Using MechGen to Create User Assignments and User-Modifiable Mechanisms

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Summary

This document describes how to use the SAPRC mechanism generation system (MechGen) to create versions of the SAPRC-18 mechanism with different mechanism assignments and with selected reactants and products represented explicitly. The system can then output mechanisms of selected reactants and the products they form, based on SAPRC-18. This can be done by any users who can access the system at http://MechGen.cert.ucr.edu, or by users who can access this system using the Telnet interface.

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Overview

The SAPRC mechanism generation system (MechGen) (Carter, 2019, 2020a) allows users to optionally create their own mechanism assignments for selected reactions, compounds or intermediates, and also create their own modified or enhanced versions of the SAPRC-18 mechanism (Carter, 2020b) containing explicit reactions of compounds or oxidation products they select. Any user-created assignments or mechanisms, referred to as "user assignments" or "user mechanisms" in this discussion, are unique to each user who has a login account on MechGen, do not affect those for any other user or the SAPRC-18 mechanism itself. These user assignments or mechanisms can be deleted or over-written by the user, though backups can be created to allow them to be restored if desired.

The MechGen system can be accessed online at http://mechgen.cert.ucr.edu, or by telnet at mechgen.cert.ucr.edu:8888. As discussed by Carter (2019), anyone can access the online system and create a free account where the user can generate reactions for selected species and use other features of the system. Telnet access, with a command-line interface, has been primarily used for programming and inputting assignments and estimation parameters into the system and requires login credentials. The user assignments and mechanism can be created and managed entirely using the web-based system, but telnet access would make it more efficient to enter large numbers of assignments or generate reactions for large user mechanisms. For this reason, the capability of web users to create login credentials for telnet access has been created. These new telnet accounts would not be able to program the system or modify SAPRC-18 assignments or estimation methods, but would be able to make their own user assignments and generate the reactions of multiple compounds if needed for large user mechanisms.

This document describes how to use the online system to create user assignments and mechanisms and to obtain and use telnet access to aid this process. It serves as a supplement to the existing MechGen documentation (Carter, 2019), and it is assumed that the reader is familiar with the major features of the system as discussed here. The first section below describes mechanism assignments and how the user can use web or telnet access to create and manage their own assignments. The second section describes what a user mechanism is and how it is used to supplement SAPRC-18 to add explicit representations of reactions of organic compounds and their oxidation products in the base SAPRC-18 mechanism, with the option to use user assigned mechanisms for these compound. It also describes how to use SAPRC box modeling software to implement and run calculations using these user mechanisms. Finally, describes how the web user can create a telnet account and use it to aid entering multiple assignments or generating reactions for large user mechanisms.

Note that many of the features discussed herein have just been programmed and have not been fully debugged. If errors difficulties are encountered, please contact the author at carter@cert.ucr.edu. In addition to error corrections, it is expected that many of the capabilities discussed here will be modified or enhanced in the future. For this reason, it is possible that future versions of the system may work somewhat differently than described in this document. Links to available documentation for MechGen is available at the login screen at mechgen.cert.ucr.edu, and also at the SAPRC mechanism web site at http://www.cert.ucr.edu/~carter/SAPRC, and those pages should be checked to obtain the latest versions. Note that the existing documentation is preliminary and does not cover all features, and more comprehensive documentation is in preparation. Note also that a discussion of the chemical mechanism assumptions, assignments, and estimation methods is beyond the scope of this document[1].

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[1] The documentation of the assignments and estimation methods incorporated in MechGen is also still in preparation. Preliminary documentation is available at the SAPRC-18 web site (Carter, 2020c). However,

User Assignments

Although the mechanism generation system is capable of estimating of generating mechanisms entirely based on estimates, it allows for rate constants and mechanisms to be manually assigned for reactions where data are available or where estimates are not considered to be possible or acceptable. The SAPRC-18 mechanism currently has rate constant and branching ratio assignments for almost 500 compounds and intermediates. These are referred to as the "SAPRC-18 Mechanism Assignments" and they cannot be modified by unauthorized users. There may be other assignment sets that the user can select but cannot modify, but if they exist they would be for special projects and are beyond the scope of the present discussion. However, each user also has the ability to create or select their own user's mechanism assignment set they are able to modify as discussed below.

Selecting Assignment Sets

The currently selected assignment set is shown near the top of the main menu that is displayed when the web user first logs in or whenever the main menu is reloaded. A link to change the assignments is shown near the top of the page where the current set is shown, and is also given nearer the bottom of the page under "Other Actions". The SAPRC-18 mechanism assignment set is the default that is normally used unless the user wants to modify assignments in the mechanism. If the "change" link is selected, the user is given the choice of available assignments, which at a minimum would include the default SAPRC-18 mechanism assignments and an option to create or select your own set of user assignments. The menu item would be to "create" the assignment if you have not done this before, then it will be to "select" the user assignment set if it already has been created but subsequently the default was selected. Note that creating the user's assignment set will also select it. Note also that you can always go back and select to use the default SAPRC-18 assignments, which will result in your user assignments not being used. However, they will still exist and you can re-select the users assignments so they can be used again.

If your users assignments are selected, then the system will check those assignments first when generating mechanisms for any compound or radical using the user's web reactor. If no assignments are found for the compound or radical whose reactions are generated, the system will then look into the default assignments in the SAPRC-18 mechanism assignment set and use those if available, or use estimation methods otherwise. Therefore, if there are no user mechanism assignments (as would be the case after your user assignment set is newly created or newly reset), the generated mechanisms would be the same if the SAPRC-18 mechanism assignments were selected, i.e., if no user assignments were available.

Note that your user mechanism assignments are only used for reactions generated in your "reactor", which is assigned for each user when they create your account. This is used generate your reactions and carry out other operations after you log in. Other users will have their own reactor and also optionally their own assignment sets, which would be different from yours. However, all users would have SAPRC-18 assignments by default, and these are also used for reactions of compounds that do not have assignments in the users assignment set.

