Response to Reviewer Comments

The SAPRC Atmospheric Chemical Mechanism Generation System (MechGen)

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We wish to thank Rolf Sander and the second (anonymous) reviewer for taking the time to review this manuscript, their thoughtful reviewing, and their support for its publication. Given below are the reviewers' comments, followed by our responses and changes made to the manuscript where applicable. Major comments, or comments or responses that are longer, are given first for each reviewer, with reviewer comments indented and given in *italic font* to clearly distinguish them from our responses. Text that was added to the manuscript or SI are indicated using underline font, and deleted text are indicted using ~~strikeout font~~. Comments that were short and had short responses are given in tables that follow for each reviewer.

We also made some other minor changes to the manuscript reflecting additional edits that we found to be appropriate, and made changes to the procedures that determine which reactions are negligible to improve efficiency, as well as modifications to parameters affecting rate constant cutoffs to avoid neglecting reactions that may be non-negligible under very low NO_x conditions. These changes are discussed below, following our responses to the reviewers.

Comments by Rolf Sander

Comment:

" I think that MechGen is a very valuable tool for the atmospheric chemistry modeling community, and the manuscript is well-written. I recommended publication in GMD."

We thank Dr. Sander for his positive comments, for which no reply is needed.

Comment:

" Lines 113-115: It is announced that MechGen could be migrated to Python or another actively supported software platform. I fully agree that this is a good idea. However, since this is about future work, it should be mentioned in an "Outlook section" near the end of the manuscript, not in the introduction."

Agreed. This sentence has been moved to the Discussion, in a paragraph describing opportunities for development and promotion.

" **Comment:**

Lines 851-853: It is speculated that MechGen is not as widely used as MCM or GECKO-A because it has not been documented in the peer-reviewed literature. While I partially agree, I think there is another reason why the MCM is much more popular: The MCM-generated mechanism can easily be exported in KPP or facsimile format. These formats are used by many atmospheric chemistry models. In contrast, an elaborate conversion of the complex MechGen output is necessary in order to implement reactions from MechGen. Although probably out-of-scope for this manuscript, I suggest to add KPP-export functionality to MechGen (Disclosure of potential COI: I am involved in the development of KPP)."

Dr. Sander makes a good point. We are actively developing toolkits to support more flexible use of MechGen, including a F0AM extension compatible with SAPRC mechanisms and a translation script to convert MechGen-derived mechanisms into F0AM format. Additionally, the SAPRC box model software referenced in the manuscript is publicly available for download and can be used alongside MechGen. While we recognize the concern, we believe it does not affect the scientific utility of the system and publishability of this paper. We will continue to improve MechGen's adaptability for the broader research community. The paragraph in question is changed as indicated below, and the new reference (Wolfe et al, 2016) is added to reference list.

Old version:

~~The main reason that MechGen has not been as widely used as MCM or GECKO-A for applications other than SAPRC mechanism development is that it has not been described or documented in the peer reviewed literature until now, including the continuous revisions that it has undergone. Most researchers have either not been aware of MechGen and have not had a stable version to cite if they do use it. This paper, along with the recently published paper of Carter et al. (2025), addresses its lack of adequate documentation. Future updates to MechGen will be documented and made available as separate versions, so work using versions prior to the updates can be duplicated.~~

Replace with:

One of the reasons that MechGen has not been as widely used as MCM or GECKO-A for applications other than SAPRC mechanism development is that it has not been described or documented in the peer-reviewed literature until now, including the continuous revisions that it has undergone. Most researchers have either not been aware of MechGen or have not had a stable version to cite if they do use it. An additional factor that may inhibit its use as an alternative to MCM is that MechGen outputs mechanisms in the format used by the SAPRC model simulation software, which is not as widely used as other modeling software systems. This paper, along with the recently published paper of Carter et al. (2025a), addresses its lack of adequate documentation. Future updates to MechGen will be documented and made available as separate versions to ensure reproducibility. We are developing software converting MechGen mechanism output to other formats and have already released a converter for the F0AM modeling system (Wolfe et al, 2016), which is available from the MechGen GitHub repository.

Note that we moved this paragraph down one paragraph, so it follows the paragraph discussing the advantages of MechGen being user-friendly. No other changes were made to the discussion section other than indicated below.

Comment:

"Throughout the text, a period "." has been used to denote radicals. This can be confused with the end of a sentence. Instead, a vertically centered dot should be used"

The period has to be used rather than a centered dot in the context of showing what MechGen uses to designate radical species or groups. This was not changed because we wanted to accurately show MechGen input and output. After carefully reviewing the manuscript, we could not find any instances where the "." used to indicate a radical center would be confused with an end-of-sentence period. Therefore, no changes were made.

