

Basic Operations for MechGen Web Users

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MechGen is a computer program that can be used to generate gas-phase reactions of volatile organic compounds and the products they form at temperatures at or near 298 K and pressures at or near 1 atmosphere. The reactions can be generated in either in "single step" mode to see the predictions and documentation for a single reaction, or in "react completely" mode to also react the intermediates formed to obtain a complete mechanism leading to stable products. The stable products can then be reacted as separate operations. Results are displayed to the user or can be downloaded for further analysis.

MechGen can be accessed using the web interface that is currently available at: <http://mechgen.cert.ucr.edu>. This quick guide will walk through the basic operations for web users. If you are unable to access this website, please contact the author, William P. L. Carter: carter@cert.ucr.edu. Documents giving more information on MechGen and how it derives chemical mechanisms are available through the MechGen web site.

When first accessing the MechGen website, the user is presented with a login page shown on Figure 1. It includes form to give a username and a password for new users to create a user-specific "reactor" system, or for returning users to access that reactor. Once created, the username and password are necessary to login back to your own reactor system in the future.

Gateway to the SAPRC Mechanism Generation System

Access System as user with password

SAPRC Mechanism Generation System
for the Atmospheric Reactions of Volatile Organic Compounds in the Presence of NO_x

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Description

The SAPRC mechanism generation system, or MechGen, derives explicit mechanisms for the gas-phase reactions of many types of emitted organic compounds and their oxidation products when they react in the atmosphere in the presence of oxides of nitrogen and other pollutants. It then uses the results to derive lumped mechanisms suitable for use in atmospheric models. A [draft users manual](#) is available, and a paper documenting the software and algorithms is in preparation. A paper documenting the scientific basis of the estimation methods and chemical assignments has been submitted and reviewed and is undergoing revisions, but a [preprint and reviewer comments](#) are available online. In addition, information about the estimates and assignments can be obtained within the system, and is also output when reactions are generated in a step-by-step manner.

Figure 1. Screen shot of the top portion of the MechGen login page.

Main Menu

When first logged into the system, the user is presented with a web page with a reactor with the default settings when a new user reactor is created. In Figure 2, one reactant has been created and fully reacted for illustration. These sections of the web page in Figure 2 are as follows:

- Header. Identifies the user and reactor and gives links to reload, log out, or restore reactor defaults. Also indicates the current lumping method that controls how mechanisms are generated and processed.
- Create VOC or radical reactant. This section has a form to create a reactant. You can input SMILES directly, or use MechGen structure notation (similar to SMILES but displays all atoms). Click the links on the website for detailed explanations of "structure" and "assigned name".
- Get information on reactants in contents. This lists reactants that previously created by the user. It has links to go to the "Reactant Information" page for the reactant (discussed later). If a reactant has been fully reacted, there are links to access the reaction results. Note that radical reactants are not displayed in this list unless they have been completely reacted.
- Reactor options. This contains links to change options that control mechanism generation and lumping options. Restoring reactor defaults sets all these options to those for a new user.
- Other information. This section includes links to obtain general information about MechGen and SAPRC.
- Advanced options. Users can employ "user assignments" to add to or override the default mechanism assignments. This might be useful for advanced users for the purpose of developing new mechanisms consistent with new data or theories, or modeling experimental data that appear to be inconsistent with default MechGen predictions. This section is not covered in this quick startup guide; please read the complete user manual on MechGen website for further details.
- User Account Section. This section has links to log out, change user password, enable telnet logins, or completely delete this web and (if applicable) telnet account, or provide optional user information.

SAPRC-22 MECHANISM GENERATION SYSTEM
Reactor for user1 [#6343] ([Reload](#)) ([Log out](#)) ([Restore defaults](#))
Lumping method = Explicit mechanism with no lumping [#22447] (type=3) ([Change](#))

Create VOC or radical reactant

- Input the [structure](#), SMILES string, or [assigned name](#) for a reactant
- Create from the list of SAPRC VOC model species by [compound type](#) or [from complete list](#) (sorted by atom nos.)