Note that mechanism assignment data are saved on a compound-by-compound basis, not on a reaction-by-reaction basis. This means that if a user assignment set is used and it has assignments for at least one reaction of a compound, the default assignments are not used for any of the other reactions of that compound unless they also entered into the user assignment set. In other words, the user assignment set "inherits" the SAPRC-18 assignments for compounds with no user assignments, but not for those with

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information on assignments and estimation methods can be viewed using the online system at mechgen.cert.ucr.edu.

any user assignments. Therefore, if it is desired to change assignments for any reaction of the compound, it is a good idea to see what default assignments exist for that compound, so the user can decide if these should be included in the user assignment set or not. How to do this is discussed in the following sections.

Making Assignments

Assignments are input using single-line <u>assignment commands,</u> each specifying either an overall rate constant for the reaction of a compound or the relative rate constant for formation of a particular set of products. These are the same regardless of whether the web or telnet access is used, and are described on Table 1, along with examples. The commands were originally developed for the telnet interface for the purpose of preparing the many assignments used in SAPRC-18, but have been adapted for use by users to input their own user assignments. These commands be input one at a time using the web interface, or by pasting or typing one or multiple assignment after the telnet login. Both of these methods are discussed below.

The four types of assignment commands are described below. Note that reactant or product species are specified using MechGen structure strings as discussed in the "help" link near the "Create reactant" control in the main menu, or as described in the available MechGen documentation (Carter, 2019). However, although SMILES strings can be used for creating reactions, they cannot be used when specifying reactants and products in assignment commands. Note that there is not a unique way to specify structures for many compounds, but the system will convert any structure input in assignment commands into the standard MechGen form that should be unique for a given structure.

- The total rate constants and optionally their temperature dependence can be assigned for the reactions of VOCs with atmospheric oxidants, and are supported for reactions of organics with OH, O_3, NO_3, O^3P, Cl atoms, or unimolecular reactions. These are in input using "k-assign-OH", "k-assign-O3", "k-assign-uni", etc. commands as shown on Table 1. Either a temperature-independent rate constant can be entered, or the parameters in the temperature-dependence expression $k = A \exp(-Ea/RT) (T/300)^B$. No other types of temperature dependences are currently supported for mechanism assignments.

- The name of a "photolysis file" giving the wavelength-dependent absorption cross sections and quantum yields as used by the SAPRC modeling software (Carter, 2020c) and optionally an overall, wavelength-independent quantum yield can be given for any photolysis reaction using a "k-assign-HV" command. Specification of an overall, wavelength-independent quantum yield is optional and gives a factor that is multiplied the photolysis frequency calculated from the data in the photolysis files to use in the model. Photolysis files have an extension ".PHF" (which is NOT included with the name in the k-assign-HV command, and their names should be no longer than 8 characters (though MechGen does not check for this). The photolysis files are not part of MechGen but are available with the distributed files for SAPRC-18 mechanism (Carter, 2020d),. The user can also enter the name of a new file (which should have no more than 8 characters that can be used in file names), and the system does not check for its existence. The user will need to create this file and have it in the same folder with the other .PHF files used in mechanism preparation for model simulations. See discussion of implementing user mechanisms using SAPRC software, below.

- The rate constants and products formed in unimolecular reactions individual radical species, and also their reactions with O_2, if applicable, can be given in "k-assign-rxn" commands. The reaction is specified using a character string with the structures of the reactants and products, with different reactants and products separated by a " + " and the lists of reactants and products are separated either by " = " or " -> " strings. The system may reorder the lists of reactants or products using a standard methodology so that any reaction would have a unique reaction string.

Table 1.   Summary of the command lines for inputting mechanisms assignments into the SAPRC mechanism generation system.

Assignment of total rate constants for atmospheric reactions of stable compounds

k-assign-*(ox) (compound)* is *(kinetic parms)* ref=*(doc)* [a]

where

(ox): an atmospheric oxidant. Currently supported are OH, O3, NO3, O3P, Cl, and uni (for unimolecular).

(compound): structure or recognized detailed model species name for a stable compound [b]

(kinetic parms): parameters for calculating absolute rate constants, optionally as follows:

k=(temperature-independent rate constant in cm, molec, sec units), or:

A=(A factor in cm, molec, sec units)

Ea=(activation energy in kcal/mole) or EaT=(activation energy in deg K) [c]

B=(B factor, where $k=A*e(-Ea/Rt)*(T/300)^B$) [c]

(doc): a character string giving the citation, documentation, or reason for the assignment.

Assignments of photolysis parameters

k-assign-HV *(compound)* is phot=*(phot file)* QY=*(overall quantum yield)* ref=*(doc)* [a]

where

(phot file): File with absorption cross-section wavelength-dependent quantum yield data [d]

(overall quantum yield): wavelength-independent quantum yield [e]

Assignment of mechanisms, branching ratios, or rate constants for individual reactions

k-assign-rxn *(reactants) = (products)* is *(kinetic parms)* ref=*(doc)* or
k-assign-rxn *(reactants) = (products)* is fac=*(ratio)* ref=*(doc)* or
k-assign-rxn *(reactants) = (products)* is fast ref=*(doc)*

where

(reactants): structures of reactants, separated by " + "s. [b,f]

(products): structures of the products, separated by " + "s [b,f]

(kinetic parms)= same as in 'k-assign-(ox)' if a total rate constant is being assigned, or

(ratio): relative amount of formation of these products from these reactants [g]

fast: This reaction is fast and the only reaction of the reactant(s) [h]

Assignments of nitrate yields in peroxy + NO reactions:

nitrate-assign *(radical)* is fac=*(nitrate yield)* ref=*(doc)* [a]

where

(radical): the structure of a peroxy radical [b]

(nitrate yield): The yield of the organic nitrate in the peroxy + NO reaction, and must be between 0 and 1. The competing NO2 + the alkoxy reaction is given a yield of 1-(nitrate yield).

