SAPRC CHEMICAL MECHANISMS, TEST SIMULATIONS, AND ENVIRONMENTAL CHAMBER SIMULATION FILES

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Summary

This distribution contains files documenting and implementing various versions of the SAPRC gas-phase atmospheric chemical mechanisms and the files and programs necessary simulate the environmental chamber experiments used to evaluate the detailed mechanism, and to run various test calculations, including those used to develop and evaluate the condensed SAPRC-07 mechanisms. Mechanism documentation is available at links at http://www.cert.ucr.edu/~carter/SAPRC/. The distributed files are as follows:

Programs and files:

- SAPRCfiles.pdf is a PDF version of this document. It summarizes the files contained in the distribution and installation instructions.
- ModelPgm.pdf gives preliminary draft documentation of the SAPRC modeling programs. This does not cover all features of this software, and will be updated as time allows. Please notify me at carter@cert.ucr.edu if you see errors, omissions, or portions that are not clear.
- MECH.ZIP contains the files implementing the following SAPRC mechanisms:
  - SAPRC-99 (published version)
  - SAPRC-07, SAPRC-07T, CS07 (Standard as published, toxics version, and condensed)
  - SAPRC-11 (published gas-phase version + unpublished PM-SAPRC-11)
  - SAPRC-18 (preliminary version, still under development and subject to change)
- PGMS.ZIP contains the SAPRC modeling programs needed to run the environmental chamber simulations and the test calculations. Templates for Excel spreadsheets with macros that can be used to summarize and plot data from the experiments and calculations are also included.
- TESTCALC.ZIP contains the files needed to run the static and multi-day dynamic test calculations discussed in the CSAPRC-07 condensed mechanism documentation report of Carter (2010b).
- CHAMCALC.ZIP contains the files necessary to use the distributed mechanisms and software to evaluate the mechanisms against the chamber data. This includes model input and experimental measurement data for a subset of the available experiments that are used for example calculations.
- CHAMEXPT.ZIP contains the model input and experimental measurement data for all the environmental chamber data in the distribution. This includes all UCR, TVA, and CSIRO experiments used to evaluate the versions of the SAPRC mechanism described in project reports or publications as of May, 2012. The latest UCR chamber experiment in the distribution was carried out in May, 2011.

- REACT.ZIP contains the files necessary to do reactivity scale calculations using the SAPRC-07 mechanism, including the MIR, MOIR, EBIR, base case, and averaged conditions scales.
- UNZIP.EXE is a freeware unzip program by Info-Zip (http://www.info-zip.org/) that can be used to extract the .ZIP files if the user does not already have such a program.
- MINGF.ZIP contains the minimum set of dynamic link library (.DLL) files needed so that the compiled programs in the distribution will run without GNU MinGW gfortran being installed. Note that these are not sufficient to compile new or modified mechanisms or change any of the programs, and they should be deleted if other compilers or new versions of gfortran are used.

The installation and organization of these files are discussed in the following section. More complete documentation of the programs and files are in preparation, but the distribution includes examples with comments to aid in the use of these files.

Installation

Installing the files.

The files in all the .ZIP files are organized into a directory structure, and should be extracted in a way that preserves this structure. If the distributed programs are to be used with the files, they must be extracted with the subfolders in all .ZIP files sharing the same root folder. The directory structure for the distributed files is shown on Figure B-1, which also indicates the zip files.

The suggested installation procedure is to copy the .ZIP files to be used to the root directory where they are to be installed, along with the distributed UNZIP program. Then open a DOS window and go to that folder and run UNZIP for each of the files (e.g., UNZIP MECH; UNZIP PGMS, etc.), which will extract the files to the proper folders. (If you are overwriting previously downloaded files with a newer version, use the "-o" option, e.g., "UNZIP -o MECH".) The ZIP files are no then longer needed and can be deleted.

Installing the GNU Fortran (gfortran)

In order to use the distributed executable programs to run, it is necessary that the GNU MinGW system and its associated GNU fortran compiler, gfortran. This is because the distributed executables requires components of MinGW and gfortran in order to run, and changing the mechanisms require that the simulation program be re-compiled. Installing the compiler will also allow you to modify the distributed Fortran programs, which are all compatible with gfortran. The location of the MinGW binaries need to be on the path in order for the programs to run or compile. Normally this is C:\MinGW\bin, but it does not have to be there.

GNU Fortran is public domain software, and the MinGW version that was used to compile these programs and it is recommended that this version be used. MinGW with gfortran can be obtained from the GNU web site at http://gcc.gnu.org/wiki/GFortranBinaries#Windows. Based on our tests on a Windows7 b4-bit laptop, using the latest MingGW graphical installer described in the Graphical User Interface Installer section at http://www.mingw.org/wiki/Getting_Started is a convenient way to get a version of gfortran for using the SAPRC programs described herein. Note that the tests were run without using the XP mode for Windows7 64-bit, which indicates using the XP mode for Windows7 64-bit computers is not required (although in some cases may be necessary). Be sure to include gfortran when prompted during the installation.