Additional comments by Rolf Sander and Responses

Comment	Response
"Line 37: "Many hundreds of types of volatile organic compounds" are mentioned here but Tab. 1 lists only 12 types. Maybe this should be species, not types?"	Changed to "Many hundreds of organic compounds …"
"Line 47: "lumping or condensations" is mentioned here. Lumping is explained later in the text but "condensations" is not. Is this the same as lumping or something different?"	Changed "condensation" to "reduction", which is the term that is used later.
"Line 203: Remove superfluous "are"."	Corrected.
"Table 4: I suggest to replace the non-standard name "2-methyl-2-ethyl butane" by "3,3-dimethylpentane"."	Changed as suggested.
"Table 4: Why are the radicals denoted as plural? Why not "radical" instead of "radicals"?"	Changed to singular to be consistent with other intermediates.
"Table 4: The acronym "MEK" is used here but not defined anywhere."	Changed "MEK oxide" to "Criegee int." in the table.
*"Table 4: The structures use the symbols *, ^ and v which seem to refer to cyclo, cis and trans. This should be explained in a table footnote."*	Footnotes added to Table 4 on first mention of applicable structures.
"Lines 480-481: It is claimed that "interconversions of hydroperoxy-substituted peroxy radicals due to rapid H-shift reactions" have been mentioned above. I cannot find this anywhere in the text. I can only see H-shifts for alkoxy radicals in Table 2."	Changed "as mentioned above" to "as discussed by Carter et al (2025a) and Vereecken and Nozière (2020)"
"Line 525: Probably change "the minimize size" to "the minimum size"."	Corrected.
"Line 552: Should this be Figure 6c instead of 6b?"	Corrected. Should be 6c.
"Table 8: What is meant by "explicit lumping"? Maybe this should be changed to "explicit (no lumping)"?"	Changed to "no lumping".
"Lines 704-705: "1 ppm" is not a "concentration" but a "mixing ratio" (or even more precise: "amount fraction". See e.g.: https://doi.org/10.1029/00EO00007"	Changed to "mixing ratio".
" Lines 830-842: The first paragraph of the Discussion section is a review about mechanism development which seems out of place. I think it can be deleted completely (or moved into the introduction section)"	We considered this suggestion from the reviewer, but opted to leave this paragraph as it is, as it provides extended context for MechGen.

Comment	Response
"Reference "Carter, 2025": I tried to open the web page https://intra.engr.ucr.edu/%7Ecarter/MechGen	This was an intermittent problem that has since been corrected.
"Throughout the text, the recommended symbol "s" should be used for a second, not "sec"."	Changed throughout the text as suggested.

Comments by Reviewer 2

Comment:

"This manuscript describes the MechGen mechanism generator that underlies the SAPRC mechanisms and builds upon the predictive chemistry described in an earlier paper (Carter et al. 2025). This work is an essential part of documenting the MechGen system, making an important contribution to FAIR research software in atmospheric chemistry. The publication is timely, as current atmospheric chemistry research relies on ever more complex kinetic models, and software assisted mechanism creation is gaining strongly in importance. The manuscript is well written, with clear and accessible descriptions despite covering a highly complex software suite.

I recommend publication of this manuscript. My comments are basically only suggestions for different presentation, and can be accepted or ignored by the authors as they please."

We thank the reviewer for the positive comments, for which no reply is needed.

Comment:

"line 244: "because these peroxynitrates are assumed to rapidly decompose at temperatures of interest": The results from Färber et al. suggest that it might be useful to have these reactions as a selectable option for specific environments (DOI: 10.1039/D3CP04163H)"

We agree with the reviewer that it is appropriate to have formation of peroxynitrates as an option for deriving mechanisms of interest at lower temperatures. The existing mechanism generation parameter "kFastUni" (Table 8) is used to determine whether a non-radical compound decomposes fast enough that it should be treated as an intermediate. Previously, the system was programmed to always ignore non-acyl peroxynitrate formation during full mechanism generations, regardless of kFastUni. In response to this comment by the reviewer, the system was modified so that peroxynitrate formation is *not* ignored if its calculated unimolecular decomposition rate constant is lower than kFastUni. The default kFastUni value is such that non-acyl peroxynitrate decompositions are estimated to be faster at the default temperature of 298 K, so their formation is ignored by default, as stated in the manuscript. However, the system will now generate the formation of peroxynitrates during full mechanism generation if the reactor temperature is low enough or if kFastUni is high enough. Both reactor temperature and kFastUni are parameters that the user can modify (see Table 8).