Table 1 (continued)

Examples:

Assignments of total rate constants

k-assign-OH CH3-CHO is A=5.200e-12 Ea=-0.640 ref=Recommended by Calvert et al (2015).

k-assign-OH M-XYLENE is k= k=2.31e-11 ref=Calvert et al (2015). [i]

k-assign-HV CH3-CO-CH3 is phot=ACET-06 QY=5.00e-1 ref=Absorption cross sections and
        quantum yields in the ACET-06.PHF file from IUPAC (2015), but the overall photolysis
        rate is multiplied by a factor of 0.5 to better fit environmental chamber data.

k-assign-rxn CH3-C[O.](OH)-OH = HO-CO-OH + CH3. is A=5.0e+13 Ea=7.367 ref=Derived
        from theoretical results given by Vereecken and Peeters (2009)

Assignments of branching ratios

k-assign-rxn HCO-CO-O-ONO2 = CO2 + HCO. + NO3 is fast ref=Assumed to dominate.

k-assign-rxn CH3-CHO + OH = H2O + CH3-CO. is fac=0.95 ref= based on IUPAC (2009).

k-assign-rxn CH3-CHO + OH = H2O + .CH2-CHO is fac=0.05 ref=see above. [f]

k-assign-rxn .CH=CH-OH + O2 = HCO-OH + HCO. is fac=0.33 ref=Carter et al (1995).

k-assign-rxn .CH=CH-OH + O2 = HCO-CHO + OH is fac=0.67 ref=See above. [f]

nitrate-assign CH3-CH(CH3)-C[OO.]*-CH2-CH=C(CH2-OH)-CH2-CH2* is fac=0.25
        ref=Adjusted to fit chamber data for sabinene.

Notes:

[a] The entire command must be in one line, which can be longer than the input box on the web interface, but should be less than ~200 characters if sent over the web. (Some examples show wrapping only so they can be shown in their entirety. Each must be input as a single long line.) The keywords "k-assign", "is", "phot=", "fac=", "fast", "QY=", "k=", "A=", "Ea=", "EaT=", and "ref=" are case insensitive.

[b] The structures of the compounds are input in the same way as when using the "Create Reactant" control on the main menu, or when giving the "build" command in the Telnet interface. If a non-standard structural designation is used, it is replaced by the standard version. However, although you can use SMILES structure formats to create reactants, this cannot be used to identify structures or reactions when making assignments.

[c] If the activation energies or "B" factors are not given, they are assumed to be zero. In this case, either "k=" or "A=" could be used to give the temperature-independent rate constant.

[d] The photolysis files provided with the SAPRC-18 mechanism are given in Table A-6 of the SAPRC-18 documentation (Carter, 2020b), and the files used for the SAPRC-18 mechanism are available with the distributed files for the SAPRC-18 mechanism (Carter, 2020d). However, any name of 8 characters or less can be used, since MechGen does not check for existence of these files. The file will need to be created and placed in the same folder as the other SAPRC-18 photolysis files if the model simulations using this mechanism are to be carried out.

[e] The overall quantum yield specification is optional, and if missing or set to 1 then the photolysis rate coefficient is the same as calculated using the photolysis file alone. If given, photolysis rates

Table 1 (continued)

calculated using the photolysis file are multiplied by this factor to give the photolysis coefficient used.

[f] Note that the "+" and "=" symbols must be surrounded by exactly one space in reaction specification input. The order of the reactants and products does not matter since the system will re-them if needed to give a standard order, which is necessary so that each reaction can be defined by a unique character string so it will be properly recognized as having assignment data if it is generated.

[g] The relative yield factors must sum up to 1.0 for all assigned reactions with the same reactants. The system will accept the assignments if not, but mechanism generation will be aborted if this is encountered. The total rate constant must be given in a separate "k-assign-(ox)" or "k-assign-HV" assignment if this is a reaction of a stable compound with an atmospheric oxidant such as OH or photolysis. If this is a reaction of a radical, it is assumed to be in steady state so the total rate constant does not affect the overall mechanism results, so the total rate constant does not need to be specified. Note that relative rate assignments for radicals can only be given for unimolecular reactions or reactions with O_2. Therefore, the "k-assign-rxn command cannot be used to derive branching ratios for reactions of peroxy radicals with NO; instead "nitrate-assign" command used for this purpose.

[h] Assignment of "fast" reaction can only be done for radicals where the steady state approximation is appropriate, and only for unimolecular reactions or reactions with O_2.

[i] The SAPRC detailed model species name can be given in place of the structure if such a name is defined for this compound. It is replaced by the structure of the compound in the assignment database.

The total rate constants and optionally their temperature dependences could be given using the same format as used in the "k-assign-OH" (etc) commands.

• The "k-assign-rxn" commands can also give branching ratios or relative rates of reactions for a given reactant or a given set of reactants. These include reactions of VOCs with oxidants such as OH and also HV, unimolecular reactions of VOCs and radicals, and reactions of radicals with O_2, when applicable. In the case of VOC + oxidant reactions or their photolyses, the total rate constant (or method for calculating photolysis rates) must be specified in separate assignment commands or reaction generation will fail. However, specification of total rate constants for radical reactions is not necessary as long as it is a reasonable approximation that the reacts rapidly enough to be in steady state. This is because the reactions involving formation and reactions of steady-state species can be by reactions forming the products they form if the steady-state approximation is applied, and this is used in part when processing MechGen output for use with SAPRC-18. The ratios of rate constants of the different pathways can be specified either by using the "fac=" input to give the relative yields, or by using the "fast" keyword to indicate that this is the only reaction route for these reactants. Note that if "fac=" input is used, the total of all factors for a given set of reactants must sum up to one or the reaction generation will fail. Unfortunately, MechGen cannot check for this when assignments are made because they are made on a reaction-by-reaction basis, therefore not all given at the same time for a given compound or set of reactants.

• The "nitrate-assign" commands are used to specify yields of organic nitrates in the reactions of peroxy radicals with NO. When peroxy radical react with NO they can form either alkoxy + NO_2 or the NO can add and rearrange and form an organic nitrate. The ratio of the rate constant for nitrate formation to the total peroxy + NO rate constant is referred to as the "nitrate yield". This is specified using the "fac=" input, which must be between 0 and 1. The yield for alkoxy + NO_2 formation is derived from this assuming that this is the only other possible reaction. Note that the

"k-assign-rxn" input cannot be used to specify nitrate yields because it only works for VOC reactions, unimolecular reactions, and reactions of radicals with O2.

Once a command is successfully entered, the system will display all the assignments for the reactions of the compound, which may include different bimolecular reactions. Note, however, that all assignments for a given compound need to be given before any reactions are generated using that compound.