Note the location where the MinGW binary files are installed. By default this is C:\MinGW\bin, but it does not have to be there. It is a good idea to have this location be in the system path, though this is not absolutely necessary if the NEWENV.BAT file is configured and used as described in the following section. The environmental settings for MinGW are discussed at http://www.mingw.org/wiki/Getting_Started.

If the user is only interested in running the programs with the existing mechanisms, and does not want to modify any programs or mechanisms, then an alternative approach is to copy the minimum number set of dynamic link library (.DLL) files to the same folder as the executables on the path. This permits the executables to run without MinGW and gfortran being installed. These are in the file MINGF.ZIP. Copying MINGW.ZIP to the root folder and running "UNZIP MINGF" will copy these three .DLL files to the PGMS folder where they will be needed. However, DON'T do this if you have MinGW and gfortran installed, or there may be an incompatibility if you install a different version that we used when compiling the programs for the distribution. If you decide to install MinGW and gfortran later, then all the .DLL files in PGMS should be deleted.

Running the Programs

The following discussion covers running the programs in PGMS.ZIP with the files in CHAMCALC.ZIP, TESTCALC.ZIP and REACT.ZIP on a Windows-based PC system. The programs have been tested on Windows 98, 2000, XP, and Windows 7 systems with XP mode.

In order for the programs to run, whether in a DOS window or using macros in the distributed Excel files and templates, it is necessary to configure the NEWENV.BAT file so that it gives the appropriate locations of the distributed files and the location of the gfortran binaries if they are not on the system path (see above). Figure B-2 shows the portion of the NEWENV.BAT file that will need to be edited, indicates the items that may need to be changed. In almost all cases, the line "SET TMPENV=" will need to be changed to the root of the distribution of files (i.e., the root of the directory structure shown on Figure B-1), since as distributed it references a temporary location used when testing the installation. No other edits should be needed if the binaries for MinGW and gfortran are C:\MinGW\bin, but the line "SET TMPGF=" would need to be changed if it is something different.

The distributed programs can be run in a DOS window or using macros in the example Excel spreadsheets and templates that are included with the distribution. One way to assure that the necessary environment exists when running the programs in a DOS window is to run NEWENV.BAT immediately after opening the DOS window, or configuring the DOS window so it runs automatically when it is opened. NEWENV.BAT is also used by the macros in the distributed Excel spreadsheets for running the calculations to assure that the necessary environment exists when the programs are run, so NEWENV.BAT needs to be configured before the macros also can be used. The Excel files and templates also need to be configured before they can be used; this is discussed in the "Excel Files for Running Calculations and Displaying Results" section, below.

The procedures to run the examples in the various distribution sets are discussed in conjunction with the descriptions of the individual example batch files and spreadsheets, below.

Distributed Files

Mechanism Files

The files and folders in MECH.ZIP, which implement versions of the SAPRC-99, SAPRC-07, SAPRC-11 mechanisms are listed on Table B-1. These include files that can be used as the starting point

for implementing the mechanisms into various modeling systems, as well as those used to implement the mechanisms on the software and calculations in this distribution.

If the programs in PGMS.ZIP are installed then the mechanism input files can be edited and modified and the mechanisms used in the TESTCALC or CHAMCALC distribution can be modified. The modified mechanisms are compiled by running the PRP program and batch file on the corresponding .PRP file (e.g., "PRP CHAMLUMP" where CHAMLUMP is a PRP filename without the .PRP extension). This requires that the files in PGMS.ZIP be extracted and the DOS environment set as described above. Compiling the mechanism also requires the GNU Fortan compiler (gfortran for MinGW), as discussed above in the "Running the Programs" section.

Program Files

The files and folders in PGMS.ZIP contain the SAPRC modeling programs needed to run the environmental chamber simulations and the test calculations. Source files for the FORTRAN programs are also included, all compiled using publicly-available GNU Fortran, (gfortran for MinGW). The executables necessary to compile the programs are not included, but can be obtained from the GNU web site as discussed above in the "Running the Programs" section.

The files and programs in PGMS.ZIP are listed in Table B-2. The procedures for installing and running the distributed programs were described above in the Installation section.

Environmental Chamber Simulation Files

The files necessary to use the distributed mechanisms and software to evaluate the mechanisms against the chamber data are included in CHAMCALC.ZIP and CHAMEXPT.ZIP. These include files needed for simulating the results of over 2900 chamber experiments using the various mechanisms, and measurement data for comparison with the results of the calculations. The experiments modeled are listed in the file Excel file CHAMEXPT.XLS which is included with the distribution. (Note that the initial concentrations given in this file are in ppm units, which are the units required by model simulation programs using the mechanisms in this distribution.) The files and folders included in this distribution are listed in Table B-3. Because of the large number of experiments, data for the full set of experiments are in CHAMEXPT.ZIP, while CHAMCALC.ZIP includes data for only a representative subset of experiments, along with all the other files needed for modeling the experiments with these mechanisms. Note that the files in CHAMEXPT.ZIP are mechanism-independent, with all the mechanism-dependent files in CHAMCALC.ZIP.