The last portion of the subject paragraph was modified as follows:

Previous version:

~~"… In addition, reactions of non-acyl peroxy radicals with NO_2 forming alkyl peroxynitrates (shown in Figure S1) are also not included during full mechanism generation because these peroxynitrates are assumed to rapidly decompose at temperatures of interest (Carter et al. 2025)."~~

Revised Version:

"… In addition, reactions of non-acyl peroxy radicals with NO_2 forming alkyl peroxynitrates (shown in Figure S1c) are not included during full mechanism generation by default because these peroxynitrates are assumed to rapidly decompose at temperatures of interest (Carter et al. 2025). These reactions can be included by either increasing the kFastUni parameter (see Table 8), or decreasing the reactor temperature such that the estimated rate constant is less than kFastUni."

Comment:

"page 29: "chemical operators": "operators" is only used ~5 times and seems equivalent to the more common phrasing "lumped species". Perhaps harmonizing the naming across the text could improve readability."

Added the following after the first sentence (in the 2nd paragraph of Section 5) that uses the term "operator":

"… (An "operator" in this discussion refers to model species that does not correspond directly to a chemical species but is added to represent overall effects of various reactions [e.g., Carter, 2020a,b]). …"

Comment:

"page S11 and elsewhere: 'sets of "cyclic" intermediates': The term "cyclic intermediates" is a bit unfortunate, as it is too similar to cyclic species. Furthermore it implies that the intermediates are connected in a 2-neighbor circle graph with n members, which is also the picture suggested by the descriptions ("intermediates react to ultimately reform themselves"). The graph topology, however, has a more general connectivity here, where connections with more/all set members are possible. I do not object strongly against the use of "cyclic" but then it needs to be clearly defined, and perhaps referred to as "cyclics" (see also below) at all times to avoid connotations of cyclic species.

p. S22, middle : "cyclics": Define 'cyclics' at the start of the paragraph, or even better when the sets of interconverting intermediates are defined.

We replaced the word "cyclic" with "interconverting" wherever it was used in this context. It is stated at the start that these are intermediates that react to ultimately reform themselves, though in some cases it may take more than one step.

Comment:

"Does MechGen support non-carbon backbone chains, e.g. -O--O- (peroxide or even higher length such as the ROOOH from RO2+OH), or (more exotic) -NH--NH-"

MechGen supports bonds between any of the groups that have bonds. However, only one bond symbol is used, unlike GECKO-A, which uses designations such as provided by the reviewer. The following was added to the first paragraph in Section 2.1:

" The leading or trailing "-", "=", "#", or "-a" indicate groups that can bond to neighboring groups by single, double, triple bonds, or aromatic/allylic bonds. Any groups with such designations can bond to other groups with such designations to form chains."

Comment:

"Page S18 middle: "30 by default, is a property of the lumping object that the MechGen programmer can modify.": Is this user-modifiable without recompilation ? I don't see it in Table 8 in the main text, but it would make sense to have that as an option."

The parameter "kEqConv", which determines the rate constant ratio in question, was omitted from Table 8 in the main manuscript, which lists the parameters that affect full mechanism generation. The following entry has been added to Table 8:

Parameters	Affects	Default
kEqConv	Peroxy radical interconversion rate constant above which the interconverting radicals can be treated as in equilibrium when the mechanisms are processed.	30 s^{-1}

The referenced text in the SI was modified as follows:

> The rate constant ratio used to distinguish between "fast" and "slow" sets of interconverting intermediates, 30 s^{-1} by default, is a property of the lumping object that the MechGen ~~programmer~~ user who created the object can modify.

The User Manual describes how the user can change this and other parameters that affect mechanism generation.

Additional comments by Reviewer 2 and Responses

Comment	Response
"line 89: "for around 298 K and 1 atm" -> "for conditions covering the lower atmosphere, i.e. around 298 K and 1 atm""	Modified as suggested.
"Table 2: "Criegee biradicals": Replace with "Criegee intermediates", as used in the remainder of the text (CI do not behave as biradicals)"	Changed as suggested.
"line 203: "rate constants are have to be estimated""	Corrected; "are" deleted.
"line 230: "representing RC(O)O·": should be "RC(O)OO.""	Corrected.
"Table 3: No CH2OO intermediate ? It shows up in the mechanism listings."	CH2OO was added to the table.
"Table 5: "Note that "RO-alpha-H" refers to the carbonyl formed when an alpha-hydrogen on an alkoxy radical is abstracted.": perhaps make this a separate footnote [d]"	Made into a separate footnote.
"Figure 1, lower left: "Reaction not supported" could perhaps read "species not supported""	This subject box on the figure was changed to "Reactions of this reactant are not supported".
"line 381: "making the fate of the reactant is independent": remove "is""	Corrected.
"line 525: "they determine the minimize size": minimal size"	Corrected to "minimum".