Get information on reactants in contents: ([Delete all reactants](#))

- [MEK](#): CH₃-CH₂-CO-CH₃ [#21153] (reacted with OH, NO₃, and HV) ([delete](#))
Reactions generated using Explicit mechanism with no lumping
Explicit mechanism has 78 reactions and 63 species. Show ([reactions and products](#)). Send ([reactions](#)) or ([products](#))
Processed mechanism has 37 reactions and 47 species. Show ([reactions](#)). Send in ([tab-separated format](#)) or in ([SAPRC RXN format](#))

Reactor options

- Temperature (°K)= ; Pressure (atm)= ; Atm PM (µg/m³)= ; O₂ in air
- H₂O is absent ([change](#))
- [Change lumping method](#), which is currently Explicit mechanism with no lumping
- [View or change standard environments](#). Currently 4 are used for product yields and 3 are used to generate mechanisms.
- Light source code is "STD640Z0". ([Info or Change](#))
- SIMPOL.1 vapor pressure estimates [#7402] ([Change](#))
- [Restore reactor defaults](#)

Obtain information

- [Show Estimation Methods](#)
- [Show assignments](#) in SAPRC-22 Mechanism Assignments (with 541 species)
- [Show information related to the SAPRC-22 mechanism](#)
- [Draft users manual](#) (opens a PDF file in a separate window)

Advanced options

- Minimum 1-step yield for competing reactions:
- Minimum estimated yields for peroxy intermediates to react during mechanism generation
- User assignments are disabled ([Enable or edit](#))
- The user mechanism option is not available when Explicit mechanism with no lumping is selected.

Web user account actions

- [Log out](#)
- Change web login password (does not affect Telnet logins):
- Telnet login enabled. [Click here](#) to get information on telnet access and commands.
- [Completely delete the web and telnet accounts for user1](#) and associated data and log out.

Web user account actions

- [Log out](#)
- Change web login password (does not affect Telnet logins):
- Telnet login enabled. [Click here](#) to get information on telnet access and commands.
- [Completely delete the web and telnet accounts for user1](#) and associated data and log out.

- Give or edit user information (optional). Clear field to delete.
Name:
Email:
Other info:

- Please email Bill Carter at carter@cert.ucr.edu if you have any comments or questions about this system or notice errors in its operation or in its chemical mechanism assignments or estimates.

Figure 2. Screen shot of most of the main menu for the web interface showing a previously created and reacted reactant but otherwise with the default settings.

Reactant Information Pages

Reactant information pages are shown when new reactants are created, or existing reactions are selected from the main menu. The content of these pages varies depending on whether the reactant is a stable compound or an intermediate, and whether the reactant has undergone a "react completely" operation. Figure 3 and Figure 4 illustrate examples of a stable reactant methyl ethyl ketone and of one of the radicals formed after it reacts. The contents of these pages are as follows:

- Header. The top section gives basic information about the reactant, including its structure in both MechGen and SMILES format, and lumping information if applicable.

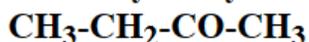
- Generate Reactions.

In the case of stable compounds, this section gives links to generate single step reactions or complete reactions of the various type that this reactant can undergo, which is reaction with OH, NO₃, and photolysis in the case of MEK, but can also include unimolecular reactions or reactions with O₃, O³P, depending on the compound. If reactions of this compound have previously been used in deriving a SAPRC mechanism, the page also includes a "Get Reaction Assignments" link to obtain information about the assignments that were used in previous complete mechanism generations for this compound.

In the case of reactant pages for intermediates, this section gives the results of a single step reaction of this radical, and a link to react this radical completely.

- Groups. This section lists MechGen groups in the molecule and how they were used to estimate the heat of formation.
- Estimated vapor pressure (stable reactants only). Information about how the vapor pressure is estimated.