In order for these simulations to run, the files in MECH.ZIP and PGMS.ZIP must also be installed, and the DOS environment must be set up as described in the Installation section, above. The simulations are run in a DOS box in the CHAMCALC subfolder created in the installation. The file EXAMPLE.BAT in CHAMCALC.ZIP runs the simulations. See the comments in EXAMPLE.BAT for a brief summary of the steps involved. Other programs are available to manage the results of these simulations, but a discussion of these is beyond the scope of the present documentation. More extensive documentation is in preparation.

Mechanism Comparison Calculation Files

Files needed to run the test calculations discussed in the condensed mechanism documentation report of Carter (2010b) that are summarized on Table 2 of that report are included in TESTCALC.ZIP. These include input files for the test calculations and files needed to run the simulations for fixed

parameter SAPRC-99 and uncondensed SAPRC-07, and for CS07A and CS07B. The files and folders included in this distribution are listed on Table B-5.

In order for these simulations to run, the files in MECH.ZIP and PGMS.ZIP must also be installed, and the DOS environment must be set up as described in the Installation section, above. The simulations are run in a DOS box in the TESTCALC subfolder created in the installation. The file EXAMPLE.BAT runs the simulations. See the comments in EXAMPLE.BAT for a brief summary of the steps involved. Other programs are available to manage the results of these simulations, and more extensive documentation can be prepared later if there is sufficient interest.

Reactivity Calculation Files

Files needed to run the reactivity scale calculations discussed by Carter (2010b,c) are included in REACT.ZIP. Comments in example batch files indicate the steps and programs used. The files and folders included in this distribution are listed on Table B-6.

In order for these simulations to run, the files in MECH.ZIP and PGMS.ZIP must also be installed, and the DOS environment must be set up as described in the Installation section, above. The simulations are run in a DOS box in the REACT subfolder created in the installation of REACT.ZIP. The file REACTEX.ZIP runs example simulations and has comments indicating the steps involved. Other batch files are available to aid complete reactivity scale calculations, as discussed in Table B-6. Other programs are available to manage the results of these simulations, and more extensive documentation can be prepared later if there is sufficient interest.

Reactivity calculation files are currently available for only the SAPRC-07 detailed mechanism, which is the version used for the latest complete VOC reactivity scale (Carter, 2010c). Files for updated mechanisms will be made available once updated reactivity scales are published.

Excel Files for Running Calculations and Displaying Results

This distribution also includes Microsoft Excel templates and example files created from them that can be used to run calculations and display plots of results of chamber simulations and chamber data. See Table B-2 for a description of the individual templates and Table B-3 and Table B-5 for a description of the examples that are distributed. These are not presently documented but include comments to assist unfamiliar users with using these files and example data. Generally data that are in red font can be modified by the user. These files contain macros that can be used to run the simulations and load the data. These macros need to know the location of the distributed files, which in general will be different for each user. Each of these files has a cell giving the root location of the distributed file, and this will have to be modified to give the location where the user installed the file before the macros will run properly. Each of the templates and example spreadsheets in the distribution should have the cell that needs to be modified when they are first opened; if not, look for comments identifying this cell, which will have bold, red font. These macros have been developed using Excel 2000 and tested using Excel 2003 and should work with newer versions of Excel but this is not guaranteed.

References

Carter, W. P. L. (2010a): "Development of the SAPRC-07 Chemical Mechanism and Updated Ozone Reactivity Scales," Revised final report to the California Air Resources Board Contract No. 03-318. January 15. Available at www.cert.ucr.edu/~carter/SAPRC. See also W. P. L. Carter, "Development of the SAPRC-07 Chemical Mechanism," Atmospheric Environment, 44, 5324-5335, 2010.

Carter, W. P. L. (2010b): “Development of a Condensed SAPRC-07 Chemical Mechanism,” Revised final Report to the California Air Resources Board, January 15. Available at http://www.cert.ucr.edu/~carter/SAPRC. See also W. P. L. Carter, "Development of a Condensed SAPRC-07 Chemical Mechanism, Atmospheric Environment, 44, 5336-5345, 2010.

Carter, W. P. L. (2010c): “Updated Maximum Incremental Reactivity Scale and Hydrocarbon Bin Reactivities for Regulatory Applications,” Report to California Air Resources Board Contract 07-339, January 28. Available at www.cert.ucr.edu/~carter/SAPRC.

Carter, W. P. L. and Gookyoung Heo (2012): "Development of Revised SAPRC Aromatics Mechanisms," Report to the California Air Resources Board Contracts No. 07-730 and 08-326, April 12, 2012. Available at http://www.cert.ucr.edu/~carter/absts.htm#saprc11.