Comment	Response
"line 743: "lower limits unless very low values of MGminYld are used.': perhaps add "... are used to minimize the amount of untreated carbon (negC)""	Revised as suggested.
"Table 9: "Rct'd" is a notation used only in this table, where it's not clear why there is an apostrophe. Is it short for e.g. "Reactants reacted"? Perhaps "Rcts", analogous to "Rxns", would be more intuitive?"	Changed "Rct'd" to "Reacted", which required widening the column slightly. Also changed "Rxns" to "Reactions"
"Figure 8, S10. The 0.5 entry seems to have a superscript "s" on the right. What does this signify?"	This stray mark was removed when the figures were revised.
"Figure 8, 9, S10, S11: The meaning of the "s" after some functionalities needs to be explained. It seems superfluous."	The group labels were modified to make them clearer. Groups are designated using leading and (if applicable) trailing "-"s. The "s" suffixes were removed.
"Line 769: "The corrected yields assuming that the distribution of products from unreacted compounds to those that were reacted are also shown.": Sentence seems malformed"	That sentence is not applicable to this version of the figure and is removed.
"Line 780: "Lumping involves representing the many predicted organic products by lumped model species representing groups of products assumed to react similarly, ": This sentence is hard to parse. Perhaps rephrase it as "Lumping involves representing a group of several predicted organic products, selected to react similarly, as a single lumped model species""	We decided that this sentence is redundant, so it was removed.
"line 782: "to reduce the numbers of intermediates": "number""	The text is discussing mechanisms in plural, referring to mechanisms for different compounds that have different numbers of intermediates. No change made.
"page S11 top: "If only a red line is seen, then both mechanisms give the same predictions.": Move this note to the caption of Figure S5, where it is more relevant."	Moved as suggested.
"page S11 bottom: paragraph of "S3.1. Initial Processing for Interconverting Intermediates": Perhaps join this title and few text lines with the bulk of the text below ?"	This comment is probably because Tables S1, S2, Figure S5, and Schemes S1 and S2 interrupt a sentence in the first paragraph of Section S3.1, making it hard to read. This is corrected in the revised version.

Comment	Response
"page S14 footnote [d]: "the fate of unreactive Criegee intermediates": "unreactive" is perhaps not the right word here, as the CI are still reactive towards bimolecular reactions. I assume the authors mean CI without fast unimolecular reactions?"	Changed to "the fate of Criegee intermediates that do not have fast unimolecular reactions".
"page S25 bottom: "deg K", "degK": Temperature in Kelvin does not have "degrees", it's just "Kelvin"."	Changed to "K".
"p. S26 top: "Further discussion of vapor pressure and SOA estimation methods is beyond the scope of this work.": Perhaps refer to the papers above for that discussion, rather than leave the reader hanging."	Deleted this sentence, which really did not add anything.

Other Manuscript Changes

Please note that we found it necessary to make minor changes to the MechGen software and default parameters that affect mechanism sizes and, in some cases, which auto-oxidation reactions are neglected or assumed to dominate. This required recalculating the example results, resulting in some changes to the figures and tables in the manuscript and SI. The changes are relatively small and affect primarily sizes of mechanisms derived with no environments (reducing them somewhat), but do not affect the discussion, conclusions, or issues that concerned the reviewers. The major changes are shown below. Other than Figure 5, whose changes are shown below, the changes in the figures with recalculated data are hardly noticeable and are not shown here.

Table 8 lists parameters affecting mechanism generation. The relevant parameter changes are indicated below. Note that the names of the parameters kMinUni and kFastUni were changed to more clearly indicate that they refer to peroxy radicals alone.

Previous version:

Parameters	Affects	Default
~~kMinUni~~	~~Minimum rate constant for unimolecular reactions of peroxy radicals not to be neglected.~~	~~2.25×10^{-3} sec^{-1}~~
~~kMaxUni~~	~~Total unimolecular rate constant for peroxy radicals above which bimolecular reactions are ignored. [a]~~	~~1000 sec^{-1}~~

Revised Version:

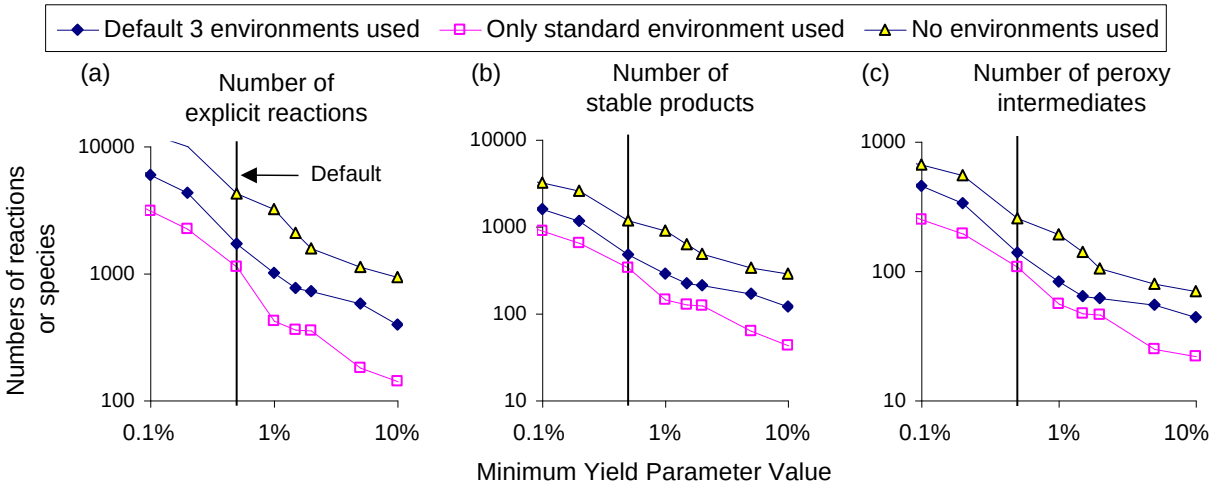
Parameters	Affects	Default
kRO2slow	Minimum rate constant for unimolecular reactions of peroxy radicals not to be neglected.	1.0×10^{-3} s^{-1}
kRO2fast	Total unimolecular rate constant for peroxy radicals above which bimolecular reactions are ignored. [a]	50 s^{-1}

Examples of effects of varying full mechanism generation options (Section 3.4)

Figure 5 in the main manuscript and Table S3 in the supplement were modified because of the changes in the single-generation derivation procedure and options. These changes are indicated below.

Figure 5 shows effects of varying the MinYld parameter and environment options on the numbers of explicit reactions in full mechanisms generated for α-pinene. There is a noticeable decrease in mechanism size statistics for the mechanism derived without environments, but not enough to affect the discussion in the text.

Previous version:



Revised version:

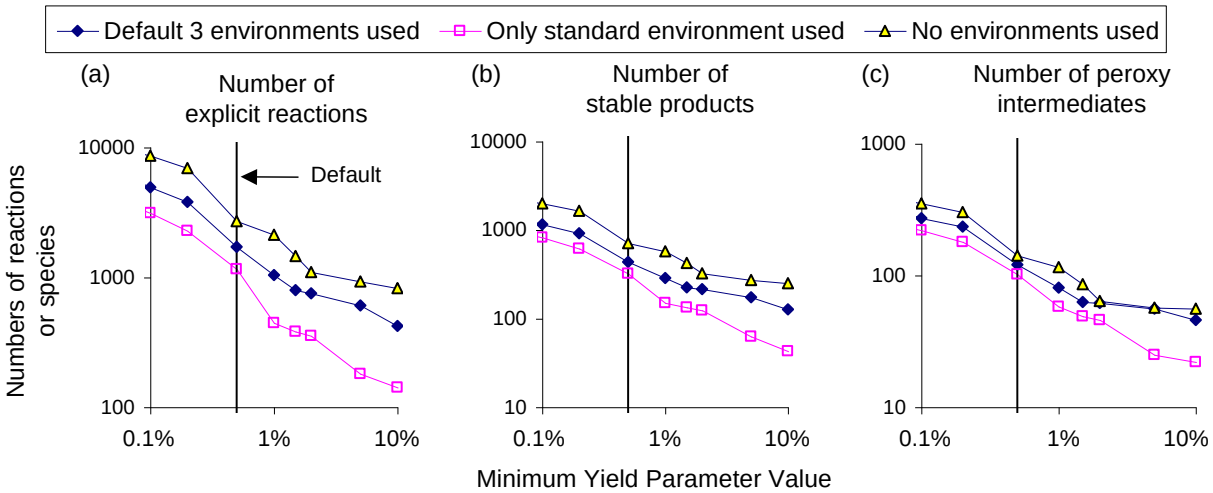


Table S3 lists representative compounds used to provide examples of results of single generation mechanism derivations. The changes can be seen to be quite small.

