distributions of selected reaction classes across SBR stages (Tables S14–S15), showing variations with both the PVOC and evaluation targets.

Sect. 6.2.2, page 39, line 829

Complementary structural analysis shows that the final multi-target mechanisms retain more RO_2 species and reactions than the corresponding SOA-focused mechanisms, consistent with their broader representation of HO_x-, NO_x-, and oxidant-coupled chemistry (Table S15; Sect. S3.3.4).

Sect. 6.4, page 42, line 885

Consistent with these pathway comparisons, the LIM multi-target mechanisms retain larger O_3- and NO_3-initiated fractions and more RO_2 species and reactions than the corresponding U8 and C12 mechanisms, indicating broader representation of initiation and peroxy-radical chemistry (Sect. S3.3.4).

Sect. 6.4.3, page 46, line 1051

These results show that SBR selectively preserves chemical pathways according to the evaluation targets, with SOA-focused reductions favoring compact representations and multi-target reductions retaining broader chemistry at increased complexity, consistent with the structural changes quantified in Sect. S3.3.4.

These results support tracers as practical integrated constraints rather than complete proxies for pathway preservation. Tracer selection is therefore mechanism- and process-dependent. Reaction-resolved or grouped pathway fluxes could provide more direct constraints and may be considered in future reductions.

RC: 9. Sections 5 and 6: Monoterpene (MT) chemistry is known to be highly complex, and this manuscript consistently shows that MT systems exhibit greater structural complexity (Figure 5) and larger reduction errors (Figure 6 and others). It would be beneficial to provide further discussion of the reasons behind this behavior. In particular, identifying which pathways are removed by GENOA during the TBR and SBR stages, and which of these pathways may be important for monoterpene SOA formation, would significantly

strengthen the analysis.

AR: Thank you for this suggestion. The newly added reaction-class and condensable-product analyses for TBR and SBR provide further chemical context for MT reduction behavior.

For TBR, Sect. S2.3 shows greater precursor-dependent variation among MTs in the relative contributions of OH-, O_3-, and NO_3-initiated reactions, with a particularly large O_3 contribution for LIM. Sect. S2.5 further shows substantial variation in the distribution of particle-phase mass among leading species: the ten leading Ref species contribute approximately 26 % for API and 60 % for CMP. Together with the absence of a consistent relationship between MT mechanism size and reduction error, these results indicate that MT reducibility depends on precursor-specific initiation and SOA product distributions rather than mechanism size alone. This interpretation is included in Sect. 5.2.1:

> *Sect. 5.2.1, page 25, line 562*
>
> In contrast, MTs show weaker and less systematic scaling with mechanism size, consistent with ~~structural isomerism and more diverse oxidation pathways~~their precursor-dependent SOA product and oxidation-initiation distributions (Sects. S2.3 and S2.5).

For SBR, Sect. S3.3.4 and Tables S14–S15 show that the LIM multi-target mechanisms retain larger O_3- and NO_3-initiated fractions and more RO_2 species and reactions than the corresponding U8 and C12 mechanisms. The pathway visualizations in Sect. S3.3 further show retention of nitrate-, peroxy-, and PAN-related products in the LIM multi-target mechanisms, whereas SOA-focused reduction retains a more compact set of SOA-related products. We added the following reference to Sect. 6.4:

> *Sect. 6.4, page 42, line 885*
>
> Consistent with these pathway comparisons, the LIM multi-target mechanisms retain larger O_3- and NO_3-initiated fractions and more RO_2 species and reactions than the corresponding U8 and C12 mechanisms, indicating broader representation of initiation and peroxy-radical chemistry (Sect. S3.3.4).

RC: 10. Section 5.2.1: The authors report that the mean tSOA reduction error exceeds the median for T10 reductions because a small number of mechanisms exhibit very large errors, suggesting a highly skewed error distribution and strong outlier influence. It would be useful to include additional statistical characterization to determine whether the mean errors are representative of typical mechanism behavior or are dominated by a small subset of reductions.

AR: To quantify the influence of the largest-error reductions, we recalculated the T10 statistics after excluding C7 and U5. The mean and median tSOA errors decrease from 12.3 and 4.2 % to 6.6 and 3.5 %, respectively. This confirms that C7 and U5 strongly influence the upper tail and overall mean, while the remaining reductions generally exhibit substantially smaller errors. We added this statistical characterization to Sect. 5.2.1:

> *Sect. 5.2.1, page 24, line 549*
>
> Across all mechanisms, tSOA is generally well preserved. T6 yields low mean and median tSOA errors (2.1 % and 0.73 %), while T10 increases these values to 12.3 % and 4.2 % ~~, remaining acceptable given the corresponding size reduction fractions. The mean exceeds the median, particularly for T10, reflecting a small number of large-error reductions~~. Excluding C7 and U5 decreases the T10 mean and median errors to 6.6 and 3.5 %, respectively, showing that these two mechanisms strongly influence the

upper tail of the error distribution.

RC: Overall, the manuscript provides a thorough evaluation of reduction performance in terms of mechanism size reduction and preservation of SOA and gas-phase metrics. However, a key question remains unanswered: what chemistry is actually removed during the reduction process? An analysis of representative systems (e.g., U8, C12, and LIM) showing the fractions of removed pathways associated with OH, O3, NOx, RO2, and related chemistry would substantially strengthen the manuscript.

AR: Thank you again for these helpful suggestions. As detailed in our responses to the specific comments above, we added complementary analyses of chemical representation during both TBR and SBR. Sects. S2.3 and S2.5 characterize changes in selected organic oxidation and RO_2 reaction classes and condensable products across the TBR mechanisms, while Sects. S3.3.4 and S3.3.5 extend these analyses through SBR for the representative U8, C12, and LIM systems. Together with the pathway visualizations in Sect. S3.3, these additions provide a broader picture of the chemistry retained or removed during reduction.

These analyses characterize structural reaction classes, retained pathways, and particle-phase product distributions, but do not quantify the kinetic contributions of individual pathways. Such pathway-resolved attribution would require more extensive flux or perturbation analyses. The present additions provide an initial basis for this chemical characterization, which will remain an important consideration when developing and testing application-ready reduced mechanisms.

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