Carter, W. P. L., Gookyoung Heo, David R. Cocker III, and Shunsuke Nakao (2012): “SOA Formation: Chamber Study and Model Development,” Final report to CARB contract 08-326, May 21. Available at http://www.cert.ucr.edu/~carter/absts.htm #pmchrpt.

Distribution	Directory structure		
MECH.ZIP	MECH	SAPRC99	
		SAPRC07	
		SAPRC07T	
		SAPRC11	
TESTCALC.ZIP	TESTCALC	INPFILES	
		CHDFILES	SAPRC07
			SAPRC11
			SAPRC18
CHAMCALC.ZIP	CHAMCALC	INPFILES (examples)	
		CHAR	LIGHT
			SAPRC99
			SAPRC07
			SAPRC18
		CHDFILES (examples)	
		CDTFILES	SAPRC99
			SAPRC07
			SAPRC07L
			SAPRC11
			SAPRC18
CHAMEXPT.ZIP	CHAMCALC	INPFILES (complete)	
		CHDFILES (complete)	
PGMS.ZIP	PGMS	SOURCE	SUBS
			UTILPGMS
			CHAMPGMS
			INT
			INTUTIL
			LMPPGMS
			LMPSUBS
			LUMPGEN
			LUMPINT
			PHK
			PREP
			REACTCAL
	TEMPLATES		
REACT.ZIP	REACT	CDTFILES	SAPRC07
		CMPFILES	
		INPFILES	
		SAPRC07	CLCFILES
			RCTFILES

Figure B-1. Directory structure for distributed files. All these directories must share the same root directory for the example simulations to run.

```
:       Sets the environment for SAPRC modeling programs
:       Use:
:               NEWENV      ... Adds the needed additional elements
:                               to the present system path
:               NEWENV TEST ... Uses the minimal system path for
:                               testing the distribution
:
:       IMPORTANT! The first two commands need to be edited for
:       your system!!
:
:       Change following to root of the location of the distributed
:       files.  ("I:\TMP\SAPRC" was used for testing, but is not
:       suitable for most systems.)
@SET TMPENV=I:\TMP\SAPRC
:
:       Change the following if the location of the MinGW binaries
:       is someting other than C:\MinGW\bin.  It can also be blank
:       (set to "") if this is already on the system path, but not
:       if the TEST option is used.
@SET TMPGF=C:\MinGW\bin
:
: ----------------------------------------------------------------
:       The remainder of this file should not need to be edited.
```

Figure B-2. Portion of NEWENV.BAT as distributed that need to be edited. The portions that may need to be changed are indicated by **bold underline font**.

Table B-1. Files and folders in MECH.ZIP, which contain files implementing various versions of SAPRC mechanisms.

Folder	Files	Description
Root	README.TXT, SAPRCfiles.PDF	README.TXT contains a brief description of files in all distribution sets, SAPRCfiles.PDF contains this document Note: these files are included in all of the distribution sets, and should be the same on all sets of the same age. If they are not the same, the older versions should be overwritten with the most recent version.
MECH*		All mechanism folders (SAPRC99, SAPRC07, SAPRC07T, SAPRC11) include files of most or all of the following types:
	*.PRP, *.MOD, *.PRO, *.EXE	Mechanism preparation input (PRP) and output (MOD, PRO, EXE) files for the mechanisms in the distribution that are used in the chamber simulations and example calculations using the software in PGMS.ZIP. Prepared mechanisms have .MOD, .PRO, and .EXE files of the same name.
	Other *.RXN	Various modules in the mechanisms, where applicable
	*.PHF	Absorption cross sections and quantum yields for the photolysis reactions. Same set used by all versions of the mechanism, though only a subset are used in the condensed versions.
	*.GNA, *.LPM	Parameter or assignment files for the detailed mechanisms, where applicable

Table B-1 (continued)