Compound	Default Options				No Environments				MinYld = 0.1% [a]			
	Explicit Rxns	Processed Prods	Int's	Yield Diff [b]	Explicit Rxns	Processed Prods	Int's	Yield Diff [b]	Explicit Rxns	Processed Prods	Int's	Yield Diff [b]
Normal Alkanes (previous version)												
~~Propane~~	~~26~~	~~11~~	~~3~~	~~0.005~~	~~46~~	~~15~~	~~4~~	~~-~~	~~37~~	~~13~~	~~4~~	~~-~~
~~n-Butane~~	~~39~~	~~14~~	~~4~~	~~0.001~~	~~52~~	~~18~~	~~4~~	~~0.001~~	~~41~~	~~14~~	~~4~~	~~0.001~~
~~n-Pentane~~	~~74~~	~~26~~	~~8~~	~~0.003~~	~~102~~	~~33~~	~~8~~	~~0.001~~	~~94~~	~~34~~	~~9~~	~~0.001~~
~~n-Hexane~~	~~138~~	~~50~~	~~14~~	~~0.003~~	~~183~~	~~62~~	~~14~~	~~0.002~~	~~161~~	~~57~~	~~15~~	~~0.001~~
~~n-Heptane~~	~~182~~	~~67~~	~~18~~	~~0.004~~	~~250~~	~~84~~	~~19~~	~~0.004~~	~~248~~	~~85~~	~~23~~	~~0.001~~
~~n-Octane~~	~~195~~	~~75~~	~~18~~	~~0.017~~	~~256~~	~~91~~	~~18~~	~~0.016~~	~~363~~	~~121~~	~~34~~	~~0.001~~
~~n-Nonane~~	~~271~~	~~103~~	~~25~~	~~0.010~~	~~356~~	~~127~~	~~25~~	~~0.010~~	~~496~~	~~165~~	~~46~~	~~0.001~~
~~n-Decane~~	~~347~~	~~130~~	~~32~~	~~0.010~~	~~467~~	~~164~~	~~33~~	~~0.009~~	~~661~~	~~221~~	~~61~~	~~0.001~~
~~n-Undecane~~	~~411~~	~~156~~	~~38~~	~~0.010~~	~~567~~	~~206~~	~~40~~	~~0.010~~	~~847~~	~~285~~	~~78~~	~~0.002~~
~~n-Dodecane~~	~~498~~	~~189~~	~~46~~	~~0.017~~	~~684~~	~~241~~	~~49~~	~~0.016~~	~~1187~~	~~401~~	~~108~~	~~0.003~~
~~n-Tridecane~~	~~621~~	~~235~~	~~58~~	~~0.014~~	~~945~~	~~334~~	~~69~~	~~0.012~~	~~1676~~	~~565~~	~~151~~	~~0.003~~
~~n-Tetradecane~~	~~781~~	~~292~~	~~73~~	~~0.020~~	~~1163~~	~~407~~	~~85~~	~~0.019~~	~~2280~~	~~766~~	~~204~~	~~0.003~~
~~n-Pentadecane~~	~~997~~	~~370~~	~~93~~	~~0.022~~	~~1489~~	~~518~~	~~110~~	~~0.020~~	~~3108~~	~~1046~~	~~277~~	~~0.003~~
~~n-Hexadecane~~	~~1140~~	~~422~~	~~106~~	~~0.024~~	~~1732~~	~~600~~	~~127~~	~~0.023~~	~~3902~~	~~1308~~	~~345~~	~~0.005~~
Normal Alkanes (replaced by)												
Propane	26	10	3	0.005	46	14	4	-	37	12	4	-
n-Butane	39	13	4	0.001	52	17	4	0.001	41	13	4	0.001
n-Pentane	74	25	8	0.003	102	32	8	0.001	94	32	9	0.001
n-Hexane	138	47	14	0.003	183	59	14	0.002	161	54	15	0.001
n-Heptane	182	64	18	0.005	250	81	19	0.004	248	82	23	0.001
n-Octane	195	72	18	0.017	256	88	18	0.016	363	118	34	0.001
n-Nonane	271	99	25	0.010	356	123	25	0.010	496	161	46	0.001
n-Decane	347	126	32	0.010	467	160	33	0.009	661	215	61	0.001
n-Undecane	411	151	38	0.010	567	199	40	0.010	847	278	78	0.002
n-Dodecane	498	182	46	0.012	684	234	49	0.011	1187	394	108	0.003
n-Tridecane	621	227	58	0.014	945	326	69	0.012	1676	557	151	0.003
n-Tetradecane	781	284	73	0.020	1163	399	85	0.019	2280	758	204	0.003
n-Pentadecane	997	362	93	0.022	1489	510	110	0.020	3108	1038	277	0.003
n-Hexadecane	1140	414	106	0.024	1732	592	127	0.023	3902	1300	345	0.004
Representative C_8 Compounds (previous version)												
~~2,2,3,3-Methyl Butane~~	~~63~~	~~21~~	~~7~~	~~0.001~~	~~80~~	~~28~~	~~7~~	~~-~~	~~67~~	~~22~~	~~7~~	~~-~~
~~2-Methyl Heptane~~	~~1057~~	~~315~~	~~77~~	~~0.006~~	~~1507~~	~~441~~	~~87~~	~~0.005~~	~~1823~~	~~510~~	~~125~~	~~0.002~~
~~Ethylcyclohexane~~	~~1586~~	~~490~~	~~130~~	~~0.008~~	~~5532~~	~~1553~~	~~267~~	~~0.006~~	~~5554~~	~~1458~~	~~352~~	~~0.001~~
~~trans-2-octene~~	~~783~~	~~237~~	~~60~~	~~0.015~~	~~1634~~	~~443~~	~~109~~	~~0.013~~	~~2442~~	~~687~~	~~199~~	~~0.002~~
~~3,5-Octadiene~~	~~661~~	~~193~~	~~39~~	~~0.014~~	~~1491~~	~~382~~	~~71~~	~~0.013~~	~~1361~~	~~385~~	~~91~~	~~0.002~~
~~1-Ethyl-cyclohexene~~	~~989~~	~~290~~	~~79~~	~~0.012~~	~~3976~~	~~1071~~	~~252~~	~~0.009~~	~~4463~~	~~1227~~	~~367~~	~~0.007~~
~~Octanal~~	~~399~~	~~136~~	~~39~~	~~0.013~~	~~1158~~	~~359~~	~~76~~	~~0.010~~	~~981~~	~~306~~	~~85~~	~~0.007~~
~~2-Octanone~~	~~268~~	~~97~~	~~27~~	~~0.031~~	~~399~~	~~137~~	~~31~~	~~0.016~~	~~397~~	~~136~~	~~37~~	~~0.001~~
~~n-Butyl Butyrate~~	~~447~~	~~129~~	~~37~~	~~0.005~~	~~602~~	~~169~~	~~37~~	~~0.005~~	~~672~~	~~179~~	~~50~~	~~0.002~~
~~m-Xylene~~	~~101~~	~~29~~	~~7~~	~~0.001~~	~~123~~	~~37~~	~~7~~	~~-~~	~~108~~	~~31~~	~~7~~	~~0.001~~
~~2,4-Dimethyl Phenol~~	~~107~~	~~39~~	~~7~~	~~0.024~~	~~115~~	~~42~~	~~7~~	~~0.024~~	~~184~~	~~56~~	~~14~~	~~-~~