MEK: Methyl Ethyl Ketone



Smiles string: CCC(C)=O

Molecular weight of C4H8O is 72.11

No assigned heat of formation.

Estimated heat of formation is -57.13 kcal/mole.

Estimated vapor pressure (SIMPOL.1) at 298.00 deg K is 1.61e-1 atm.

Fraction in particle phase (with PM=50 ug/m3): 1.1e-7

VOC Type = Ketone

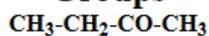
Generate Reactions

React with OH:	(Single step)	(Select to react completely <input type="checkbox"/>)
React with NO3:	(Single step)	(Select to react completely <input type="checkbox"/>)
React with HV:	(Single step)	(Select to react completely <input type="checkbox"/>)

[React completely with all.](#) or

[Get reaction assignments](#)

Groups



#	Group	Bonded To	Heat of Formation
1	-CH ₃	2	-10.04 C_(C)
2	-CH ₂ -	1,3	-5.26 C_(C)(CO)
3	-CO-R	2,4	-31.79 CO_(C)(C)
4	-CH ₃	3	-10.04 C_(CO)

Notes on heat of formation estimate:

- Hf(-CH₃[1])= -10.04 C_(C) (Holmes and Aubry (2011))
- Hf(-CH₂-[2])= -5.26 C_(C)(CO) (Holmes and Aubry (2011))
- Hf(-CO-R)= -31.79 CO_(C)(C) (Holmes and Aubry (2011))
- Hf(-CH₃[4])= -10.04 C_(CO) (Holmes and Aubry (2011))

Estimated vapor pressure at 298.00 deg K is 1.61e-1 atm.

Vapor pressures estimated using the SIMPOL1. method.
Estimated for T = 298.00 deg K

Prm	Description	N	Parm	Log(VP)
b0	zeroeth group (constant term)	1	1.842	1.84
b1	carbon number	4	-0.425	-1.70
b9	ketone	1	-0.936	-0.94

For CH₃-CH₂-CO-CH₃ at T=298.0K:

- Estimated vapor pressure (atm) = 10^{-0.79} = 1.61e-1

Figure 3. Screen shot of the reactant menu for a newly created reactant with default reactor settings, using MVK as an example.

RAD-4

CH₃-CO-CH₂-CH₂O.

Radical type: A primary alkoxy radical center.

Smiles string: CC(=O)CC[O]

Molecular weight of C₄H₇O₂ is 87.10

No assigned heat of formation.

Estimated heat of formation is -40.96 kcal/mole.

Vapor pressure cannot be estimated: Cannot estimate VP for radicals

VOC Type = This is a -CH₂O. radical.

[React completely](#)

Unimolecular or O₂ reactions

CH₃-CO-CH₂-CH₂O. → [CH₃-CO-CH₂](#) + [HCHO](#) (5.5%)

- Decomposition (T= 298K): k= 3.73e+3 s⁻¹.
- k= A*e^{-Ea/RT}; A= 1.00e+14 s⁻¹; Ea= Base Ea contributions + corrections = 14.22 kcal/mol. A factor estimate based on recommendations of Orlando et al (2003).
- Base Ea contribution for decompositions forming a HCHO carbonyl product = 0.00 kcal/mol. Assigned to be zero (not independent).
- Base Ea contributions for decompositions forming -CH₂(.) radicals = 15.51 kcal/mol. Adjusted to fit activation energies derived for decompositions of acyclic saturated hydrocarbon alkoxy radicals.
- Correction for -CO- substituent on the radical formed = -1.29 kcal/mol. Adjusted to fit activation energies for decompositions of various types of acyclic, non-alkyl alkoxy radicals. All the parameters for radicals formed from alkanes were optimized first.
- Warning: This reaction is estimated to be endothermic by 6.85 kcal/mole. However, this is less than the estimated activation energy of 14.22 kcal/mole, so the estimated activation energy is not modified.