Making and Displaying Assignments using the Web Interface

In order to make assignments, it is necessary to create and/or select the user's mechanism assignment set. Once this is done, the Main Menu will have a "(view)" link next to the name of the assignment set near the top of the page, and also where will be a "Show or modify your mechanism assignments" link under "Other Actions. If you click on this link, you will see an input box to "Give assignment command" where you can enter or paste a single assignment command line. This must be entered as one line, which may be longer than the input box, so it is recommend that it be pasted into the box if the reference citation is long. Unfortunately, due to network issues that the programmer does not understand, it is not possible to input multiple lines of assignment commands without losing data, so assignments can be entered only one line at a time.

The assignment input/display page can also give the assignments that have already been entered, though how they are displayed depend on the number of species for which assignments have been made. If there are fewer than 10 species, then all the assignments are displayed. If there are more than 10 and fewer than 50 that then all the species with assignments are listed on a table, and one can select the "(show)" link to see them (they are displayed at the top, then the page is re-loaded). Either way, the assignments for the compound can be deleted using the "(delete)" link. It is generally best to delete all assignments for a compound and re-enter them if mistakes are found that need to be corrected. If there are more than 50 assignments, then you can search and select compounds to display assignments as discussed below. This will probably not be applicable to most users assignments.

The users assignment page also has a link to delete all data in the user's assignments, so that only standard SAPRC-18 assignments will be used when all reactions are generated. Note that the users assignment set is still selected, though it has no data. You can then add new assignments to it as discussed above.

Although it is not possible to use the web system to modify the standard SAPRC-18 assignments, it is possible to search and display them. In order to do that, the SAPRC-18 assignments need to be selected, which would be the case if your user assignment set has never been created. If you have your user assignments selected, you need to re-select the SAPRC-18 assignments in order to view them. You can always re-select your user assignments when done, and your previously entered assignments will still be there. If you select "view" or "show assignments" when SAPRC-18 assignments are selected, you will get a page without options to enter or delete assignments, but you will see a number of viewing and searching options. These options should be fairly clear from viewing the page, but a discussion of this is beyond the scope of this document. Note that these include the option of displaying or downloading assignment commands used to create then, which can be useful if at least some SAPRC-18 assignments are to be preserved for compounds for which any user assignments have been made.

In addition, the assignment web page gives you options to download the assignments in either csv format for loading into spreadsheets or in command format so they can be re-entered if needed. This can be done with either all SAPRC-18 assignments or with the user's assignments, depending on which set is created. It your work involves creating many user's assignments, it is strongly recommended that to create

a backup these assignments be created by downloading them in command format so they can be re-created. This may be necessary as general updates to the MechGen system may sometimes result in some user accounts being deleted. This allows the assignments to be re-entered after the user account is re-created.

Making or Displaying Assignments using the Telnet (Command) Interface

Because the web system can only be used to enter one assignment line at a time, it is recommended that the user create a telnet access account so multiple assignments can be entered at once. The process of getting a telnet account using the web system is discussed in a separate section below. Once logged in using the telnet access, the user can type in the assignment commands to his reaction generator, which is the same as the one used during web access, as shown on Table 1. Note that the format of the commands are the same as those given in the web system through the input box as discussed above.

It is not recommended that multiple assignment commands be simply pasted into the system at once because MechGen is based on a multi-user system that allows commands to be carried out essentially simultaneously, which may result in conflicts if more than one command is being processed at once. Instead, first give the command "input-asns", and the system will prompt you to enter multiple assignment commands, terminated by a "." by itself. The system will then execute one command at a time, waiting for each to finish before starting on the next. If you get a message stating that you cannot "modify SAPRC-18 mechanism assignments", then you need to select your user assignment set. This can be done using the web system, or by giving the "select-user-asns" command at the telnet interface.

Table 2 lists the commands that are available to the user logged in using the telnet interface that may be useful for creating assignments or managing a user's mechanism. These also include commands for managing the user mechanism, as discussed in the next section. The commands listed on Table 2 are not all the commands that are available using the telnet system, though many of the others will only work for authorized users. However, the commands listed on Table 2 are sufficient to duplicate the capabilities available through the web system for this purpose.

Note that Table 2 also includes commands so you can send the assignment information or commands to redo the assignments to a file that you can retrieve at an FTP site with anonymous access. This is discussed further in footnote [b] to that table. This information can also be obtained using the web interface.

User Mechanisms

This system can allow you to create modified version of the SAPRC-18 mechanism with reactions of compounds you select and can optionally modify using user assignments. You can then output the mechanisms generated for the selected compounds, with or without the other reactions in the base SAPRC-18 mechanism. If you select including the base reactions, the mechanism will include the inorganic + C_1 reactions, plus reactions of the lumped or explicit SAPRC-18 model species needed to represent any organic products your compounds form that are not included in your user mechanism species list.

If the reactions you generate for any compound forms one of the compounds in your user's mechanism list, the generated mechanism will have it form that compound explicitly, rather than forming the SAPRC-18 model species that would otherwise be used for it. This gives you a means to force the mechanism to represent products you select explicitly, rather than using lumped species. Note that this is

Table 2.   Commands available to users logged in using the telnet (command) interface.

Command [a]	Description
Assignment Commands	
assignment command	Executes a single assignment command. The types of commands that can be used are listed on Table 2.
input-asns *assignment command #1* *assignment command #2* *…* .	Used to input multiple assignment commands. The system then prompts for the commands, which could be any of the commands listed on Table 2. Any number of commands can be input, terminated by a line with only ".". To input multiple lines at once, copy all the commands, starting with "input-asns" and ending with ".", and paste them into the telnet window.
k-assign *species* k-assign-all	Show the assignments for the compound or radical *species* or for all species with assignments. "Species" is the structure or detailed model species name of the compound or radical.
remove-k-assign *species*	Deletes all assignments for a compound or radical.
select-user-asns select-default-asns	Select (or create than select) user's assignments or select the default SAPRC-18 mechanism assignments. Note that that the user assignments need to be selected for the "k-assign" or "input-asns" commands to work.
Assignment Display or Output	
Show-asns [(compound)]	Shows the assignments for a particular compound or for all compounds in the currently selected assignment set. The compound can be specified using a MechGen structure string (SMILES is not supported) or a SAPRC detailed model species name. If the compound is not given (or the name "all" is used), then all assignments are shown. Note that this will create many lines of output if the default SAPRC-18 assignments are used.
Show-asncmds [(compound)]	As above, but the commands to create the assignments are output.
@ftpout cmds on userasns @ftpout dump on userasns @ftpout csvdump on userasns [b]	Sends a file with user assignment information to the MechGen FTP site. The option "cmds" sends the assignment commands used to create the assignment. The "dump" and "csvdump" option send the information in a form that can be loaded into spreadsheets, with the data either tab- ("dump") or comma- ("csvdump") separated.
@ftpout userasns	Sends a file giving user assignment information in the format shown in a human-readable format as shown when the "show-asns" command is done.
User Mechanism Commands	
usermech	Updates users mechanism if needed and outputs summary of reactants and status. Indicated if the mechanism is complete and ready to output.
usermech create *compound1 name1* *compound2 name2* *…* .	Creates a user's new user's mechanism and inputs a list of the compounds and species names. The system prompts for a list of lines giving compound and (if needed) model species names, which are terminated by a line with only ".". Any previously created users mechanism is over- written. Note that the complete users mechanism must be given if there