Representative C_8 Compounds (replaced by)												
2,2,3,3-Methyl Butane	63	20	7	0.001	80	27	7	-	67	21	7	-
2-Methyl Heptane	1126	312	80	0.006	1588	441	90	0.005	1894	510	128	0.002
Ethylcyclohexane	1535	453	118	0.008	2183	659	125	0.006	2806	765	199	0.001
trans-2-octene	783	212	52	0.016	1292	321	62	0.015	2206	512	113	0.002
3,5-Octadiene	653	171	33	0.016	1135	281	41	0.015	1141	289	52	0.004
1-Ethyl cyclohexene	987	256	67	0.011	2061	460	91	0.009	3080	682	151	0.007
Octanal	366	118	34	0.013	512	158	36	0.010	541	167	45	0.007
2-Octanone	268	93	27	0.031	399	133	31	0.016	397	132	37	0.001
n-Butyl Butyrate	445	126	37	0.005	600	166	37	0.005	658	172	48	0.002
m-Xylene	109	29	7	0.001	131	37	7	-	116	31	7	0.001
2,4-Dimethyl Phenol	107	36	7	0.024	115	38	7	0.024	196	55	14	-
Representative Terpenes (previous version)												
~~a-Pinene~~	~~1717~~	~~488~~	~~139~~	~~0.013~~	~~4270~~	~~1193~~	~~256~~	~~0.012~~	~~5982~~	~~1597~~	~~457~~	~~0.003~~
~~b-Pinene~~	~~3852~~	~~1071~~	~~288~~	~~0.020~~	~~12064~~	~~3121~~	~~650~~	~~0.016~~	~~12418~~	~~3154~~	~~902~~	~~0.006~~
Representative Terpenes (replaced by)												
a-Pinene	1720	440	121	0.013	2710	714	142	0.012	4949	1143	272	0.003
b-Pinene	3389	876	216	0.016	5966	1465	264	0.016	8590	1895	429	0.002