Folder	Files	Description
	STD640.FZS	Parameters for calculating solar actinic fluxes as a function of zenith angle used for reactivity and test calculations (mechanism independent but expected to be in the mechanism folder)
	PRPALL.BAT	Complies all the mechanisms with PRP files
	KZSPREP.BAT PHF.LIS	Calculates photolysis rates as a function of zenith angles for ambient simulations. PHF.LIS lists the photolysis files. STD640.FZS is one of the outputs.
MECH\SAPRC99		SAPRC-99 mechanism files
	CHAMCALC.PRP CHAMMIX.PRP CHAMS99L.PRP TSTS99.PRP	Input files for preparing mechanism for various purposes: CHAMCALC - chamber simulations using detailed mechanism; CHAMS99L - chamber simulations using fixed-parameter (airshed version) mechanism; TSTS99 - mechanism comparisons
	CHAMLUMP.LPC	Lumping control file used when evaluating the detailed mechanism against chamber data
	CHAMS99L.LCC	Assignments of detailed model species to lumped model species used for the fixed parameter of SAPRC99 for chamber simulations.
MECH\SAPRC07		SAPRC-07, CS07, and SAPRC-07T mechanism files
	CHAMLUMP.PRP CHAMCL.PRP CHAMS07L.PRP TST*.PRP AIRLMP*.PRP	Input files for preparing mechanism for various purposes: CHAMLUMP and CHAMCL - chamber simulations using detailed mechanism (CHAMCL with chlorine chemistry) ; CHAMS07L - chamber simulations using fixed-parameter (airshed version) mechanism; TST* - mechanism comparisons for various versions; AIRLMP* - reactivity simulations.
	SAPRC07B.MEC, SAPRC07B.RXN	Uncondensed, fixed-parameter SAPRC-07 mechanism in CMAQ (MEC) or SAPRC (RXN) format. (RXN used in CHAMS07L and TSTS07B.PRP)
	SAPRC07C.MEC, SAPRC07C.RXN	Same as above, but uses the explicit reactions for the peroxy radical operators. This has more reactions but is more compatible for some solver software systems, such as that using MEC files. (Used in TSTS07C.PRP)
	CS07A.MEC, CS07A.RXN	Condensed mechanism CS07A in CMAQ format in CMAQ (MEC) or SAPRC (RXN) format. (Used in TSTCS07A.PRP)
	CS07B.MEC, CS07B.RXN	Condensed mechanism CS07B in CMAQ format in CMAQ (MEC) or SAPRC (RXN) format (Used in TSTS07B.PRP)
	S07TB.MEC, S07TB.RXN	SAPRC-07T mechanism in CMAQ (MEC) or SAPRC (RXN) format using peroxy radical representation “B”. This is the representation used in the standard SAPRC mechanism as documented in the report to the CARB, but is not compatible for some model solver software systems. The MEC file has input that is not yet implemented in CMAQ.
	S07TC.MEC, S07TC.RXN	Same as above, but uses the explicit reactions for the peroxy radical operators. This has more reactions but is more compatible for some solver software systems, such as that using MEC files.
	CHAMLUMP.LPC	Lumping control file used when evaluating the detailed mechanism against chamber data

Table B-1 (continued)

Folder	Files	Description
	CHAMS07L.LCC	Assignments of detailed model species to lumped model species used for the fixed parameter of SAPRC07 for chamber simulations.
	SAPRC07L.LCC	Assignments of detailed model species to lumped model species used for the fixed parameter of SAPRC07 for ambient and mechanism test simulations.
	PHOTKS.XLS	Photolysis rates as a function of zenith angle for the actinic fluxes used for the reactivity scenario calculations (STDZA640.JZS). The actinic fluxes at the various zenith angles are also included.
	SAPRC07T.LCC	Assignments of detailed model species to lumped model species used for SAPRC07T for ambient and mechanism test simulations.
	SAPRC07T.XLS	Excel file containing species and reactions in both versions of the SAPRC-07T mechanism.
MECH\SAPRC11		SAPRC-11 mechanism files. Mechanisms for non-aromatic compounds the same as SAPRC-07. Note that this mechanism can calculate SOA formation from aromatics, but the SOA formation mechanism is subject to change.
	CHAMLUMP.PRP TESTS11.PRP	Input files for preparing the mechanism for chamber simulations (CHAMLUMP) or for test calculation comparisons with other mechanisms (TESTS11)
	AIRLMP*.PRP REACT.LPC TESTLUMP.LPC	Input files for preparation of mechanism for reactivity simulations. The .LPC files are used for preparation of model simulation input for various compounds.
	CHAMLUMP.LPC	Lumping control file used when evaluating the detailed mechanism against chamber data
	SAPRC11.LCC	Assignments of detailed model species to lumped model species used for the fixed parameter mechanism for ambient and mechanism test simulations.
MECH\SAPRC18		Mechanism files for preliminary SAPRC-18. Please check for latest version before using for research.
	S18CHAM.PRP S18CHAM2.PRP	Mechanism preparation files for chamber simulations.
	SAPRC18.PRP	Mechanism preparation file for ambient simulations.
	S18CHAM.LCC SAPRC18.LCC	Fixed parameter lumping control files for chamber and ambient simulations, respectively. (Note: SAPRC-18 does not use parameter lumping and .LCC files.)

Table B-2. Files and folders in PGMS.ZIP, which contain the distributed executable and program source files.