Table 2 (continued)

Command [a]	Description
Note: name input not needed if there is a detailed model species name assigned to the compound.	are to be any changes in species used or their model species names. Warning messages are given if model species names provided are not used because they are already assigned for the compound, but that will not cause the process to fail. Error messages are given and the process fails if there is at least one reactant input that does not have a valid structure given or name provided when it is needed. In that case, correct the error and try again.
usermech react usermech react all	Reacts or re-reacts all species in the user mechanism. If the "all" option is specified, all the compounds in the mechanism are reacted or re-reacted, and created first if they are not in the reactor. Otherwise, only the compounds in the reactor that have not been reacted and whose reactions are needed for the mechanism are reacted.
usermech reset	Removes all reactions from the user mechanism. The species and names are unchanged, and no reactants are deleted from the reactor.
usermech delete	Deletes all species and reactions in the user mechanism
read usermech	Outputs the commands used to create the user mechanism. This only lists the species and model species names, and not the status of the reactions.
@ftpout usermech [b]	Same as above, except that the output goes in a file that is sent to the MechGen FTP site.
@ftpout rxns on usermech @ftpout all on usermech @ftpout base on usermech [b]	Creates files with completed user or base mechanisms and sends them to the MechGen FTP site. Following options available: rxns includes only reactions of user mechanism species all includes reactions of user mechanism species they form from the base mechanism, and the base inorganic + C_1 reactions. base outputs the base mechanism in its entirety, ignoring the users mechanism.
read usermech read *option* on usermech	Same as @ftpout, except that file is written to the telnet screen. Note that this is not generally satisfactory for large users mechanisms (or the base option) because many lines are output, causing some to be lost over the network.

General Mechanism Generation Commands

Command	Description
build *name* as *structure* [c]	Creates a compound in the reactor, whose structure is indicated by *structure*, the MechGen structure string. The compound is given the name *name* to identify it in the reactor, this may not be the name assigned to it in the users mechanism. This should not be necessary for compounds in the users mechanism, which can be reacted by the "usermech react" or "usermech react all" commands.
DMS *name* [c]	Creates the compound given the SAPRC detailed model species name *name*. This assures that the compound will have the same name as used for it in a users mechanism. This also should not be necessary for user mechanisms.

Table 2 (continued)

Command [a]	Description
reactants	Lists all reactants in the reactor. The list will indicate whether they have been reacted. The list may include intermediate radicals from failed reaction generations.
fullreact *name* [c] fullreact *structure*	Reacts or re-reacts the selected compound, where *name* is the name given to the compound in the reactor or *structure* is the MechGen structure string or a recognized SAPRC detailed model species name. The compound is created if it is not already in the reactor. Note that the name should be the same user mechanism name if the compound is in the user mechanism. This may be useful if there are many compounds in the mechanism, but only a few need to be reacted.
read failed on *name* [c]	Lists the intermediates for which reaction generation failed, if any in attempts to react the compound with name (name). You will need to assign reactions for these intermediates if you want to generate mechanisms for this compound.
clear *name*	Deletes any generated mechanisms from the reactant named *name*. This does not affect mechanisms loaded into the user mechanism, but requires that the reactions be re-generated after the user mechanism is reset using the "usermech reset" command. This is useful if a changed assignment or user mechanism product species may affect the mechanism for the compound.
zap-reactants	Deletes all reactants in the reactor.
options	Show options for this reactor, which includes the temperature, pressure, mechanism assignment set, and lumping method used.
@quit	Log out to end Telnet session.

[a] Not case sensitive. Input that may vary are indicated using *italic*, and optional input is surrounded by brackets.

[b] The file is sent to the FTP site at mechgen.cert.ucr.edu, which has anonymous FTP access to read and delete user-created files. This can be accessed using a web browser at ftp://mechgen.cert.ucr.edu, or using an FTP program. To retrieve the file, you can access the site as an anonymous user with no password, and download the file named *user*-dat.txt, where *user* is your web and telnet login name. (If you don't see the file, look in the folder "userdata"). Although anonymous users can download and delete files in this folder, please only download or delete your own files. You also should retrieve your files fairly soon after creating them, since files left in this folder are subject to deletion at any time.

[c] The term "*name*" is the name given to the reactant by the system. Structures recognized as SAPRC detailed model species are given the SAPRC detailed model species name regardless of whether they are in the users mechanism. Other structures are given the user mechanism name if the compound is in the user mechanism, or system assigned names are used. The system assigns the compound names such as "ORG-*nnnn*" if this is one of the many compounds used to derive SAPRC-18 mechanisms for organic product species, or are given temporary names such as "VOC-*n*" (where *n* is a 1-digit number), which are used only as long as the species is in the reactor. The ORG-*nnnn* or VOC-*n* names should only be used for compounds not in the users mechanism.

only applicable to mechanisms generated in your own web reactor, but are used regardless whether the compound whose mechanism you are generating is on your user's mechanism list.

The system also allows you to modify mechanism assignments of the compounds you select, so you can optionally specify how they react. Otherwise, the reactions would be based on default SAPRC-18 mechanism assignments or estimation methods. This could include assignments for radicals or intermediates that these compounds form. These assignments are only applicable to reactions generated in your web reactor, but are also used regardless whether the compound or intermediate whose mechanism you are generating is on your user's mechanism list.