Examples of Results for Multi-Generation Mechanisms (Section 4.2)

The multi-generation mechanisms also had to be recalculated because of changes in the single mechanism generation procedures and parameters. The changes to Table 9, which summarizes the calculations and gives the results, are shown below. When recalculating the examples where the environment was varied (middle part of the table), we decided to use only the environment used for determining product yields for the multi-generation derivations in the single-generation derivation, unlike the others where the three default environments were used. This gives the same product yield results but results in fewer reactions, as discussed in section 3.1. To reflect this, the following changes were made to Section 4.2

First paragraph of Section 4.2

"To illustrate the results of multi-generation mechanism derivation operations and their dependence on selected options, mechanisms were derived for several example compounds ranging from propane to α-pinene using a standard set of options, and additional multi-generation mechanisms were derived for α-pinene using differing sets of options. The compounds and mechanism derivation options are summarized in Table 9, which gives the sets of options, the numbers of explicit reactions, information on lost or low yield carbon, and estimated SOA formation for the mechanisms. In ~~all cases~~ the cases where the compound or MGminYld parameter was varied, the single-generation mechanisms for individual reactants were derived using the three default environments listed in Table 7 and the default mechanism generation options given in Table 8. In the cases where the environments were varied, the single-generation mechanisms were derived using the stated environment only, with defaults used for the other parameters. Table 9 shows that, as expected, the results depend significantly on the MGMinYld parameter and the multi-generation environment used."

Fifth paragraph of Section 4.2

"Examples of effects of using different environments on multi-generation mechanisms derived for α-pinene are shown in Table 9 and Figure 9. In those examples, the single-generation mechanisms were derived using only the subject environment rather than the three default environments, which is the reason that the number of reactions derived for α-pinene in these calculations is smaller than in those where the compound or MGminYld parameter was varied (see Figure 5), though the overall product yields are essentially the same. As discussed earlier, …

Table 9 gives mechanism sizes and other results for the example multi-generation mechanisms that were derived. The number of reactions decreased by 15-30% but the other quantities changed by less than 5% in most cases. The changes are indicated below.

Compound	Options [a] MGminYld	Environ [b]	Mech Size [c] Reactions	Reacted	Neg /Rct'd C [d]	SOA [e]
		Previous Version				
~~Propane~~			~~339~~	~~37~~	~~0.03%~~	~~~0~~
~~n-Butane~~		~~Mid NO_x~~	~~1457~~	~~110~~	~~0.2%~~	~~0.01%~~
~~1-Butene~~	~~0.01%~~	~~urban~~	~~1582~~	~~125~~	~~0.3%~~	~~0.02%~~
~~n-Octane~~	~~(default)~~	~~(default)~~	~~82,076~~	~~1433~~	~~6%~~	~~7%~~
~~Trans-2-octene~~			~~32,698~~	~~934~~	~~4%~~	~~5%~~
~~α-Pinene~~			~~113,379~~	~~1698~~	~~12%~~	~~52%~~
		~~High NOx~~	~~76,652~~	~~1278~~	~~8%~~	~~35%~~
~~α-Pinene~~	~~0.01%~~	~~Mid NO_x~~	~~113,379~~	~~1698~~	~~12%~~	~~52%~~
		~~Low NOx~~	~~92,495~~	~~1340~~	~~9%~~	~~50%~~
		~~Night~~	~~8493~~	~~95~~	~~0.3%~~	~~7%~~
	~~0.02%~~		~~78,098~~	~~1080~~	~~16%~~	~~50%~~
~~α-Pinene~~	~~0.01%~~	~~Mid NO_x~~	~~113,379~~	~~1698~~	~~12%~~	~~52%~~
	~~0.005%~~		~~151,139~~	~~2569~~	~~9%~~	~~55%~~
		Replaced by				
Propane			299	37	0.03%	~0
n-Butane		Mid NO_x	1203	109	0.2%	0.01%
1-Butene	0.01%	urban	1381	126	0.3%	0.02%
n-Octane	(default)	(default)	50235	1466	6%	7%
Trans-2-octene			24570	945	4%	5%
α-Pinene			82375	1695	12%	52%
		High NOx	20819	1252	8%	36%
α-Pinene	0.01%	Mid NO_x	56446	1683	12%	52%
		Low NOx	44933	1337	9%	51%
		Night	5961	95	0.3%	7%
	0.02%		56952	1088	16%	49%
α-Pinene	0.01%	Mid NO_x	82375	1695	12%	52%
	0.005%		116426	2587	9%	54%