Folder	Files and folders	Description

Table B-2 (continued)

Folder	Files and folders	Description
Root	README.TXT, SAPRCfiles.PDF	README.TXT contains a brief description of files in all distribution sets, SAPRCfiles. PDF contains this document Note: these files are included in all distribution sets, and should be the same on all sets of the same age. If they are not the same, the older versions should be overwritten with the most recent version.
	NEWENV.BAT	Batch file to set DOS environment to execute and compile programs. Before using, it needs to be edited to change the "SET TMPENV=" line to refer to the full path name of the root directory where these files are installed.
PGMS		Location of executable files needed to run the model and example calculations. This folder must be on the path for the programs to run.
	*.EXE	Executable files included with the distribution. All of these are Fortran programs whose source files are included under the SOURCE folder. All these programs were installed using the version of gfortran for MinGW that is current at the time the distribution was created.
	*.DLL (in MINGF.ZIP, not PGMS.ZIP)	These are the dynamic link libraries needed for the executables to run if the system does not have MinGW and gfortran installed. The versions used when the distributed executables were compiled are in MINGF.ZIP. These files should be copied to the PGMS folder ONLY IF MinGW and gfortran or another fortran compiler is not installed, and should be deleted if a compiler is installed later and the programs are re-compiled. These DLL's should be sufficient to run the programs but are not sufficient to compile mechanisms and programs.
PGMS\SOURCE		Source files
	BLDALL.BAT	Execute BLDALL in all the program subfolders to compile all the programs. Note: NEWENV.BAT needs to be edited and run first.
	AllSource.BAT	Used by BLDALL.BAT. Runs a specified batch file for all SOURCE subdirectories.
	SUBS.LIB	Library of compiled subroutines used by most of the programs. Re-created using BLDALL.BAT
PGMS\SOURCE*		Subfolders that contain the source files and batch files to compile the various types of programs, as summarized below. The source files are *.FOR and can be compiled using GFORTRAN. Most also contain the bile BLDALL.BAT which compiles all the programs or libraries, as applicable. See that file for the list of specific programs that are created from the source files.
	SUBS	Source files for subroutines used by most of the programs. BLDALL.BAT creates PGMS\SOURCE\SUBS.LIB from them.
	PREP	Source files for mechanism preparation programs.
	INT	Source files for the mechanism-independent portions of the model simulation programs. BLDALL.BAT creates PGMS\SOURCE\INT\INT.LIB with the compiled programs that are linked with the mechanism-specific subroutines prepared by PREP to produce the mechanism-specific executable.

Table B-2 (continued)

Folder	Files and folders	Description
	INTUTIL UTILPGMS CHAMPGMS	Source files for the various utility programs for running model simulations and obtaining selected results and experimental data.
	LUMPINT LUMPGEN LMPPGMS LMPSUBS	Source files for various lumping programs. Note that LMPSUBS contains only common subroutines that are used when compiling the programs in the other folders. See BLDALL.BAT in these folders (except LMPSUBS) for the programs that are compiled.
	REACTCAL	Source files for reactivity simulation programs and utilities.
	PHK	Source files for the program PHK, which calculates photolysis rates given spectral distribution data.
TEMPLATES		Templates that can be used to create spreadsheets to run calculations and display selected results. These have been developed and tested using Microsoft Excel 2000 and 2003 and may not necessarily work with newer version of Office. These include macros to load experimental and calculation data and run calculations. These are not presently documented, but have comments that should be helpful to show how they can be used. Before they can be used, the cells containing the root location of the distributed files need to be changed. The cell that needs to be changed should be selected when the file is opened.
	RunCalc.xlt	Template to plot selected experimental and model calculation data for one or two experiments. This was used to create the example file CHAMCALC\RunCalcEx.xls.
	RunsFit.xlt RunsFitPlt.xlt	RunsFit.xlt is the template to plot selected experimental and model calculation data for multiple experiments. The template contains no plots, but contains a macro to create the number of plots needed, which will vary depending on the number of data channels and experiments being plotted. RunsFitPlt.xlt is used by this macro, and is not intended to serve other purposes. RunsFit.xlt was used to create the example files CHAMCALC\RunsFitEx.xls and TESTCALC\TestCalcs.xls.

Table B-3. Files in CHAMCALC.ZIP, containing files used to conduct the environmental chamber simulations used in the SAPRC mechanism evaluations.

Folder	Files or folders	Description
Root	README.TXT, SAPRCfiles.PDF	README.TXT contains a brief description of files in all distribution sets, SAPRCfiles.PDF contains this document Note: these files are included in all distribution sets, and should be the same on all sets of the same age. If they are not the same, the older versions should be overwritten with the most recent version.
CHAMCALC		Folder where chamber simulation calculations are carried out

Table B-3 (continued)