The user mechanism is defined by a list of one or more stable compounds (not radicals) that are to be explicitly represented in the mechanism, together with the name that is to be used for it in the mechanism. The species name is required and must be no longer than 8 characters to be compatible for use with SAPRC modeling software[2] (Carter, 2020d,e). Many compounds have defined SAPRC detailed model species, and these are used for users mechanisms with these compounds and cannot be changed. However, most of the oxidized product compounds do not have model species names assigned to them, so the user needs to provide these before the mechanism can be processed.

Once a user mechanism is defined, it can be filled in with reactions of the selected compounds once they are created and their reactions are generated in the user's reactor. The user first creates the reactants and then has the system generate their reactions. It is best not to react any of the compounds until the users mechanism is completely defined and all user assignments have been entered and verified. This is because these may affect the mechanisms that are generated. The reaction generation uses any of the user assignments that may have been created if the user assignment set is selected and has assignments for the reactant, or the standard assignments otherwise. After the explicit reactions are generated, the system creates the lumped SAPRC-18 version by applying the various lumping rules associated with these mechanism (Carter, 2019, 2020b), except that any reaction products formed that are represented explicitly, using the name assigned to it, rather than by SAPRC-18 lumped model species. These results are incorporated into the users mechanism every time the user mechanism menu is selected in the web system, or if a command to update it is entered during a telnet session.

Once the user mechanism has been updated by incorporating the reactions of all the compounds selected for the mechanism, the resulting mechanism can be sent to the user in a file using the web system or to the MechGen FTP site if the Telnet interface is used[3]. This mechanism will include the reactions of the compounds selected for the user mechanism, and optionally portions of the SAPRC-18 base mechanism necessary to represent the reactions in a complete mechanism. The latter includes the base inorganic and C_1 organics, and any C_2+ product species needed to represent the reactions of the product species formed in the generated reactions of the user mechanism compounds. Note that if the user's mechanism includes a compound that is represented explicitly in the base SAPRC-18 mechanism, it's generated mechanism, which may be different if user assignments are given for it, is used rather its standard mechanism in SAPRC-18. Therefore, outputting the users mechanism along with the base mechanism is the required approach if the users mechanism includes an explicit SAPRC-18 model

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[2] Model species names can be no more than 8 characters and normally should contain only uppercase characters, numbers, or "-" or "_" characters. The system will convert any lower case character to uppercase to avoid confusion between systems that are case-sensitive or not. The system will not permit you to give more than one user mechanism compound the same name, nor can you assign a name that is already used in the base mechanism if it is used for a different compound or lumped species.

[3] See Footnote [b] to Table 2 for information on accessing files from the MechGen FTP site.

species, since appending the user mechanism to a complete base mechanism would result in the reactions of that species appearing twice in the combined mechanism.

The users mechanisms can be created, modified, and sent to the user using either the web or telnet interface, and the procedures for each are discussed below. Generally the web interface should be sufficient unless there are to be a large number of compounds in the user's mechanism, as would be the case if one wanted to create a version of SAPRC-18 mechanism where all or most of the oxidation major products are to represented explicitly, as is the case for MCM (2020). In that case, the telnet interface would be more convenient for creating and generating the reactions for the large numbers of species involved. On the other hand, the web interface provides a more convenient means to transfer the output mechanism to the user without having to use FTP to access the data. But FTP transfer may be more reliable for large files.

Creating and Modifying User Mechanisms Using the Web System

The process of creating and updating a users mechanism using the web system is discussed in this section. The starting point is the "main menu", which is the page that appears when the user first logs in, and or after selecting the "reload main menu" link that should be visible on most pages. However, most of the operations are done using the "user mechanism menu", which can be accessed from the main menu as discussed below. The steps involved are as follows:

- If you have not created a user's mechanism before, you should see an option under "other actions" in the main menu called "Enable user mechanism". After you click on that, you will see that option changed to "Manage your user's mechanism", and it will indicate how many species you added to it, which would be zero to start with.

- If you click on the option "Manage your user's mechanism", you will get the user mechanism menu, where you can add species to it and (once you have done the other steps below) output the results. The many also gives you the option to delete all species in it and start over.

- The top of the menu will be a table listing the names and structures for all species in the users mechanism. If reactions have been generated for this compound, the table will also have the number of lumped reactions and lumped model species required to represent the compound. Below that will be a blank input box where you can give the structure of compounds you want to add to the mechanism. When you start or after you delete the mechanism there will be no table and only the input box for new species.

- To add a compound, give its structure in the input box and press the "Add Species" control. You can also give the model name in the input box (after the structure, separated by a single space), if there is no SAPRC detailed model species assigned for the compound. (If you don't know if a SAPRC detailed model species is assigned for a compound, just input the structure without the name, and you will be able to add the name at a later step if needed. The structure is specified the same way as you create a reactant using the main menu, except that SMILES strings are not recognized. Note that this must be stable compound, not a radical. If this is successful, you will see the species on the table giving the list of species in the mechanism. It may or may not give a compound name -- see below. This will also create the compound and add it to the list of reactants in your reactor's contents, but will not generate reactions for it, so the "Lumped Rxns" column on the table will not indicate that it had reacted.

- Each compound in your mechanism must also have an assigned species name that is used in the model. If the compound is represented by a standard SAPRC detailed model species it will already have an assigned name that must be used, and it will be automatically. If the user attempts to give such a compound a different name in the input box, the name provided will be ignored

with a warning message. If the model species name is needed and not given in the input box when the species is added to the mechanism, or the model species name was not acceptable because it is too long or has a space, you will see an input box for the name after the compound is listed on the table. You must enter the model name there in order for this reactant to be processed, though not having them all defined doesn't prevent you from adding new species.

- If you decide you don't want the compound in your mechanism after all, you can click the "(remove)" link in the "Action" column in the row listing the compound you want to remove. This will remove the compound from the list, but will not remove it from your reactor.

- The compounds need to be in the reactor in order for you to generate reactions for them and then for the user mechanism to obtain the results. They are automatically created in your reactor when you add them to the users mechanism, unless they are there already. They are also created if they are subsequently deleted before the users mechanism has been updated to include their reactions. However, if the user deletes the reactant after its reactions have been included in the user mechanism during a previous update, the reactant is not re-created since the information about its mechanism has already been copied to the users mechanism. However, if assignments are subsequently made, new product compounds are added to the users mechanism, or there is some other reason to update the reactions of the compound, it should be re-created and reacted again. The table of reactants in the user mechanism menu includes a link to re-create reactants that have been deleted, as well as links to react or re-react compounds after they are created.