CH₃-CO-CH₂-CH₂O. → [CH₂-CO-CH₂-CH₂-OH](#) (0.3%)

- 1,4 H-shift isomerization: k(298K)= 2.25e+2 s⁻¹
- - A = 4.00e+10 x 3 = 1.20e+11 cm³-mole⁻¹ s⁻¹. The A factor per H atom used for 1,4-H shift isomerizations is 4.0e+10 sec⁻¹, as recommended by Vereecken and Peeters (2009) for structure-reactivity estimation purposes.
- - Base Ea for abstractions from -CH₃[1] groups = 7.549 kcal/mol. Activation energies derived from fits of experimental 1,4-H-shift isomerization rate constants for 1-butoxy an 1-pentoxy radicals (Atkinson, 2007).
- - Ring strain for 1,4 H-shift isomerizations = 0.000 kcal/mol. No ring strain correction is used for 1,4 H-shift isomerizations.
- - Ea correction for substitution by -CO- on the group with the abstracted hydrogen is 0.030 kcal/mole. Correction to the activation energy due to this substituent derived from the correction factor for the effect of this substituent on rate constants for abstractions by OH from various organics.
- - Ea correction when a -CO- is in the transition state ring next to a CH₃ group with the shifted hydrogen is 4.314 kcal/mole. Adjusted to be consistent with the rate constant for CH₃-CO-CH₂-CH₂O. → [CH₂-CO-CH₂-CH₂-OH](#) as calculated by Vereecken and Peeters (2010).
- - Overall Ea including and all corrections = 11.893 kcal/mole.

CH₃-CO-CH₂-CH₂O. + O₂ → [CH₃-CO-CH₂-CHO](#) + HO₂. (94.2%)

- O₂ reaction (T= 298K, 20.9% O₂): k*[O₂]= 6.43e+4 s⁻¹
- k= 2.38e-14 * exp(-0.38/RT) = 1.25e-14 cm³ mole⁻¹ s⁻¹; T= 298 K.
- Kinetic parameters are estimated to be approximately the same for reactions of O₂ with all alkoxy radicals with -CH₂O. groups. The 300K rate constant was derived by averaging the recommended values from measurements for n-propoxy and n-butoxy radicals, with the Arrhenius parameters estimated by assuming that the A factor is the same as that given for 1-propoxy.

Groups

CH₃-CO-CH₂-CH₂O.

#	Group	Bonded To	Heat of Formation	
1	-CH ₃	2	-10.04	C_(CO)
2	-CO-R	1,3	-31.79	CO_(C)(C)
3	-CH ₂ -	2,4	-5.26	C_(C)(CO)
4	-CH ₂ O.	3	-7.89	C_(C)(O*)
			14.02	O*(C)

Notes on heat of formation estimate:

- Hf(-CH₃[1])= -10.04 C_(CO) (Holmes and Aubry (2011))
- Hf(-CO-R)= -31.79 CO_(C)(C) (Holmes and Aubry (2011))
- Hf(-CH₂-[3])= -5.26 C_(C)(CO) (Holmes and Aubry (2011))
- Hf(-CH₂O.)= -7.89 C_(C)(O*) (Assume no beta substituent effect on BDE's. Set to [C_(C)(O)])

Figure 4. Screen shot of the reactant page for a newly created radical reactant with default reactor settings, using one of the radicals formed in the initial reactions of OH with MEK as the example.

Generating Single Step Reactions

Generating single step reactions is the best means to obtain information about reactions of individual compounds or radicals, and obtaining documentation information about how the results are derived or assigned. Once a single step reaction is generated, an associated single step reaction results page will be displayed.

These consist of lists of reactions and estimation methods, or mechanism assignments used. Example of single step reaction output for a stable reactant is shown in Figure 5.