Folder	Files or folders	Description
	CHAMEXPT.XLS	Excel file containing list of all chamber runs in the distribution (i.e., all runs in CHAMEXPT.ZIP) and related information.
	RunsFitEx.XLS RunCalcEx.XLS	Examples of spreadsheet showing plots of model simulations against experimental data. RunsFitEx was created from RunsFit.xlt and contains the 27 selected toluene experiments whose data are included as example runs in CHAMCALC.ZIP. RunCalcEx was created from RunsCalc.xlt and contains a single experiment. Before these can be used, the cell containing the root location of the distributed files needs to be changed. This cell should be selected when the distributed files are first opened.
	SAPRC99.PRM SAPRC07.PRM SAPRC11.PRM	Parameter file for simulating runs using the detailed SAPRC99, SAPRC07 and SAPRC11 mechanisms. A similar file can be added for any new mechanisms to be used -- see comments in the SAPRC07.PRM.
	SAPRC07L.PRM SAPRC07T.PRM	Parameter file for simulating runs using the lumped SAPRC07 or SAPRC07T mechanisms. Same as detailed except that lumped model species are used for compounds that are not represented in the base mechanism. SAPRC07T has more compounds represented explicitly.
	MODELING.PRM	Default parameters and file locations for all simulations
	EXAMPLE.BAT	Batch file to show example for simulating a test calculation with the two mechanisms. Requires files in PGMS.ZIP and MECH.ZIP
	CLEANUP.BAT	Batch file to remove files created by example.bat and other simulations
CHAMCALC\INPFILES [a]		Folders containing input files (RunID.INP) for simulations for representative chamber experiments. Runs are listed in CHAMEXPT.XLS. Some runs require .CMP files to input mixture compositions, and outdoor chamber runs require .VSA files to give actinic fluxes as a function of time, and these files are also included here when applicable.
CHAMCALC\CHAR		Input files with characterization data for chamber simulations.
	LIGHT*.SDR	Spectral distribution files
	SAPRC99 SAPRC07	Folder with characterization files for simulations using the SAPRC99 and SAPRC07 mechanism. Note that SAPRC11 uses the same characterization assignments as SAPRC07.
CHAMCALC\CHDFILES [a]		Folder containing files with measurement data for representative chamber experiments (RunID.GDT).
CHAMCALC\CDTFILES		Folder for calculation results. Subfolders are created for each mechanism PRM file used for the simulations
	SAPRC99*.CDA SAPRC07*.CDA SAPRC07L*.CDA SAPRC07T*.CDA SAPRC11*.CDA	Calculation data files. These are ASCII files containing the list of species and the concentrations at each simulation time output. By default their names are the same as those for the input (.INP) file used to run the simulation. These folders are initially empty, but are created by EXAMPLE.BAT and deleted by CLEANUP.BAT.

Table B-3 (continued)

[a] Note that CHAMCALC.ZIP only has a representative subset of these files, while all these files are in CHAMEXPT.ZIP.

Table B-4. Files in CHAMEXPT.ZIP, containing additional files used to conduct the environmental chamber simulations used in the SAPRC mechanism evaluations

Folder	Files or folders	Description
Root	empty	This is intended to be merged with the files in CHAMCALC.ZIP, as listed on Table B-3.
CHAMCALC		Folder where chamber simulation calculations are carried out
	CHAMEXPT.XLS	Excel file containing list of all chamber runs modeled and related information. This is also in CHAMCALC.ZIP.
CHAMCALC\INPFILES		Folders containing input files (RunID.INP, and also *.CMP, and RunID.VSA where applicable) for simulations of all the chamber experiments modeled. Runs are listed in CHAMEXPT.XLS.
CHAMCALC\CHDFILES		Folder containing files with measurement data for all the chamber experiments modeled (RunID.GDT).

Table B-5. Files in TESTCALC.ZIP, containing files used to run mechanism comparison calculations associated with the SAPRC-07 condensed mechanisms documentation.

Folder	File(s)	Description
Root	README.TXT, SAPRCfiles.PDF	README.TXT contains a brief description of files in all distribution sets, SAPRCfiles.PDF contains this document Note: these files are included in all distribution sets, and should be the same on all sets of the same age. If they are not the same, the older versions should be overwritten with the most recent version.
TESTCALC		Folder to run test calculations
	SAPRC99.PRM SAPRC07.PRM SAPRC07T.PRM	Parameters used to run test calculations with the fixed-parameter SAPRC-99, SAPRC-07 or SAPRC07T mechanisms
	CS07A.PRM CS07B.PRM	Parameters used to run test calculations with CS07A or CS07B mechanisms.
	MODELING.PRM	Default parameters and file locations for all simulations
	TESTCLCS.TXT	List of test calculations included and file names used for them
	EXAMPLE.BAT	Batch file to show example for simulating a test calculation with all mechanisms. Requires files in PGMS.ZIP and MECH.ZIP
	CLEANUP.BAT	Batch file to remove files created by example.bat and other simulations

Table B-5 (continued)

Folder	File(s)	Description
	TESTCALCS.XLS	Spreadsheet created from RunsFit.xlt that plots selected calculation data from the ambient simulation and aromatic test calculations used when developing the condensed SAPRC-07 mechanism. Note that this file does not display experimental data because these examples are not simulations of experiments or real scenarios. Before this can be used, the cell containing the root location of the distributed files needs to be changed. This cell should be selected when the file is first opened.
TESTCALC\INPFILES		Input files used for test calculations.
	*.INP	Input file for a particular test calculation. See TESTCLCS.TXT
	Z0.SDR	Spectral distribution used for solar irradiation with Z=0.
	ARBROG.CMP	Composition of base ROG mixture used for some test calculations.
TESTCALC\CDTFILES*		Folder for calculation results. Subfolders are created for each mechanism PRM file used for the simulations (e.g., SAPRC07, CS07A, etc.)
	**.CDA	Calculation data files. Initially empty, but created using EXAMPLE.BAT. Same name as input (.INP) file, in folder named for the parameter (.PRM) file used.