- The species list will be in the order that you enter it, and this is also the order they will be output when you generate your user's mechanism. You can change this order by clicking on the "(first)" link in the table under the "Action" column in the row listing the compound you want first. This only affects the order the reactions are output, not the predictions of the mechanism itself.

- In order to create the user's mechanism, you must react all the compounds on the list. To react the compounds, either click on the "(react)" link in the table listing that species in the user's mechanism menu, and the compound will react[4]. Alternatively, you can click the "(view)" link at the users menu and then click the "React Completely With …" link at the bottom of the table to start the reaction. In either case the species the compound reacts with depends on the type of compound[5], and are the same regardless of which link is used. If it is a large compound the process may take a up to a minute or more, and if takes more than around 10 seconds you will get a page telling you it is not finished and gives you a choice between going to the main menu, going to the users mechanism menu, or aborting the process. If you chose to abort the process the compound will still be in the reactor but will be unreacted and you will be returned to the main menu. If you chose to go to a menu but the process is not finished, you will see the same page again asking you to wait or abort, so you can wait a while and try again. If the process is finished you will go to the menu you select. If the reaction is successful, you will see information about the results where the compound is listed on the page.

- If the reaction is not successful you will not see that the reaction has not completed when you return to the main or users mechanism. In this case, it is suggested you try the reaction using the telnet interface as discussed below. It is unlikely to be any more successful but you will get more information on what is happening and can get better information on the reason for the failure. It may well be that MechGen cannot estimate the reactions of a particular intermediate that is

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[4] You will not see a "(react)" link if your user mechanism has a compound with no model species assigned. This is because generated reactions could have errors when this is the case.

[5] The atmospheric oxidant the VOC reacts with is determined by finding the lumped model species that represents this compound in the SAPRC-18 mechanism, and generating reactions for all oxidants (or photolysis) that react with the model species in the mechanism.

predicted, and you might find which intermediate it is from the telnet output (see "read failed" on Table 2). If it is a simple enough compound you could do the reactions step-by-step using the web interface as discussed by Carter (2019) and maybe found the intermediate causing the failure. If it is found, you can assign its mechanism so it does not have to be estimated. Otherwise, you won't be able to include this compound in a users mechanism because MechGen is unable to process it.

- Once you complete the process and reacted all compounds in your mechanism, the processing for the users mechanism will be complete when you see the users menu. This will be indicated by links under "Actions" section below the table of reactants to send files with the reactions of these compounds, both with and without the reactions required from the base mechanism. Your web browser will then give you the option to either open the file or save it on your own computer.

If you want to start again, select the action "Delete All" and can then create a new mechanism. Note that this does not delete any species in the reactor. You can do this using the main menu.

Creating and Modifying User Mechanisms Using the Telnet Interface

Although users mechanisms can be completely managed using the web interface, the telnet interface may be more efficient for processing large mechanisms, or if attempts to generate reactions for some reactants fail for unknown reasons. Table 2 lists the commands that can be given after logging in with your web user name to the telnet interface. The main command for creating and managing user mechanisms is "usermech", and typing this by itself will output a help message indicating how it can be used. Table 2 also lists other mechanism generation commands that may be useful for managing users mechanisms.

Unlike the web interface, all user mechanism definition input must be given in a single command that completely defines the mechanism, over-writing any previous mechanisms, if any. This is the "usermech create" command as shown on Table 2. The system prompts for lines of input giving structures and (when needed) model names, with one line for each compound, terminated by a line containing only ".". This can be pasted into the telnet screen for large mechanisms. The process will fail if even a single error is encountered, so all data would have to be entered again once the error is corrected -- which is one reason why pasting in the user mechanism definition commands from a file is a good idea. Note that giving a model name for a compound that is already assigned a different model name is not treated as an error -- a warning message is given saying that the name input was not used, but the mechanism is still processed using the already assigned name.

If the "usermech create" command is successful, the species listed will be created in the reactor but they will not be reacted. As shown on Table 2, The "usermech react all" command will react all the compounds in the mechanism, or the "fullreact (name)" command will react a selected compound. When the reactions are generated you will see output indicating the progress, and also messages if the reaction generation has failed. This is another way the telnet interface is more useful than the web, since with the web interface you usually do not get useful information if the process fails. However, you may miss the error messages if you have a large mechanism and try to react them all at once using the telnet interface, since the fullreact command produces a lot of output when showing the progress of the mechanism generation. The telnet command "read failed on (name)", where (name) is the name of the compound, will list intermediate species for which reaction generation has failed, if any. The mechanisms for the compound cannot be generated until reactions of these intermediates are assigned. Note that assigning these reactions may result in additional intermediates being formed that cannot be reacted, so this may need to be done iteratively.

The "usermech" command (Table 2) will tell you if all the compounds in the mechanism have been reacted and the user mechanism is prepared. Once this has happened, you can obtain the resulting mechanism (with or without the base reactions) from users mechanism menu using the web interface, or using "@ftpout" commands during the Telnet session as shown on Table 2. The files sent by @ftpout can be retrieved with anonymous ftp access to mechgen.cert.ucr.edu (or going to ftp://mechgen.cert.ucr.edu on web browsers). They should be retrieved relatively soon after being sent, since files at that site are subject to periodic deletion.

Running Simulations with the User Mechanism and SAPRC Software

The output files MechGen creates for your users mechanism contain data that can be used by the SAPRC box modeling software to prepare the mechanism for model calculations. Note that these are Fortran programs that are intended to be run in DOS windows on Windows systems. The programs, files, and documentation needed to use the SAPRC software and use it to conduct model simulations using SAPRC-18 and other mechanisms is available at the SAPRC web pages (Carter, 2020d,e). A discussion of the SAPRC modeling software is beyond the scope of this document (see Carter, 2020d for the available documentation), so the discussion here assumes that the user is familiar with it or has read the documentation. For discussion purposes, we assume that the model will be named "USERMECH", but any name that is a legal file name with no more than 8 characters could be used.