MVK: Methylvinyl ketone
CH₂=CH-CO-CH₃
Smiles string: C=CC(C)=O
Molecular weight of C₄H₆O is 70.09

No assigned heat of formation.
Estimated heat of formation is -28.16 kcal/mole.
Estimated vapor pressure at 298K is 1.26e-1 atm.
Fraction in particle phase (with PM=50 ug/m3): 1.4e-7.
VOC Type – Alpha unsaturated ketones

Reactions with OH

CH₂=CH-CO-CH₃ + OH -> [CH₃-CO-CH₂-OH](#) (70.0%)

- Assigned total rate constant = 2.01e-11 = 2.60e-12 * exp(1.212/RT) (T=298) cm³ molec⁻¹ s⁻¹. From the Compilation of McGillen et al (2020), as updated to version 2.1.0, June 23, 2021. <https://doi.org/10.25326/mh4q-y215>
- Rate constant for this reaction = 1.41e-11 cm³ molec⁻¹ s⁻¹ (70.0%). Based on product distribution of Tuazon and Atkinson (1989), as discussed by Carter and Atkinson (1996)

CH₂=CH-CO-CH₃ + OH -> [CH₃-CO-CH\(CH₂\)-OH](#) (30.0%)

- Rate constant for this reaction (see above for total) = 6.04e-12 cm³ molec⁻¹ s⁻¹ (30.0%). Based on product distribution of Tuazon and Atkinson (1989), as discussed by Carter and Atkinson (1996)
- Assigned Total kOH for T = 298 and 1.00 atm. = 2.01e-11 cm³ molec⁻¹ s⁻¹.
- From the Compilation of McGillen et al (2020), as updated to version 2.1.0, June 23, 2021. <https://doi.org/10.25326/mh4q-y215>

Figure 5. Screen shot of the portion of the single step reaction results page from reacting MVK with OH radicals.

Full Mechanism Generation

The full mechanism generation process involves reacting all radicals formed in the initial reactions, then reacting the intermediates formed that need to be reacted, until only stable or species or basic species that do not need to be reacted remain. This can take a significant amount of time for larger molecules.

If the compound has more than 9 groups, the "Generate Reaction" section will not contain any active links to generate full reactions -- only single step reactions can be generated using the web system for such compounds. Telnet logins are required to generate mechanisms for login compounds. The main menu (Figure 1) has links to create a telnet login.

Once the full reaction generation is completed, a page showing the generated reaction is displayed with links for downloading the reaction or product lists. An example of the portions of such a page is shown as Figure 6.

In Figure 6, the top part of the page has links for downloading the list of products and reactants in the explicit, minimally processed, and (if applicable) lumped mechanisms in various formats. The download options include the following:

Full mechanism (reactions): Reactions, rate constant parameters, and branching ratios in tab-separated format. Columns in this spreadsheet include reaction number, A, Ea, and B parameters for calculating temperature dependences where $k(T)=A*\exp(-Ea/T)*(T/300)^B$, the weighting factor used during mechanism generation, the rate constant at the default temperature, and the reaction itself. For photolysis reactions, the name of the SAPRC-22 photolysis file is given in the column used for Ea and the overall quantum yield is in the column used for B, and the rate constant is shown for overhead sunlight for standard reaction conditions.

Full mechanism (Products): List of products and their estimated yields for the standard environmental conditions.

Processed mechanism (reactions & tab-separated format): List of products and intermediates (steady state species) in the minimally reduced processed mechanism. The product and intermediate listings include columns with the product or intermediate number, the name used for the product or intermediate in the reaction listings (either a standard SAPRC name or system generated), and the structure. The reaction section includes columns with the reaction number, A, Ea, and B parameters and rate constant at the default temperature (or photolysis file names and quantum yields and photolysis rates for overhead sunlight for photolysis reactions), and the reactions.