Table B-6. Files in REACT.ZIP, containing files used to run reactivity scale calculations with the SAPRC-07 mechanism

.Folder	File(s)	Description
Root	README.TXT, SAPRCfiles.PDF	README.TXT contains a brief description of files in all distribution sets, SAPRCfiles.PDF contains this document Note: these files are included in all distribution sets, and should be the same on all sets of the same age. If they are not the same, the older versions should be overwritten with the most recent version.
REACT		Folder to run reactivity calculations
	REACTEX.BAT	Runs example reactivity simulations and contains comments on the steps and programs involved
	SCENARIO.PRM	Defines the base case scenarios that are currently supported in the distribution, including the "averaged conditions" (AVGARBBS) and the 39 city-specific EKMA scenarios.
	MODELING.PRM	Contains parameters needed to run reactivity simulations for SAPRC-07
	LUMPALL.BAT	Prepares lumped VOC and mixture mechanism files needed for reactivity simulations. Not needed for SAPRC07 because the files are already in the distribution, but included for completeness.

Table B-6 (continued)

.Folder	File(s)	Description
	BASECALC.BAT	Can be used to run base case calculations for a type of scenario. Runs base calculation for base case scenario, then finds MIR, MOIR, and EBIR NOx levels then runs base case calculations for these adjusted NOx scenarios. (The commands to do this are also in REACTEX.BAT, but this is useful for complete reactivity scale calculations with many scenarios.)
	RCTALL.BAT	Runs reactivity calculations and prepares complete reactivity listing for all VOCs in SAPRC-07 for a given scenario
	ALLSCEN.BAT	A batch file that can be used to run a selected batch file for all the 39 city-specific scenarios. ALLSCEN BASECALC will run all base calculations, and ALLSCEN RCTALL will calculate the reactivity scales for all the scenarios. The CASE environment variable can be set to either BS, MR, MO, or NL to run base case, MIR, MOIR, or EBIR scenarios, respectively.
	CLEANUP.BAT	Cleans up all files created by REACTEX.BAT and all other reactivity files. Used primarily to prepare the files for distribution.
REACT\SAPRC07		Contains files and subfolders with inputs specific to SAPRC-07
	TESTC.INS	Contains model input parameters for all VOCs and mixtures whose reactivities can be calculated (not VOCs that are represented using the "lumped molecule" method). Created by LUMPALL.BAT
	ARBMIX1.RXP	Composition of base ROG mixture in terms of model species. Created by LUMPALL.BAT
	ALOFT.LMO	Composition of aloft mixture in terms of model species. Created by LUMPALL.BAT
REACT\SAPRC07\CLCFILES		Contains reactivity output files created by REACTCAL. These are all deleted by CLEANUP.BAT
	*.BAS	Selected base case calculation results for a given scenario.
	*.CLC	Reactivity calculation results for final ozone for a given scenario
	*.CLD	More extensive reactivity calculation results for a given scenario, including integrated O3, PAN, and H2O2
REACT\SAPRC07\RCTFILES		Contains reactivity scale created from the .CLC files by DMSRCT, which are read by REACTAB. Includes reactivities for mixtures and "lumped molecule" species that are calculated from reactivities of other compounds. These are all deleted by CLEANUP.BAT
	*.RCT	Reactivity values for all VOCs that have been calculated for a given scenario.
REACT\CMPFILES		Mixture compositions used for the reactivity calculations
	*.CMP	Composition file for each mixture whose reactivities can be calculated. Also has ARBMIX1.CMP that have the base ROG mixture and ALOFT.CMP that has the aloft mixture used in the calculations. (ARBROG.CMP is the same as ARBMIX1.CMP except that it is normalized to 1 ppmC.)
REACT\INPFILES		Scenario input files used for reactivity calculations.
	*.INP	Input file for a particular type of base case reactivity scenario.

Table B-6 (continued)

.Folder	File(s)	Description
	*.JZS	Solar spectral distributions at various zenith angles used to do ambient simulations. STDZA640.JZS is used for the standard reactivity simulations (renamed to STD640).
REACT\CDTFILES		Folder for calculation results, with subfolders for each mechanism used. Initially empty, and files created by REACTEX.BAT deleted by CLEANUP.BAT
	SAPRC07*.CDA	Results files for base case reactivity simulations. File names give the scenario used and folder gives the mechanism (only SAPRC07 in this case).