The user mechanism output file should be saved in the folder with the SAPRC-18 files (MECH\SAPRC18) using the name "USERMECH.RXN". This can be referenced in a mechanism preparation file called "USERMECH.PRP", which is listed on Table 3. If your assignments included referencing photolysis sets that are not included with SAPRC-18, you will need to create the .PHF file for any sets you reference, and put them in the same folder. The command "PRP USERMECH" will prepare the mechanism. You should examine the model preparation listing output "USERMECH.PRO" to see if there are any problems. The first thing to look for is warning messages and the list of "buildup-only" species to see if there are compounds formed whose reactions are not given, but which should react.

To conduct simulations with it, you will need to create a parameter file that gives the locations of the files needed for this mechanism, including the locations of the PRP output files and lumping control files needed to process model-independent input. This file goes into any folder where you are conducting model simulations. An example of such a file is shown on Table 4.

As indicated on Table 4, you can use the standard SAPRC-18 lumping control files if your mechanism assignments does not change how compounds are lumped in the mechanism. However, users mechanism may have new compounds, or compounds that are lumped in SAPRC-18 or otherwise represented using a different model species. To address this, you should create a separate lumping control file for the mechanism by copying either SAPRC18.LCC and editing the file so that the user mechanism species are assigned the proper model species. In most cases, this would involve just assigning the compound name to a model species with the exact same name for compounds in the users mechanism, and deleting other assignments for these names. Look up the 8-character compound names (shown under the "name" column in the user mechanism species listings) under the "ASSIGN" command and change the model species name (in the 2nd column) given for it, if necessary. Note that these names how you would reference the compound in simulation input files.

Once the mechanism is successfully compiled and necessary lumping control and parameter files are created, simulations can be carried out using this mechanism. The process of conducting simulations and managing the results are discussed in the SAPRC modeling program documentation (Carter, 2020d).

Table 3.   Example of a mechanism preparation file in for the SAPRC modeling program to compile a users mechanism.

Line	Discussion
Users mechanism based on SAPRC-18	Comment line used for output but otherwise ignored.
TEMP 300.0	Default temperature for simulations
.UNITS=PPM	Tells the program that rate constants are to be converted from
@USERMECH.RXN	Reactions in the users mechanism. Use another name if you named the user mechanism output file something other than USERMECH.RXN
! @SAPRC18.RXN	Include this only if you output the users mechanism without the base reactions. It is recommended that the users mechanism file include the base mechanism, so presently this line has a "!" in column 1, which results in this input line being ignored.
@WALLS.RXN	Include this if you intend to use this mechanism to model environmental chamber experiments. Not needed otherwise.
.END	Tells the program this is end of input and to prepare the mechanism.

Table 4.   Example of a model parameter file that can be used when conducting model simulations using the users mechanism with the SAPRC software distribution.

Line	Discussion
MDC=_text_	Mechanism ID added to title during simulation output. Text should be no more than 8 characters.
MOD=..\MECH\SAPRC18\	Location of mechanism executable and other mechanism files
DFLMOD=USERMECH	Mechanism executable file used by default. Change "USERMECH" if another name is used for the .PRP file.
LCC=..\MECH\SAPRC18_file_ Where _file_=SAPRC18 or the name of a lumping file for this user mechanism	Lumping control files used. The file used depends on whether a separate lumping control file is required for this user mechanism. If not, use "SAPRC18". Otherwise, create a copy of this and edit it to give the model species names assigned to the user mechanism species.
MECH=..\MECH\SAPRC18\	Location of any files referenced by the lumping control file.
LMPPGM=LUMPGEN	Lumping program used .

Using the Telnet (command) Interface

As discussed above, while the web interface is sufficient for creating user assignments and mechanisms, the Telnet interface is more suitable when many assignments or large mechanisms are involved, or if there are mechanism generation problems. Telnet access requires a username and password that must be previously assigned. However, users with an account on the web system can create an account and password to log onto the system using the Telnet interface. This Telnet user will not have the full capabilities as the login used to program the system, but will be able to carry out the commands need for user assignments and mechanisms, as listed in Table 2.

Telnet access can be enabled from the main menu of the web interface. Under "Other Actions" there should be an "Enable telnet logins" link if it has not been enabled previously. Click on this link, and this item on the menu will be replaced by "Telnet login enabled. Log in as *username* after you give your password here," where *username* is the user name for the telnet login, which should be the same as your web user name[6]. Under that will be an input box where you need to give a password before you log in, since passwords are stored in an encrypted manner. This input box will still be there after you supply a password, and you can use it to change it when desired or if you forget it.

Once telnet login is enabled and you provided a password, you can open use telnet program to connect to mechgen:cert.ucr.edu:8888. Once you are connected you will see an opening login screen stating, in part, that "This is test of the development of a MOO system for applications to atmospheric chemistry research". Give the command "connect *username userpass*", where *username* is the telnet (and usually also web) user's name, and *userpass* is the telnet password. If the login is accepted, you will see a message saying you are in your user's web chamber (the same one you access using the web system) and giving the environmental conditions for reactions generated in the chamber[7]. You can then give the commands for managing assignments or users mechanisms as discussed above and listed in Table 2. Give the command "@quit" to end your telnet session, or just close telnet.

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[6] If your web login name is the same as an existing MechGen telnet user name, your telnet login name will be your web name with a "-*n*" appended to it, where *n* is a number (usually 1). This would happen, for example, if used a name such as "mechgen", "owner", "anonymous", "guest" and several others.

[7] The MechGen system is actually a version of a "Multiuser Object Oriented" (MOO) system that was originally developed for text-based games (MOO, 2014, 2016). This type of text-based system is no longer widely used for online virtual reality experiences and the programming system is no longer being developed or supported, but features of the MOO object-oriented programming language (MOO, 1998), which is very similar to Python (Python, 2016), made it much better suited for mechanism generation applications than Fortran or other programming languages that the author happens to be familiar with, so that is why it was used for its initial development. This system uses "virtual rooms" that affect which users commands are available, and the users' "reaction chambers" are types of virtual rooms. When a telnet user is created using the web system the user goes to this "room" when logging in, which will will not be able to move to different rooms or reactors. Although normally MOO users should be able to move from room to room, this is not allowed for unauthorized users to avoid confusion and possible interferences with other reactors used by other users.

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