Processed mechanism in (SAPRC .RXN format): This gives the processed mechanism in the format that can be used with SAPRC base mechanism and the SAPRC box modeling software. Links to obtain the SAPRC mechanism files and software are available at <https://intra.engr.ucr.edu/~carter/SAPRC/SAPRCfiles.htm>.

Mechanism generated using Explicit mechanism with no lumping
 Full mechanism has 39 reactions and 35 species. Download tab-separated files with [\(reactions\)](#) or [\(products\)](#)
 Processed mechanism has 16 reactions and 20 species. Show [\(reactions\)](#). Send in [\(tab-separated format\)](#) or in [\(SAPRC .RXN format\)](#)

Full set of reactions with OH

Full set of reactions with OH

Rxn	k	Fac	Weight	Reaction
1	3.15e-13	28%	28.4%	CH3-CH2-CH3 + OH -> CH3-CH2-CH2. + H2O
2	7.94e-13	72%	71.6%	CH3-CH2-CH3 + OH -> CH3-CH[.] -CH3 + H2O
3		100%	71.6%	CH3-CH[.] -CH3 + O2 -> CH3-CH[OO.] -CH3
4	8.75e-12	96%	68.7%	CH3-CH[OO.] -CH3 + NO -> CH3-CH[O.] -CH3 + NO2
5	3.70e-13	4%	2.9%	CH3-CH[OO.] -CH3 + NO -> CH3-CH(CH3) -ONO2
6	2.30e-12	100%	71.6%	CH3-CH[OO.] -CH3 + NO3 -> CH3-CH[O.] -CH3 + NO2 + O2
7	9.92e-12	100%	71.6%	CH3-CH[OO.] -CH3 + HO2 -> CH3-CH(CH3) -O-OH + O2
8	7.80e-15	50%	35.8%	CH3-CH[OO.] -CH3 + RO2 -> CH3-CH[O.] -CH3 + O2 + RO.
9	3.90e-15	25%	17.9%	CH3-CH[OO.] -CH3 + RO2 -> CH3-CH(CH3) -OH + O2 + RO-alpha-H
10	3.90e-15	25%	17.9%	CH3-CH[OO.] -CH3 + RO2 -> CH3-CO-CH3 + O2 + ROH
11	1.28e-11	80%	57.3%	CH3-CH[OO.] -CH3 + RC03 -> CH3-CH[O.] -CH3 + O2 + RC02.
12	3.20e-12	20%	14.3%	CH3-CH[OO.] -CH3 + RC03 -> CH3-CO-CH3 + O2 + RC0-OH
13	3.63e+2	1%	2.4%	CH3-CH[O.] -CH3 -> CH3-CHO + CH3.
14	3.56e+4	99%	230.9%	CH3-CH[O.] -CH3 + O2 -> CH3-CO-CH3 + HO2.
15		100%	28.4%	CH3-CH2-CH2. + O2 -> CH3-CH2-CH2O0.
16	8.75e-12	96%	27.3%	CH3-CH2-CH2O0. + NO -> CH3-CH2-CH2O. + NO2
17	3.70e-13	4%	1.2%	CH3-CH2-CH2O0. + NO -> CH3-CH2-CH2-ONO2
18	2.30e-12	100%	28.4%	CH3-CH2-CH2O0. + NO3 -> CH3-CH2-CH2O. + NO2 + O2

(not all reactions shown)

37	1.22e-11	90%	2.1%	CH300. + RC03 -> CH30. + O2 + RC02.
38	1.35e-12	10%	0.2%	CH300. + RC03 -> HCHO + O2 + RC0-OH
39	8.21e+3	100%	7.5%	CH30. + O2 -> HCHO + HO2.

* SAPRC-22 photolysis rates (sec-1) for Z=0, calculated using actinic fluxes used by the Carter (1994) reactivity scale

Mechanism Generation options: T=298; P=1.0; O2=0.2095; MinYld=0.0050; Lumptype=3; Environ: HighNOxEnv, LowNOxEnv, NightEnv

Products from reacting under standard conditions

Explicit products formed when PROPANE reacts with OH under the following conditions:

Condition Description

Mid NOx	Mid NOx standard urban conditions (near EBIR)
High NOx	High NOx urban conditions (near MIR)
Low NOx	Low NOx downwind conditions (NOx = MOIR NOx/10)
Night	Nighttime conditions for multi-day, mid-NOx scenario

Products listed in descending order of maximum yield

Mid NOx	High NOx	Low NOx	Night	Explicit product or reacted
92.07%	96.63%	79.10%	64.14%	NO2
88.10%	95.94%	65.00%	64.51%	HO2.
65.33%	67.98%	57.50%	59.78%	CH3-CO-CH3
26.07%	27.13%	22.94%	23.84%	CH3-CH2-CHO
2.77%	2.91%	2.38%	-	CH3-CH(CH3) -ONO2
2.80%	-	11.10%	11.12%	CH3-CH(CH3) -O-OH
1.10%	1.15%	0.95%	-	CH3-CH2-CH2-ONO2
0.78%	0.84%	0.63%	0.60%	HCHO
0.66%	0.69%	0.57%	0.58%	CH3-CHO
1.11%	-	4.40%	4.41%	CH3-CH2-CH2-O-OH
0.13%	0.14%	0.12%	0.09%	LostRads
-	-	0.05%	0.07%	CH3-O-OH
0.01%	-	-	0.00%	Total < 0.05%

Figure 6. Portions of the web page displaying following a full reaction of propane with OH showing the explicit mechanism generated with the default (explicit) lumping approach

Modifying Mechanism Generation Options

The options that affect mechanism generation and results processing in the reactor that the user can modify are listed and summarized in Table 1, which also gives the defaults for these options. These can be modified using links or input boxes in the "Reactor options" or "Advanced Options" sections of the main menu.

Table 1. List of reactor options that can be modified by MechGen users

Option	Default	Description
Temperature	298 K	Default temperature in K
Pressure	1.0 atm	Default pressure in atmospheres
O2 in air	20.95%	Mole fraction of O ₂ in the reaction environment
Atm PM	50 µg/m ³	Atmospheric particle levels used to estimate fractions of reactants in the particle phase if their vapor pressures can be estimated
H2O	Present	Used to determine if some intermediates react with water
Lumping method	Explicit	Lumping method used when generating full reactions and processing results. Currently available options are "Explicit" or SAPRC-11 or versions of SAPRC-22.
Standard Environments	3 Daytime and 1 nighttime (urban)	Determines which environmental conditions are used for deriving estimated product yields and allows the user to control whether they are used to determine which reactions can be treated as negligible.
Vapor pressure estimator	SIMPOL.1	Method used to estimate the vapor pressure that is displayed on the reactant information page for stable compounds. Available options are SIMPOL.1 ^a or EVAPORATION ^b .
Advanced options		
Minimum 1-step yield	0.5%	The minimum yield for a competing process in a single step reaction for it to be considered non-negligible during full mechanism generations
Minimum yield to react	0.5%	The minimum estimated yield for a peroxy radical intermediate to be reacted during full mechanism generation.
Mechanism Assignments	No user assignments	This option is selected if the user wants to use user assignments that the user can create to add to or replace the standard used by MechGen.
User mechanisms	No user mechanisms	Users who select the SAPRC-22 lumping method can optionally add versions of the mechanism with selected reactant and product compounds being represented explicitly.

[a] Pankow, J. F. and W. E. Asher, *Atmos. Chem. Phys.*, 8, 2773-2796, 2008. <https://doi.org/10.5194/acp-8-2773-2008>. [b] Compernelle, S., K. Ceulemans, and J.-F. Muller (2011), *Atmos. Chem. Phys.*, 11, 9431-9450. <https://doi.org/10.5194/acp-11-9431-2011>.